A comprehensive modeling approach for BMP impact assessment considering surface and ground water interaction

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Abstract

The overall goal of this study was to develop a comprehensive tool for assessing the effectiveness of selected BMPs on both hydrology and water quality and to demonstrate the applicability of the system by considering 1) temporally and spatially changing land use management practice in an agricultural watershed and 2) interaction between surface and ground water over the entire system. A user interface and Dynamic Agricultural Non-point Source Assessment Tool (DANSAT) were developed to achieve this goal. DANSAT is the only distributed-parameter, physically-base, continuous-simulation, and multi-soil layer model for simulating impacts of agricultural BMPs on hydrology and water quality in small agricultural watersheds. DANSAT was applied to QNB plot (18m × 27m) and two agricultural watersheds in Virginia, including Owl Run watershed (1140 ha) and QN2 in the Nomini Creek watershed (216 ha), to evaluate the model components and its performance in predicting runoff, sediment yield, and pesticide load. DANSAT performed well in predicting total runoff and temporal variations in surface runoff for both field-scale and watershed-scale applications. Total percent errors between the measured and predicted results were less than 10% except for one case (39.8% within a subwatershed of Owl Run watershed), while the daily Nash-Sutcliffe model efficiencies were greater than 0.5 in all applications. Predicted total sediment yields were within ±35% of observed values in all applications. However, the performance of DANSAT in predicting temporal trend and spatial distribution of sediment loads was acceptable only within Owl Run watershed, where high correlations between flow rates and sediment loads exist. The predicted total pesticide loads were within ±100% of observed values. DANSAT failed to simulate the temporal occurrence of pesticide loads with a 0.42 daily Nash-Sutcliffe efficiency value. The Dual-Simulation (DS) was developed within the linked ground water approach to resolve problems encountered due to the existence of different temporal scales between DANSAT and the existing ground water models such as MODFLOW and MT3D. The linked approach performed better in predicting the seasonal trend of total runoff compared to the integrated approach by showing an increase in monthly Nash-Sutcliffe efficiency value from 0.53 to 0.60. Surface and subsurface output variables were sensitive to the changes in spatially distributed soil parameters such as total porosity and field capacity. A maximum grid size of 100
m was recommended to be appropriate for representing spatial distribution of topographic, land use, and soil characteristics based on accuracy analysis during the GIS manipulation processes. Larger time-step based on predefined acceptable maximum grid size, decreased the computational time dramatically. Overall sensitivity to different grid sizes and time-steps was smallest for hydrology components followed by sediment and pesticide components. Dynamic crop rotation was considered by DANSAT, and the model successfully simulated the impacts of temporal and spatial changes in crop rotations on hydrology and water quality for both surface and subsurface areas. DANSAT could prove to be a useful tool for non-point source pollution managers to assess the relative effectiveness of temporally and spatially changing BMPs on both surface and ground water quantity and quality.
Dedication

I would like to dedicate this work to my lovely advisor Dr. Saied Mostaghimi. None of my research work would have been completed without his continuous support.
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First, I would like to thank God for bringing me to Blacksburg and delivering me to the way of eternal life in death. Thank God for the wonderful grace and endless love you showed me through the cross of our Lord Jesus Christ. I turn all glories to God, who is still working on me in Christ.

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# Table of Contents

Dedication ........................................................................................................................................ iv

Acknowledgements ......................................................................................................................... v

Table of Contents ........................................................................................................................... vi

List of Tables .................................................................................................................................. xi

List of Figures ................................................................................................................................. xv

Chapter 1: Introduction ................................................................................................................. 1
  Water Quality Problems by NPS Pollution ................................................................................... 1
  Best Management Practices (BMPs)............................................................................................... 2
  Approaches for Assessing BMP Effectiveness ............................................................................ 3
  Limitations of Current NPS Models ........................................................................................... 4
  Goal and Objectives: .................................................................................................................... 5
  Dissertation Overview .................................................................................................................. 6
  References ................................................................................................................................... 7

Chapter 2: Literature Review ......................................................................................................... 11
  Introduction ................................................................................................................................ 11
  Watershed-scale NPS Models ..................................................................................................... 13
    AnnAGNPS ............................................................................................................................... 13
    ANSWERS-2000 .................................................................................................................... 15
    MIKE-SHE ............................................................................................................................ 17
    Selection of a Base Model ........................................................................................................ 18
  Agrochemical Models .................................................................................................................. 19
    GLEAMS ............................................................................................................................... 19
    PRZM .................................................................................................................................... 20
    RZWQM ............................................................................................................................... 21
    LEACHM ............................................................................................................................... 22
    Opus ..................................................................................................................................... 23
    Selection of a Base Model ........................................................................................................ 23
  Ground Water Models .................................................................................................................. 24
    MODFLOW and MT3D ........................................................................................................... 24
    HST3D .................................................................................................................................... 25
    VS2D ..................................................................................................................................... 25
    Selection of a Base Model ........................................................................................................ 26
<table>
<thead>
<tr>
<th>Chapter</th>
<th>Pages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Development of Input Parameters</td>
<td>166</td>
</tr>
<tr>
<td>Model Calibration</td>
<td>176</td>
</tr>
<tr>
<td>Results and Discussion</td>
<td>178</td>
</tr>
<tr>
<td>Watershed-scale Evaluation</td>
<td>193</td>
</tr>
<tr>
<td>Study Area</td>
<td>193</td>
</tr>
<tr>
<td>Development of Input Parameters</td>
<td>194</td>
</tr>
<tr>
<td>Model Calibration and Validation</td>
<td>197</td>
</tr>
<tr>
<td>Results and Discussion</td>
<td>198</td>
</tr>
<tr>
<td>Watershed-scale Evaluation</td>
<td>215</td>
</tr>
<tr>
<td>Study Area and Methods</td>
<td>215</td>
</tr>
<tr>
<td>Development of Input Parameters</td>
<td>216</td>
</tr>
<tr>
<td>Results and Discussion</td>
<td>221</td>
</tr>
<tr>
<td>Summary and Conclusions</td>
<td>227</td>
</tr>
<tr>
<td>References</td>
<td>229</td>
</tr>
<tr>
<td>Chapter 6: Sensitivity Analysis</td>
<td>233</td>
</tr>
<tr>
<td>Introduction</td>
<td>233</td>
</tr>
<tr>
<td>Parameter Sensitivity Analysis</td>
<td>236</td>
</tr>
<tr>
<td>Methods</td>
<td>236</td>
</tr>
<tr>
<td>Results and Discussion</td>
<td>241</td>
</tr>
<tr>
<td>Grid Size Sensitivity Analysis</td>
<td>277</td>
</tr>
<tr>
<td>Methods</td>
<td>277</td>
</tr>
<tr>
<td>Results and Discussion</td>
<td>281</td>
</tr>
<tr>
<td>Time-step Sensitivity Analysis</td>
<td>297</td>
</tr>
<tr>
<td>Methods</td>
<td>297</td>
</tr>
<tr>
<td>Results and Discussion</td>
<td>298</td>
</tr>
<tr>
<td>Summary and Conclusions</td>
<td>308</td>
</tr>
<tr>
<td>References</td>
<td>311</td>
</tr>
<tr>
<td>Chapter 7: Model Application</td>
<td>314</td>
</tr>
<tr>
<td>Introduction</td>
<td>314</td>
</tr>
<tr>
<td>Methods</td>
<td>315</td>
</tr>
<tr>
<td>Results and Discussion</td>
<td>318</td>
</tr>
<tr>
<td>Hydrology</td>
<td>318</td>
</tr>
<tr>
<td>Sediment</td>
<td>322</td>
</tr>
</tbody>
</table>
List of Tables

Table 2.1. Descriptions of AGNPS and AnnAGNPS (Bosch et al., 1998; Young et al., 1987) .......... 14
Table 2.2. Description of ANSWERS and ANSWERS-2000 .......................................................... 16
Table 2.3. Description of each component of water movement (WM) and advection and dispersion (AD) modules of MIKE-SHE (DHI, 2000a; DHI, 2000b) ........................................... 18
Table 3.1. Summary of major issues considered from previous recommendations by developers of ANSWERS-2000 .................................................................................................................. 36
Table 3.2. Physical variable data blocks and input parameters ......................................................... 39
Table 3.3. Temporal variable data block and parameters for DANSAT ........................................ 40
Table 3.4. Spatial variable data block and parameters for DANSAT ............................................. 40
Table 3.5. Possible output files of the integrated modeling approach ............................................. 42
Table 3.6. Potential evapotranspiration (PET) methods used in DANSAT ..................................... 48
Table 3.7. Sediment delivery ratio for each particle size (adapted from Foster, 1982) ................. 66
Table 3.8. Assumptions for the four sediment routing cases ......................................................... 71
Table 3.9. List of selected and defined plant types in DANSAT ....................................................... 94
Table 3.10. A summary of DANSAT’s characteristics ..................................................................... 108
Table 5.1. Selected quantitative criteria for field-scale validation of DANSET .................................. 134
Table 5.2. Selected qualitative and quantitative criteria for the watershed-scale validations of DANSET ................................................................................................................................................. 135
Table 5.3. Observed and predicted daily and monthly runoff over the monitoring period from QNB plot ........................................................................................................................................... 141
Table 5.4. The depth-wise distributions of observed and simulated soil water content in soil layers (0 - 0.9m) on the field sampling dates for QNB plot ................................................................. 144
Table 5.5. Observed and predicted daily and monthly sediment yield over the monitoring period for QNB plot ........................................................................................................................................... 148
Table 5.6. Observed and predicted daily and monthly atrazine losses in runoff over the monitoring period for QNB plot ................................................................................................. 151
Table 5.7. Observed and simulated atrazine amounts in the top 0.9 m soil depth on the field sampling dates for QNB plot ........................................................................................................... 154
Table 5.8. Measured and predicted daily and monthly metolachlor losses in runoff over the monitoring period for QNB plot ................................................................................................. 159
Table 5.9. Measured and simulated metolachlor amounts in the top 0.9m soil profile on the field sampling dates for QNB plot .......................................................... 162

Table 5.10. Data source and derived spatially distributed input parameters for the Owl Run watershed .............................................................................. 169

Table 5.11. Typical rotation information for crop areas in the Owl Run watershed ................................................................. 173

Table 5.12. Summary of the Owl Run land uses and Manning’s roughness coefficients, (adapted from Kilgore, 1997) .......................................................... 175

Table 5.13. Summary of sensitive watershed-scale parameters used for the calibration of hydrology and sediment in Owl Run watershed................................................................. 178

Table 5.14. Comparison of observed and simulated annual total runoff and summary of model performance criteria for Owl Run watershed ...................................................................... 179

Table 5.15. Comparison of observed and simulated annual total sediment load and summary of model performance criteria ................................................................................................. 189

Table 5.16. Comparison of typical dates and application types of agricultural management during the calibration and validation period .......................................................... 197

Table 5.17. Summary of sensitive parameters calibrated for model application at QN2 ................. 198

Table 5.18. Comparison of observed and simulated annual total runoff and summary of model performance criteria for calibration and validation periods at QN2 ................................................................. 200

Table 5.19. Comparison of observed and simulated annual sediment yields and a summary of model performance criteria for calibration and validation periods at QN2 ................................................................................................. 204

Table 5.20. Comparison of observed and simulated total pesticide loss and summary of model performance criteria for the calibration and validation periods at QN2 ................................................................................................. 211

Table 5.21. Perviousness, and annual average recharge value for each land use type .................. 221

Table 5.22. Results of steady-state calibration of MODFLOW for the QN2 Subwatershed .......... 222

Table 5.23. Comparison of observed and simulated annual total runoff and sediment yields by the linked GW approach for calibration period at QN2, along with the summary of model performance criteria ................................................................................................. 225

Table 6.1. List of field-scale, watershed-scale, and channel related parameters used in sensitivity analysis ................................................................................................. 238

Table 6.2. Summary of preliminary field-scale sensitivity analysis of DANSAT for surface and subsurface output variables ................................................................................................. 242

Table 6.3. Sensitivity index of DANSAT for surface and subsurface output variables for
different soil layer depths. .................................................................259

Table 6.4. Summary of sensitivity index for changes in field-scale and watershed-scale parameters. .................................................................264

Table 6.5. Summary of sensitivity index values based on spatial location of soils in a field. .................................................................273

Table 6.6. Procedures used for conducting grid size sensitivity analysis. .................................................................................................................277

Table 6.7. Selected sensitive parameters used for calculation of watershed average values. .................................................................281

Table 6.8. Watershed delineation and rasterization errors for each grid resolution. ...............................................................................................284

Table 6.9. Summary of the response of hydrology component of DANSAT to different grid size on user-created rectangular watershed. ..................................................................................................................286

Table 6.10. Summary of response of sediment component of DANSAT to different grid sizes on a user-created rectangular watershed. .................................................................................................................287

Table 6.11. Summary of response of the pesticide component of DANSAT to different grid size on a user-created rectangular watershed. .................................................................................................................288

Table 6.12. Summary of overall response of hydrology component of DANSAT to different grid sizes on QN2. ..................................................................................................................291

Table 6.13. Variation in elevation and slope for various grid sizes. .................................................................................................................292

Table 6.14. Summary of overall response of sediment component of DANSAT to different grid sizes in QN2. ..................................................................................................................294

Table 6.15. Summary of response of pesticide component of DANSAT to different grid sizes on QN2 ..........................................................................................................................296

Table 6.16. Summary of the model response of hydrology component to different time-steps without considering baseflow component. ..................................................................................299

Table 6.17. Summary of the model response of sediment component to different time-steps without considering baseflow component. ..................................................................................300

Table 6.18. Summary of the model response of hydrology component to different time-step by considering baseflow components. ..........................................................................................302

Table 6.19. Summary of the model response of sediment component for different timesteps by considering baseflow component. ..........................................................................................304

Table 6.20. Summary of the model response of pesticide component for different time-steps by considering baseflow components. ..........................................................................................307

Table 6.21. Response of pesticide leaching components to different time-step in QNB plot. .................................................................308

Table 7.1. Dates and types of agricultural management information for the typical rotation
approach in QN2.................................................................................................................. 317

Table 7.2. Comparison of surface and subsurface hydrology results using the two rotation
approaches........................................................................................................................................ 319

Table 7.3. Comparison of surface and subsurface hydrology results for the two crop rotation
information levels used in this study. ............................................................................................. 323

Table A.1. Soil layer parameters in DANSAT and corresponding column name and numbers
in the horizon table. ....................................................................................................................... 336

Table A.2. Hierarchical menu structure of the interface ................................................................ 339

Table A.3 Required directories for the interface and necessary files for each directory.................. 342

Table A.4. Descriptions for the source codes included in the compressed file............................. 386
List of Figures

Figure 1.1. Selected steps in developing a hydrologic and water quality model (adapted from Refsgaard, 1997) ................................................................. 7
Figure 2.1. Evolution tree of agricultural water quality models (adapted from Chung, 1995) .... 12
Figure 3.1. Schematic representation of the impacts of spatial and temporal land use changes
on crop, soil, and residue parameters................................................................. 37
Figure 3.2. Input files for DANSAT and the data structure of the main input file ................. 38
Figure 3.3. Multiple soil layers defined by DANSAT ........................................... 41
Figure 3.4. Temporal, spatial, and vertical scale of DANSAT outputs ...................... 42
Figure 3.5. Components of DANSAT Model ........................................................ 44
Figure 3.6. Time-steps in the DANSAT ............................................................... 45
Figure 3.7. Flowchart of hydrology components of DANSAT ................................ 46
Figure 3.8. Conceptual representation of (a) an actual interflow, (b) layer based interflow
approach, and (c) lumped interflow pool approach ........................................... 56
Figure 3.9. Comparison of integrated modeling approach and linked modeling approach .... 57
Figure 3.10. Overall concept of baseflow component .......................................... 58
Figure 3.11. Schematic procedures for baseflow calculation in DANSAT ................... 59
Figure 3.12. Concept of overland and channel flow routing in DANSAT .................... 62
Figure 3.13. Daily flowchart of sediment components of DANSAT ......................... 65
Figure 3.14. Flow chart of pesticide components ............................................... 74
Figure 3.15. Pesticide application methods in DANSAT ....................................... 76
Figure 3.16. Conceptual movement of instantaneously injected pesticide in a one-
dimensional flow field ................................................................................. 83
Figure 3.17. Approaches for GIS and model coupling: (a) GIS-based loose coupling; (b)
model-based loose coupling; (c) GIS-based close coupling; (d) model-based close
coupling; (e) GIS-based tight coupling; and (f) model-based tight coupling ........ 102
Figure 3.18. The overall concept and major functions of the DANSAT interface .......... 105
Figure 3.19. The flowchart for DANSAT Model and time-steps used for various components 107
Figure 4.1. Conceptual model of linked approach used in this study ......................... 118
Figure 4.2. Flowchart representation of time-steps for various model components .... 120
Figure 4.3. Flowchart of the dual simulation approach used in this study ............... 121
Figure 4.4. Temporal, spatial, and vertical scale of ground water output within the linked modeling approach

Figure 5.1. The four steps of model verification procedure used in DANSET

Figure 5.2. Location and layout of the plots (QNB) in the Nomini Creek Watershed

Figure 5.3. Structure and description of the rotation data block of main input file for plot-scale application

Figure 5.4. Time-series of observed and simulated daily runoff for QNB plot

Figure 5.5. Scatter-plot of observed and simulated monthly runoff for QNB plot

Figure 5.6. The depth-wise distributions of observed and simulated soil water content in soil layers (0 - 0.9m) on the field sampling dates for QNB plot: a) day 118, b) day 128, c) day 145, d) day 167, e) day 209 and f) day 272

Figure 5.7. Observed and simulated depth-averaged soil water content in the top 0.9 m soil depth on sampling dates for QNB plot

Figure 5.8. Time-series of observed and simulated daily sediment load for QNB plot

Figure 5.9. Scatter-plot of observed and simulated monthly sediment load for QNB plot

Figure 5.10. Time-series of observed and simulated daily atrazine load for QNB plot

Figure 5.11. Monthly comparison of observed and simulated monthly atrazine load for QNB plot

Figure 5.12. The depth distributions of measured and simulated atrazine amounts in the top 0.9 m soil depth on the field sampling dates: a) day 118, b) day 128, c) day 145, d) day 167, e) day 209 and f) day 272

Figure 5.13. Measured and simulated depth-averaged atrazine mass in the top 0.9 m of the soil profile on various sampling dates

Figure 5.14. Simulated temporal changes in atrazine mass in storage and losses during the simulation period

Figure 5.15. Time-series of observed and simulated daily metolachlor load for QNB plot

Figure 5.16. Monthly comparison of observed and simulated Metolachlor load for QNB2 plot

Figure 5.17. The depth-wise distributions of observed and simulated metolachlor amount in soil layers (0 - 0.9m) on the field sampling dates: a) day 118, b) day 128, c) day 145, d) day 167, e) day 209 and f) day 272

Figure 5.18. Observed and simulated depth-averaged metolachlor mass in the top 0.9 m soil
depth on different sampling dates. ........................................................................................................164

Figure 5.19. Location and monitoring network of Owl Run watershed..............................................165

Figure 5.20. Spatial distribution of impermeable soil layers within the Owl Run watershed. ....167

Figure 5.21. Average monthly runoff to rainfall ratio at the outlet (QOA) of Owl Run watershed. ........................................................................................................167

Figure 5.22. DEM of 30 m grid resolution for the Owl Run watershed...........................................170

Figure 5.23. Stream network and stream shape types for each stream segment in the Owl Run watershed. .................................................................................................171

Figure 5.24. Spatial distribution of major soil types in the Owl Run watershed. .........................172

Figure 5.25. Spatial distribution of representative land uses in the Owl Run watershed in 1992 (April through October). ........................................................................................173

Figure 5.26. Spatial distribution of thiessen polygon in the Owl Run watershed. .....................176

Figure 5.27. Comparison of observed and simulated runoff volumes for QOA: (a) scatter-plots for daily flow, (b) scatter-plots for monthly flow, (c) time-series for daily flow, and (d) time-series for monthly flow. .....................................................................................................................182

Figure 5.28. Temporal changes in thiessen averaged rainfall intensity for (a) 6/18/1991 and (b) 8/9/1991 storm events. ..........................................................................................183

Figure 5.29. Actual rainfall intensity in (a) QPB, (b) QPD, (c) QPF, and (d) QPH raingauge stations. .........................................................................................................................184

Figure 5.30. Comparison of observed and simulated flow for QOC: (a) scatter-plots for daily flow, (b) scatter-plots for monthly flow, (c) time-series for daily flow, and (d) time-series for monthly flow.............................................................185

Figure 5.31. Comparison of observed and simulated flow for QOD: (a) scatter-plots for daily flow, (b) scatter-plots for monthly flow, (c) time-series for daily flow, and (d) time-series for monthly flow. .....................................................................................................................186

Figure 5.32. Comparison of daily runoff and sediment load from 6/15/92 to 10/30/92 for QOA. ........................................................................................................................................189

Figure 5.33. (a) Scatter-plot and (b) time-series of observed and simulated monthly sediment load for QOA.................................................................190

Figure 5.34. (a) Scatter-plot and (b) time-series of observed and simulated monthly sediment load for QOC.........................................................................................191

Figure 5.35. (a) Scatter-plot and (b) time-series of observed and simulated monthly sediment
load for QOD. .......................................................................................................................... 192
Figure 5.36. Location and monitoring network of Nomini Creek watershed. .................. 194
Figure 5.37. Major GIS layers used for creating spatially distributed parameters in Nomini
Creek watershed: (a) DEM; (b) Channel network; (c) soil; (d) land use; and (e) Thiessen
polygon. .................................................................................................................................... 196
Figure 5.38. Comparison of observed and simulated flow for calibration period: (a) scatter-
plots for daily flow, (b) scatter-plots for monthly flow, (c) time-series for daily flow, and
(d) time-series for monthly flow. ................................................................................................. 201
Figure 5.39. Time-series of simulated monthly total runoff and monthly average flux from
intermediate to ground water zone. ............................................................................................. 202
Figure 5.40. Spatial distribution of annual simulated total flux from intermediate to ground
water zone (unit is mm/year-cell). ............................................................................................... 202
Figure 5.41. Comparison of observed and simulated flow for validation period: (a) scatter-
plots for daily flow, (b) scatter-plots for monthly flow, (c) time-series for daily flow, and
(d) time-series for monthly flow. ................................................................................................. 203
Figure 5.42. (a) Scatter-plot and (b) time-series of observed and simulated monthly sediment
load for the calibration period at QN2. ......................................................................................... 206
Figure 5.43. (a) Scatter-plot and (b) time-series of observed and simulated monthly sediment
load for the validation period at QN2. .......................................................................................... 207
Figure 5.44. Relationship between observed daily discharge and daily total sediment load in
QN2. ............................................................................................................................................... 208
Figure 5.45. Example of flow rate, sediment concentration, and representative interval for
daily sediment load calculation (December 1987). .................................................................. 208
Figure 5.46. Temporal changes in flow rates and sediment concentrations during five biggest
runoff events: (a)-(e) from QN2 watershed and (f) from Owl Run watershed. ..................... 209
Figure 5.47. Daily sediment load for triangular and rectangular stream cross sections. ....... 210
Figure 5.48. Effect of stream cross sections on accumulated sediment load. .................... 210
Figure 5.49. Observed and simulated daily atrazine loads for the (a) calibration and (b)
validation periods at QN2. ........................................................................................................... 212
Figure 5.50. Observed and simulated daily metolachlor loads for the (a) calibration and (b)
validation periods at QN2. ........................................................................................................... 213
Figure 5.51. Atrazine mass balance during the calibration period. ....................................... 214
Figure 5.52. Location of ground water monitoring wells in Nomini Creek watershed. ........215
Figure 5.53. Location of ground water monitoring stations and selected stream points and
   generated contours of average ground water table in the Nomini Creek Watershed. ......217
Figure 5.54. Spatial distribution of hydrologic soil groups in QN2 sub-watershed. ............219
Figure 5.55. Spatial distribution of land use categories in QN2 Sub-watershed.....................221
Figure 5.56. Observed and simulated hydraulic head at monitoring wells of QN2. ............223
Figure 5.57. Time-series comparison of observed and simulated monthly runoff by integrated
   and linked GW approaches. ..................................................................................................226
Figure 5.58. Time-series comparison of observed and simulated monthly sediment yields by
   integrated and linked GW approaches. ....................................................................................226
Figure 5.59. Spatial distribution of ground water table elevation (GWT) at the end of the
   simulation period. ..................................................................................................................227
Figure 6.1. Spatial distribution of soil groups for the soil location sensitivity analysis
   according to (a) cell number and (b) actual soil types. .......................................................241
Figure 6.2. Sensitivity of parameters to changes in total porosity. .........................................248
Figure 6.3. Sensitivity of parameters to changes in field capacity........................................248
Figure 6.4. Sensitivity of parameters to changes in clay percent............................................249
Figure 6.5. Sensitivity of parameters to changes in sand percent.........................................249
Figure 6.6. Sensitivity of parameters to changes in silt percent.............................................250
Figure 6.7. Sensitivity of parameters to changes in organic matter content..........................250
Figure 6.8. Sensitivity of parameters to changes in Green-Ampt effective hydraulic
   conductivity...............................................................................................................................251
Figure 6.9. Sensitivity of parameters to changes in saturated hydraulic conductivity in soil
   layer ..........................................................................................................................................251
Figure 6.10. Sensitivity of parameters to changes in interrill erodibility..................................252
Figure 6.11. Sensitivity of parameters to changes in maximum root depth..........................252
Figure 6.12. Sensitivity of parameters to changes in depth to ground water table..................253
Figure 6.13. Sensitivity of parameters to changes in random roughness of secondary tillage...253
Figure 6.14. Sensitivity of parameters to changes in pesticide half-life in soil..........................254
Figure 6.15. Sensitivity of parameters to changes in pesticide partitioning coefficient............254
Figure 6.16. Sensitivity of parameters to changes in pesticide application depth....................255
Figure 6.17. Sensitivity of parameters to changes in rill space..............................................255
Figure 6.18. Sensitivity of parameters to changes in fraction of dissolved chemical available for runoff. ..................................................................................................................... 256

Figure 6.19. Comparison of sensitivity index based on changes in clay percent at various soil depths. ................................................................................................................ 259

Figure 6.20. Comparison of sensitivity index based on changes in sand percent at various soil depths. ............................................................................................................. 260

Figure 6.21. Comparison of sensitivity index based on changes in very fine sand percent at various soil depths. ............................................................................................... 260

Figure 6.22. Comparison of sensitivity index based on changes in total porosity at various soil depths. ............................................................................................................. 261

Figure 6.23. Comparison of sensitivity index based on changes in field capacity at various soil depths. ............................................................................................................. 261

Figure 6.24. Comparison of sensitivity index based on changes in saturated hydraulic conductivity at various soil depths. ................................................................. 262

Figure 6.25. Comparison of sensitivity index based on changes in organic matter percent at various soil depths. ................................................................. 262

Figure 6.26. Comparison of sensitivity index values for total runoff for changes in field-scale and watershed-scale parameters. ................................................................. 267

Figure 6.27. Comparison of sensitivity index values for sediment load for changes in field-scale and watershed-scale parameters. ................................................................. 268

Figure 6.28. Comparison of sensitivity index valued for pesticide load for changes in field-scale and watershed-scale parameters. ................................................................. 269

Figure 6.29. Comparison of sensitivity index values for recharge to ground water for changes in field-scale and watershed-scale parameters. ................................................................. 270

Figure 6.30. Comparison of sensitivity index values for pesticide flux to ground water zone for changes in field-scale and watershed-scale parameters. ................................................................. 271

Figure 6.31. Comparison of sensitivity index values for changes in total porosity soil parameter at different locations in the watershed. ................................................................. 273

Figure 6.32. Comparison of sensitivity index values for changes in field capacity soil parameter at different locations in the watershed. ................................................................. 274

Figure 6.33. Comparison of sensitivity index values for changes in clay percent soil parameter at different soil locations in the watershed. ................................................................. 274
Figure 6.34. Comparison of sensitivity index values for changes in sand percent soil parameter at different soil locations in the watershed. .................................................................275
Figure 6.35. Comparison of sensitivity index values for changes in OM content soil parameter at different soil locations in the watershed. .................................................................275
Figure 6.36. Comparison of sensitivity index values for changes in saturated hydraulic conductivity soil parameter at different soil locations in the watershed. .................................276
Figure 6.37. Procedures used for analysis of watershed delineation error. .................................................................278
Figure 6.38. Procedures used for rasterization error analysis. .................................................................................................279
Figure 6.39. User-created watersheds used for evaluating overland component and channel routing components for different grid sizes. .................................................................279
Figure 6.40. A user-created rectangular watershed with constant overland and channel slopes and homogeneous soil and rotation type. .................................................................................................280
Figure 6.41. Watershed boundary and channel network maps for various grid resolutions. .................................................................282
Figure 6.42. Variations in spatial distribution of the soil type for QN2 watershed. .................................................................283
Figure 6.43. Variations in spatial distribution of crop rotation type for QN2 watershed. .................................................................283
Figure 6.44. Hydrologic response of (a) overland routing and (b) channel routing components to a storm event with constant intensity (0.3 mm/min) for different grid sizes. .................................................................285
Figure 6.45. Summary of response of hydrology component to different grid size on user-created rectangular watershed. .................................................................286
Figure 6.46. Summary of response of sediment component to different grid sizes on a user-created rectangular watershed. .................................................................................................287
Figure 6.47. Comparison of simulated (a) daily total runoff and (b) daily sediment yield at 30 m grid size for the different shapes of stream cross sections. .................................................................288
Figure 6.48. Summary of response of the pesticide component of DANSAT to different grid size on a user-created rectangular watershed. .................................................................289
Figure 6.49. Summary of overall response of hydrology component to different grid sizes on QN2 .................................................................291
Figure 6.50. Response of ground water recharge to different grid sizes. .................................................................................................292
Figure 6.51. Comparison of temporal changes in daily total runoff for different grid sizes. .................................................................292
Figure 6.52. Spatial distribution of ground water recharge and streams for different grid sizes in QN2. .................................................................293
Figure 6.53. Summary of overall response of sediment component to different grid sizes in QN2. ................................................................. 294
Figure 6.54. Comparison of daily (a) total runoff and (b) sediment yield for different grid sizes in a rectangular stream of QN2 watershed. ......................................................... 295
Figure 6.55. Summary of response of pesticide component of DANSAT to different grid sizes in QN2. .............................................................................. 296
Figure 6.56. Ratio of pesticide flux to 30 m grid size based on average and maximum values. 296
Figure 6.57. Summary of the model response of hydrology component to different time-steps without considering baseflow component................................................................. 299
Figure 6.58. Maximum and average rainfall intensity for different time-steps. ......................... 300
Figure 6.59. Summary of the model response of sediment component for different time-steps without considering baseflow component................................................................. 300
Figure 6.60. Summary of the model response of hydrology component to different time-steps by considering baseflow component. .............................................................. 302
Figure 6.61. Response of ground water recharge to different time-steps in the rectangular stream......................................................................................................................... 303
Figure 6.62. Time-series of daily total runoff for different time-steps........................................ 303
Figure 6.63. Summary of the model response of sediment component for different time-steps by considering baseflow component. .............................................................. 305
Figure 6.64. Possible cases for sediment detachment in streams for various stream shape and flow rates................................................................................................................. 305
Figure 6.65. Summary of the model response of pesticide component for different time-steps by considering baseflow component. .............................................................. 307
Figure 6.66. Response of pesticide flux from intermediate to ground water zone for different storm event time-steps .......................................................................................... 307
Figure 6.67. Comparison of daily pesticide flux to ground water for different time-steps in QNB plot.................................................................................................................. 308
Figure 7.1. Procedures used for manipulating land use data for the crop rotation input. ........... 316
Figure 7.2. Comparison of (a) daily total runoff and (b) monthly total recharge in each cell for the two levels of information on crop rotation......................................................... 320
Figure 7.3. Temporal comparison of difference in monthly total runoff (monthly total runoff by typical approach – monthly total runoff by dynamic approach) and difference in
spatially averaged monthly recharge (spatially averaged monthly recharge by typical
approach – spatially averaged monthly recharge by dynamic approach) for the two
levels of information on crop rotation. .................................................................321
Figure 7.4. Comparison of effective hydraulic conductivity values for Green-Ampt for the
two rotation approaches at cell number 86. .......................................................321
Figure 7.5. Spatial distribution of difference in average monthly recharge for the two crop
rotation approaches. .......................................................................................322
Figure 7.6. Comparison of the simulated daily total sediment loads for the two crop rotation
approaches used in this study. ..........................................................................323
Figure 7.7. Time-series of differences in monthly total sediment loads (monthly total
sediment load by typical approach – monthly total sediment load by dynamic approach)
during the simulation period. ...........................................................................324
Figure 7.8. Comparison of (a) interrill erodibility, (b) rill erodibility, and (c) critical shear
stress in a rill for the two crop rotation approaches at cell number 86. ..............325
Figure A.1. Main window of the interface and main menus. .................................339
Figure A.2. Example of define activity window of the interface. ...........................341
Figure A.3. Example of Edit Database window (tillage). ......................................341
Figure A.4. General tab of the General Block Generator window to control directory and file
names. ...........................................................................................................343
Figure A.5 Flags tab of the General Block Generator window to control component, output,
and method flags ............................................................................................344
Figure A.6 Create Database Table window ................................................................345
Figure A.7 Interface window for creating cell number ascii file. ............................345
Figure A.8 General tab of the Input/Output Block Generator interface window ........346
Figure A.9 Output tab of the Input/Output Block Generator interface window ..........347
Figure A.10. Interface window for creating initial data block ..................................348
Figure A.11 Required input ascii files for creating cell data block .........................349
Figure A.12 Edit Channel Database window and available channel types ...............350
Figure A.13 Soil Block Generator interface window ..............................................351
Figure A.14 Overview of linkages between activity related interface windows ..........352
Figure A.15. Leaf Area Index Table window ......................................................353
Figure A.16 Edit Depth Distribution window ......................................................354
Figure A.17 Generate Rotation Data Block window for individual inserting of management information..................................................................................................................356
Figure A.18 Rotation Initial Value window. ..................................................................................357
Figure A.19 Control panel and spreadsheet of Rotation Builder Excel workbook. ..................358
Figure A.20. Interface window for creating break-point rainfall input file. ............................359
Figure A.21 Overview of the proposed research. ..................................................................361
Chapter 1: Introduction

Water Quality Problems by NPS Pollution

The United States Environmental Protection Agency (USEPA) estimated that 45 percent of the rivers, 54 percent of the lakes, and 54 percent of the estuaries, among 32 percent of U.S. waters assessed, are threatened or polluted (USEPA, 2000). The nation’s waters are still threatened by pollutants such as sediment, bacteria, nutrients, and metals in spite of more than 30 years clean up efforts. Non-point source (NPS) pollution transported by precipitation and runoff from both urban and agricultural areas is the most significant source of water quality problem in the United States (USEPA, 2000). NPS pollution is difficult to monitor and control because the pollutants are generated over an extensive area of land and enter receiving water bodies in a diffused manner. NPS pollution is low in concentration and high in total load, while point source pollution is generally high in concentration and low in total load. Therefore, NPS pollution abatement is usually focused on land and runoff management practices. Agricultural activities may introduce sediments, nutrients, pesticides, and other organic matter to the water bodies. It is reported that agriculture is the most widespread source of pollution in impaired rivers and lakes (USEPA, 2000).

Pesticides mainly originate from agricultural activities. Over 76% of the 1.2 billion pounds of pesticides’ active ingredients used in the United States during the 90s were used in agricultural areas (Donaldson et al., 2002). It is estimated that the annual amount of pesticide (active ingredient) used in the U.S. is about 20% of the total amount used in the world (Aspelin, 1997). Growing evidence shows that pesticides exist in the environment, such as atmosphere, surface, and ground water, far from the areas of their application. About 50% of the U.S. population, primarily in urban areas, relies on streams and reservoirs for drinking water. Surface waters are vulnerable to pesticide contamination because runoff from source areas, including agricultural and urban areas, can carry pesticides into streams. Although surface water problems by pesticides have been investigated because of their acute effects, more attention has been given to soil and ground water contamination by pesticides because ground water is a major source of drinking water in Western Europe and the United States (Van Den Berg and Van Den Linden, 1994). Furthermore, continued contamination of surface water resources has increased our dependence on ground water to meet growing water needs. Contamination of soil and ground water by NPS pollutants is serious, because areal extent of contamination is usually large and effective...
remediation is very difficult (Corwin and Wagenet, 1996). Ground water and surface water quality were examined as part of the National Water Quality Assessment (NAWQA) Program by the U.S. Geological Survey in 1991. The results of the NAWQA study of pesticides in surface water indicated that more than 95% of the samples collected from 58 rivers and streams across the U.S. contained at least one pesticide or pesticide byproduct (Larson et al., 1999). Results from the first set of ground water/land use studies conducted in the first 20 NAWQA study units during 1993-1995 indicated that the concentration and frequency of pesticide detection was closely related to the use and properties of pesticides and land use categories (Kolpin et al., 1998). Overall, the results of the national study demonstrated that pesticides were commonly detected in shallow ground water of both agricultural and urban areas, with about 54% of 1034 sites sampled containing one or more pesticide compounds. However, agricultural areas showed higher frequency of pesticide detection in ground water than urban areas (Kolpin et al., 1998).

**Best Management Practices (BMPs)**

Best management practices (BMPs) have been used to reduce or eliminate the losses of pollutants from diffuse sources into receiving waters (Line et al., 1999; Line et al., 1994; Spooner et al., 1992). The effectiveness of BMPs varies according to their placement and time of installation. Selection of appropriate systems of BMPs for a particular condition is difficult because the extent of pollution is related to uncontrollable climatic events as well as site-specific conditions such as soils, topography, and land use (Novotny and Olem, 1994). BMPs should be economically feasible and well suited to a specific site. Several factors such as crop yields, machinery costs, labor, and field conditions should be considered when the effectiveness of BMPs are evaluated (Hairston, 1995). Selection of BMPs should take into consideration the BMP effect on both surface and ground water. Some BMPs implemented for reducing surface water quality problems may accelerate pollutant transport to ground water (Smith et al., 1991). The interaction between surface water and ground water in many perennial streams has significant influence on chemical and biological conditions of both surface and subsurface systems. Ground water in the alluvium aquifer adjacent to the stream is the principal source of solute in the stream (Squillace et al., 1993). Therefore, investigation of the interaction of surface water and ground water is critical in order to determine the effects of land use changes on water resources, especially during low-flow conditions when the baseflow from ground water may be the only source feeding streams.
Approaches for Assessing BMP Effectiveness

Estimates of BMP effectiveness are essential for 1) selecting the most appropriate BMP for a particular problem and site, 2) estimating the benefits of BMP implementation, 3) ranking alternative BMPs in terms of their cost effectiveness, and 4) determining an optimum BMP program based upon program objectives (Dillaha, 1990). Two approaches have been used to evaluate BMP effectiveness: monitoring and modeling.

Monitoring is the most straightforward method to assess BMP effectiveness. Watershed-scale monitoring projects, including 21 Rural Clean Water Program (RCWP) projects, were established in an attempt to evaluate the impacts of BMPs. However, the effectiveness of BMPs at the watershed-scale has not been well identified. Difficulty in linking BMP implementation with water quality at the watershed-scale exists because of complexity and uncertainty from: 1) the interconnection between the surface and ground water, 2) lack of actual implementation data and insufficient BMP implementation level, and 3) lag time between the BMP implementation and water quality responses (Shukla, 2000). In addition, the monitoring approach is hampered by a number of complicating factors inherent in measuring NPS pollution. The BMP effectiveness is site-specific depending on land use, topography, and climatic factors. Therefore, it is not possible to extrapolate the monitoring results to other ungaged watersheds (Dillaha, 1990), since monitoring reflects only past activities.

Because watershed-scale monitoring programs require a long period of data collection, many NPS pollution studies have been based on modeling approaches. The modeling approach provides a number of benefits including 1) predicting the effect of BMPs prior to their implementation and 2) ranking BMP alternatives and determining the most appropriate system of BMPs for a particular situation. The modeling approach is considered to be a cost-effective tool for preliminary evaluation of the effectiveness of agricultural BMPs at watershed-scale.

Deterministic models can be classified into: 1) lumped or distributed models, 2) continuous or event-based models, and 3) conceptual or physically-based models, depending on the treatment of space, time, and process, respectively (Borah and Bera, 2003; Chow et al., 1988). Among eight combinations of model type, physically-based, distributed parameter, and continuous simulation NPS models are ideal for predicting the effectiveness of BMPs in agricultural watersheds (Bouraoui and Dillaha, 1996). Section 208 of the 1972 amendments to the Federal Water Pollution Control Act (PL 92-500) requires States to identify area-wide pollution problems and develop and implement plans to control non-point sources. Furthermore, section 319 of the Water
Quality Act of 1987 (PL 100-4) requires each State to develop a non-point source management program on a watershed basis (Ribaudo, 1991). Numerous studies have indicated that a few critical areas are responsible for a disproportionate amount of the pollution. As a result, pollution control resources should be targeted to those critical areas for cost-effective improvements in downstream water quality. Identification of critical area within the watershed is one important aspect of a watershed management project that can easily be accomplished through the use of models (Osmond et al., 1997). Distributed parameter models such as SLOSS and PHOSPH (Tim et al., 1992), AGNPS (Osmond et al., 1997; Srinivasan and Engel, 1994), ANSWERS (Beasley et al., 1981; Dillaha and Beasley, 1983), and ANSWERS-2000 (Bouraoui and Dillaha, 1996) can be used to identify critical areas within the watershed. Estimation of effectiveness of BMPs requires the use of continuous simulation models because continuous models are known to be useful for evaluating long-term effects of land use changes and watershed management practices, while storm event models are appropriate for analyzing actual or design storms, especially for structural practices. Long-term simulation is necessary to consider the lag time between the BMP implementation and water quality responses. In addition, required data for model calibration and validation are not available in many agricultural watersheds. Physically-based models use physical parameters that can be either measured or determined using appropriate relationships in order to describe the physical, chemical, and biological mechanisms of the system. Physically-based models require minimum calibration in contrast to empirical models.

Borah and Bera (2003) reviewed eleven watershed-scale hydrologic and non-point source pollution models based on model capability, temporal and spatial representation, mathematical strength, and applicability of hydrology, sediment, chemical, and BMP components. Frequently used watershed-scale hydrologic and water quality models include AGNPS (Young et al., 1987), AnnAGNPS (Bingner and Theurer, 2001), ANSWERS (Beasley et al., 1980), ANSWERS-2000 (Bouraoui et al., 2002), CASC2D (Ogden and Julien, 2002), DWSM (Borah et al., 2002), HSPF (Bicknell et al., 1993), KINEROS (Woolhiser et al., 1990), MIKE-SHE (Refsgaard and Storm, 1995), PRMS (Leavesley et al., 1983), and SWAT (Arnold et al., 1998).

Limitations of Current NPS Models

Among the eleven NPS models investigated in this study, AGNPS, ANSWERS, DWSM, KINEROS, PRMS, and CASC2D have difficulties in evaluating long-term impacts of BMPs on hydrology and water quality because they are single-event models. AnnAGNPS and SWAT models use curve number (CN) and Universal Soil Loss Equation (USLE) methods for simulating
runoff and soil erosion components, respectively. Bouraoui (1994) and Byne (2000) reported on major limitations of the CN and USLE methods, respectively. These empirically derived methods restrict the capability of the model to simulate the impacts of spatially and temporally changing BMPs on hydrology and water quality because it is difficult to select appropriate CN values and USLE factors according to the different BMP scenarios. HSPF is a semi-distributed model based on conceptual equations. The capability of the HSPF can be limited in application to ungaged watersheds where measured data are not available and significant land use changes have occurred and model parameters are not directly linked to the physical conditions of a watershed (Refsgaard and Knudsen, 1996). There is difficulty in using HSPF for an ungaged watershed or simulating the impacts of temporally changing BMPs because HSPF uses conceptual equations, which require intensive model calibration. In addition, HSPF has semi-distributed model characteristics, which limits the ability of the model to simulate the impacts of BMP application in different locations within a subwatershed on hydrology and water quality. Model characteristics of ANSWERS-2000 and MIKE-SHE are appropriate as ideal NPS models. However, MIKE-SHE is a commercial model and the source code is not available for public use. There is difficulty in obtaining information on the model such as sediment and BMP related components (Borah and Bera, 2003). Extensive requirement of input parameters and the lack of available data are also known to be limiting factors in applications of MIKE-SHE (Bouraoui et al., 1997). ANSWERS-2000 does not simulate interflow and baseflow contributions to streams (Borah and Bera, 2003), and it may cause difficulties in evaluating the impacts of BMP on subsurface areas and interaction between surface and ground water.

As a result, none of the models discussed in this section seem to be appropriate for evaluating long-term impacts of temporally and spatially changing BMPs on hydrology and water quality at the watershed-scale by considering the interaction between surface water and ground water.

**Goal and Objectives:**

The overall goal of this study was to develop a comprehensive tool for assessing the effectiveness of selected BMPs on both hydrology and water quality and demonstrate the applicability of the system on a watershed-scale by considering 1) temporally and spatially changing land use management practice in an agricultural watershed and 2) interaction between surface and ground water over the entire system. The specific objectives of this study were to:
1. Define the necessary characteristics of the system and design the structure of the system for considering the overall research goal.

2. Develop a distributed parameter, continuous simulation, and physically-based NPS model to predict hydrology, sediment, and pesticides, and evaluate the capability of the model in assessing the effectiveness of spatially and temporally changing BMPs at the watershed-scale.

3. Develop a comprehensive approach for considering dynamic surface and ground water interactions and evaluate the performance of the approach by comparing its predictions with the simulated results by other approaches.

4. Analyze the sensitivity of the model's surface and subsurface output to changes in input parameters, grid-size, and time-step to identify critical model parameters and provide guidelines for deciding appropriate grid-size and time-step.

5. Evaluate the applicability of the comprehensive modeling system for assessing the impacts of dynamically changing agricultural managements on an entire surface and subsurface system by considering different levels of crop rotation information based on actual and typical land use changes.

Dissertation Overview

Figure 1.1 shows the five steps of the modeling protocol developed in this study, including design, development, evaluation, sensitivity, and application. Chapter 1 contains the background information and overall modeling goal and objectives. Literature review of watershed-scale NPS model, ground water model, and agrochemical models are contained in chapter 2 in order to select a suitable code and methods for the various components required for the newly developed model. Chapter 3 explains the selected method and relationships used in the hydrology, sediment, pesticide, and dynamic parameter components of newly developed model, Dynamic Agricultural Non-point Source Assessment Tool (DANSAT). Development of the model interface is also included in Chapter 3. Development of the linked approach for the interaction between surface water and ground water is explained in chapter 4. Chapter 5 includes the input parameter preparation, model calibration, and validation in one field plot and two watersheds of different hydrologic characteristics. Chapter 6 contains the sensitivity analysis of the model’s output to different cell size, time step, and function input parameters. Application results of the model is
included in chapter 7 in order to demonstrate the responses of the newly developed comprehensive modeling system to different levels of crop rotations based on actual and typical land use changes.

Figure 1.1. Selected steps in developing a hydrologic and water quality model (adapted from Refsgaard, 1997).

References


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Chapter 2: Literature Review

Introduction

Three different groups of models are necessary to achieve the goal of this research. A physically-based, distributed, continuous, and watershed-scale non-point source pollution (NPS) model is necessary for assessing the effectiveness of selected BMPs on both hydrology and water quality by considering temporally and spatially changing land use management practice in an agricultural watershed. An agrochemical model and a ground water model are also necessary for considering interaction between surface and ground waters by simulating the movement of pollutants in the unsaturated zone and saturated zone, respectively. The three models, including 1) watershed-scale NPS model for simulating surface hydrology and water quality, 2) agrochemical model, which covers the soil profile between ground surface and ground water table, and 3) ground water model for saturated zone, should be integrated or linked in one system.

A large number of NPS models have been developed for simulating the generation and movement of water and its related pollutants from the point of origin to receiving waters (Borah and Bera, 2003). Current continuous simulation, watershed-scale NPS models that contain a surface component include AnnAGNPS (Bingner and Theurer, 2001), ANSWERS-2000 (Bouraoui et al., 2002), MIKE-SHE (Refsgaard and Storm, 1995), HSPF (Bicknell et al., 1993), and SWAT (Arnold et al., 1998). Conceptual models such as HSPF and SWAT require intensive calibration, and the results are not transferable to other watersheds (Heng and Nikolaidis, 1998). Due to the focus of this study, only distributed-parameter, continuous-simulation, physically-based, and watershed-scale models, such as AnnAGNPS, ANSWERS-2000 and MIKE-SHE, are reviewed in this chapter.

Both qualitative and quantitative models can be used to evaluate the fate and movement of agrochemicals in the subsurface. Qualitative models are referred to as index models that are generally used for evaluating ground water vulnerability to contamination. Several index models have been applied to large-scale assessment, using geographic information systems (GIS). Examples of index models include DRASTIC (Aller et al., 1985), Attenuation Index (AF) (Rao et al., 1985), Mobility and Degradation Index (MDI) (Mahmood and Sims, 1986), Ground water Ubiquity Score (GUS) (Gustafson, 1989), Leaching Pesticide Index (LPI) (Meeks and Dean, 1990), and Ground water Vulnerability Index for Pesticides (GWVIP) (Kellogg et al., 1994). Several quantitative models have been developed to describe the fate and movement of...
agrochemicals, such as pesticides and nitrate in the vadose zone (Figure 2.1). Addiscott and Wagenet (1985) categorized pesticide leaching models into three types: 1) detailed research models such as LEACHM (Wagenet and Hutson, 1989) and RZWQM (Hanson et al., 1998), 2) management models such as GLEAMS (Leonard et al., 1987) and PRZM (Carsel et al., 1985), and 3) screening models such as PESTAN (Enfield et al., 1982). Research models provide quantitative estimates of water flow and pesticide behavior, but comprehensive data are required for these types of models. Management models are less quantitative and data-intensive in predicting water and pesticide movement under transient field conditions compared to research models. This type of model cannot be used as an absolute predictor of pollutant loading. Screening models are intended for evaluation of pesticide behavior under constrained and limited conditions using an analytic solution, but few data inputs are required for this category of models (Wagenet and Rao, 1990). Therefore, only quantitative research and management agrochemical models are reviewed in this chapter.

![Figure 2.1. Evolution tree of agricultural water quality models (adapted from Chung, 1995)](image)

In addition, only the groundwater models using Finite Difference Method (FDM) are reviewed in this section, because the grid-based FDM is conceptually appropriate for the linkage between distributed surface, unsaturated zone, and saturated zone models, compared to the irregular grid of Finite Element Method (FEM). Furthermore, three modeling approaches for the simulation of flow and solute in saturated zone are reviewed, ranging from a complicated approach to a simple one.
Watershed-scale NPS Models

AnnAGNPS

The Agricultural Non-Point Source (AGNPS) model was developed in early 1980s (Young et al., 1987) and is widely applied throughout the world because of its ease of use, flexibility, and relative accuracy. However, it had serious limitation in that it was originally developed as an event-based model. In the early 1990s, a group of scientists developed a continuous-simulation version of the model, Annualized Agricultural Non-Point Source model (AnnAGNPS). Detailed information on different versions of the AGNPS model is provided in Table 2.1.

The AnnAGNPS is a continuous simulation, multi-event, watershed-scale model developed for evaluating non-point source pollution from agricultural watersheds of up to 300,000 ha in size. Several additional features, such as pesticides, snowmelt, and frozen soil, were incorporated to the capabilities of the original AGNPS (Bosch et al., 1998). Depending on the soil type, land use, and land management, the cells can be of any shape instead of the square grids used by AGNPS. The AnnAGNPS can be used to compare the effectiveness of alternative BMPs and select the most appropriate BMPs for a specific site and problem. In general, AnnAGNPS can simulate surface water, sediment, nutrient, and pesticide transport. Special components, such as feedlot and point source (only dissolved nutrients), gully erosion, cropping and tillage systems, impoundment and irrigation, are also included.
Table 2.1. Descriptions of AGNPS and AnnAGNPS (Bosch et al., 1998; Young et al., 1987).

<table>
<thead>
<tr>
<th>Models</th>
<th>Description</th>
</tr>
</thead>
</table>
| AGNPS    | • Hydrology  
  - Runoff: SCS curve number (CN) method  
  - Peak runoff: TR-55 method  
  - Regular cells  
  • Sediment  
  - 5 different particle size classes  
  - Soil erosion by USLE  
  - Transport capacity: Bagnold (1966) stream power equation  
  - Includes gully erosion and impoundments  
  • Chemical transport  
  - Nitrogen, Phosphorous, and COD  
  - Dissolved and adsorbed form  
  - Include point source input: feedlot, waste water plant discharges |
| AnnAGNPS | • Converted from event-based model to continuous simulation model  
  - Added snow melt, frozen soil, irrigation, and winter routines  
  - Evapotranspiration: Penman equation  
  - Percolation: hydraulic conductivity based on soil moisture content (Brooks-Corey equation)  
  - Two layers: tillage layer (20 cm) and static sub-layer  
  - Irregularly shaped cells  
  • Nutrients  
  - Daily mass balance of nitrogen, phosphorus, and organic carbon  
  - Plant uptake, residue decomposition, downward movement  
  - Sediment bound N, soluble N in runoff, sediment bound P, soluble P in runoff, and sediment bound organic carbon  
  • Add pesticide modules  
  - Unlimited number, dissolved and attached  
  - Wash-off from foliage  
  - Downward and upward pesticide movement in the soil profile  
  - Degradation base on the pesticide half-life  
  - Pesticide routing in streams based on travel time, water temperature, and pesticide half-life. |

The soil profile is divided into two layers. The top layer is a tillage layer of 200mm depth and its properties could vary. The properties of the remaining layers are static over time and space. The soil moisture budget of applied water, runoff, evapotranspiration, and percolation is calculated on a daily basis. The curve number method is modified on a daily basis based on tillage operation, soil moisture, and crop stage to calculate runoff. The modified TR-55 methods (Theurer and Cronshey, 1998) are used to compute overland flow, shallow concentrated flow, and concentrated flow. Actual evapotranspiration is a function of potential evapotranspiration, which is calculated using the Penman equation and the soil moisture content. The erosion module includes overland erosion, gully erosion, and streambed and bank erosion. Overland erosion is estimated by the Revised Universal Soil Loss Equation (RUSLE) (Renard et al., 1997). Gully erosion is a function of surface runoff volume. Streambed and bank erosion are determined from the transport capacity. The nutrient model simulates nitrogen (N), phosphorous (P), and organic carbon (OC). Soluble
and sediment-adsorbed N and P are simulated by considering plant uptake, fertilization, residue decomposition, and transport. The daily mass balance of each pesticide is calculated based on the GLEAMS (Leonard et al., 1987) pesticide module. Major processes in the pesticide module include foliage wash-off, vertical transport in the soil profile, and degradation. Runoff, sediment, nutrients, and pesticides are routed from each cell through the channel network to the watershed outlet. Sediment is routed considering five particle size classes based on transport capacity relationships explained by the Bagnold stream power equation (Bagnold, 1966). Each pesticide component is decayed during the reach routing, based upon the reach travel time, water temperature, and an appropriate pesticide half-life. Soluble pesticides can further be lost by infiltration through the bottom of reaches. The sediment-attached pesticides are adjusted by considering changes in clay particle sizes in the sediment from the upstream to downstream.

ANSWERS-2000

The original ANSWERS (Beasley et al., 1980) model, a distributed parameter and event-based planning model, was modified to simulate long-term continuous simulation of runoff, sediment, and nutrients (Bouraoui and Dillaha, 1996; Bouraoui and Dillaha, 2000). Byne (2000) developed and incorporated a process-oriented sediment detachment and channel scour submodel into ANSWERS-2000. Bouraoui et al. (1997) modified the model to include the simulation of water transport in the vadose and saturated zones. ANSWERS-2000 was coded using FORTRAN language. Detailed information on different versions of the ANSWERS model is provided in Table 2.2. In addition to ANSWERS-2000, an ArcView and MS Visual Basic based user interface, QUESTIONS, was developed to help create the input files for ANSWERS-2000 and display the cell-by-cell output (Veith et al., 2000).

Soil detachment and transport of the various particle size classes are modeled as a function of precipitation and overland flow. Soil particle detachment by overland flow does not occur unless excessive energy is available, after considering the amount required to transport suspended sediments. Within an element, the material available for transport is the combination of detached sediment within the element and entering sediment from adjacent elements. If the computed transport capacity is insufficient to carry the available material, the excess sediment is deposited in the element.

The current nutrient submodel in ANSWERS-2000 is adapted from GLEAMS. The model simulates dissolved and sediment-bound nutrients. The dissolved nutrient component is based on a mass balance approach, which simulates dissolved nutrient losses in runoff and percolation. The
input of dissolved nutrients come from the mixing of rainfall with dissolved nutrients present in the top portion of the soil (EDI), which is assumed to be 1 cm. Sediment-bound nutrient losses are based on the principle of conservation of mass. The initial nutrient content of the soil is distributed among the different particles’ size classes. The sum of sediment-bound nutrients comes from adjacent cells and the newly generated nutrients within the cell due to detachment.

Table 2.2. Description of ANSWERS and ANSWERS-2000.

<table>
<thead>
<tr>
<th>Models</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANSWERS</td>
<td>• Hydrology</td>
</tr>
<tr>
<td></td>
<td>- Interception: Huggins and Monke (1966)</td>
</tr>
<tr>
<td></td>
<td>- Detention: Huggins and Monke (1966)</td>
</tr>
<tr>
<td></td>
<td>- Infiltration: Holtan’s equation</td>
</tr>
<tr>
<td></td>
<td>- Runoff: continuity equation combined with a stage-discharge relationship</td>
</tr>
<tr>
<td></td>
<td>- Permitted rain gauges: up to 4</td>
</tr>
<tr>
<td></td>
<td>• Sediment</td>
</tr>
<tr>
<td></td>
<td>- Different particle size classes: up to 10</td>
</tr>
<tr>
<td></td>
<td>- Detachment by raindrop: function of kinetic energy of the rainfall (Meyer and Wischmeier, 1969)</td>
</tr>
<tr>
<td></td>
<td>- Detachment by overland flow: Meyer and Wischmeier (1969) as modified by Foster and Meyer (Foster, 1976)</td>
</tr>
<tr>
<td></td>
<td>- Transport: Yalin’s equation (1963) modified by Foster and Meyer (1972)</td>
</tr>
<tr>
<td></td>
<td>- Channel erosion is not simulated</td>
</tr>
<tr>
<td>ANSWERS-2000</td>
<td>• Converted from event-based model to continuous simulation model*</td>
</tr>
<tr>
<td></td>
<td>- Improved infiltration model: Green-Ampt infiltration equation</td>
</tr>
<tr>
<td></td>
<td>- Evapotranspiration submodel: adaptation of Ritchie’s method (Ritchie, 1972)</td>
</tr>
<tr>
<td></td>
<td>- Permitted rain gauges: up to 8</td>
</tr>
<tr>
<td></td>
<td>- A single homogeneous soil layer</td>
</tr>
<tr>
<td></td>
<td>• Nutrient modules: based on GLEAMS model</td>
</tr>
<tr>
<td></td>
<td>- Nitrogen: 4 nitrogen pools (stable organic N, active organic N, nitrate, and ammonium) and transformations (ammonification, nitrification, and plant uptake)</td>
</tr>
<tr>
<td></td>
<td>- Phosphorous: 4 phosphorous pools (stable mineral P, active mineral P, soil organic P, and labile P)</td>
</tr>
<tr>
<td></td>
<td>• Process-oriented sediment module‡</td>
</tr>
<tr>
<td></td>
<td>- Critical shear rill detachment subroutine based on WEPP (Flanagan and Nearing, 1995).</td>
</tr>
<tr>
<td></td>
<td>- Improved interrill detachment subroutine based on WEPP.</td>
</tr>
<tr>
<td></td>
<td>- Channel scour subroutine based on WEPP model</td>
</tr>
<tr>
<td></td>
<td>• Interaction between surface and subsurface†</td>
</tr>
<tr>
<td></td>
<td>- 4 layers: 2 (root zone), 1 (vadose zone), 1 (saturated zone)</td>
</tr>
<tr>
<td></td>
<td>- Root depth: sinus function of number of days after planting and before maturity</td>
</tr>
<tr>
<td></td>
<td>- Drainage in the unsaturated zone: based on Darcy’s approach</td>
</tr>
<tr>
<td></td>
<td>- Travel time through a particular soil layer: linear storage equation</td>
</tr>
<tr>
<td></td>
<td>- Drainage during a specific time step: exponential function (Williams et al., 1985)</td>
</tr>
<tr>
<td></td>
<td>- No lateral subsurface flow from one cell to another in the unsaturated zone</td>
</tr>
<tr>
<td></td>
<td>- Average daily aquifer discharge is distributed to each cell and new piezometric head is determined</td>
</tr>
</tbody>
</table>

* Bouraoui and Dillaha, 1996 and 2000
‡ Byne, 2000
† Bouraoui et al., 1997
MIKE-SHE

MIKE-SHE (Refsgaard and Storm, 1995) has been developed based on the SHE (Abbott et al., 1986) modeling concept to simulate water quality and soil erosion. The model can be applicable to a wide range of problems including the dynamic interaction between surface and ground water systems on different spatial scales ranging from a single soil column to a large river basin. MIKE-SHE is a distributed parameter, physically-based, continuous simulation model. Water Movement (WM) is the basic module of MIKE-SHE and is used to simulate the entire hydrologic cycle as well as individual processes in the cycle. MIKE-SHE WM module consists of six process-oriented components, including 1) interception, 2) overland and channel flow, 3) unsaturated flow, 4) ground water flow, 5) snowmelt, and 6) aquifer-river exchange (Table 2.3). These processes may operate at different time steps consistent with their own most appropriate temporal scales. In the case of different time steps, accumulation of simulated values over a period is required to transfer from one component to another. Furthermore, add-on modules for specific processes include: advection and dispersion of solutes (AD), geochemistry (GM), biological (BM), sorption and degradation (SD), macropore flow (MP), linear reservoir (LR), particle tracking (PT), crop growth and nitrogen processes in the root zone (DAISY), soil erosion (SE), and irrigation (IR).

MIKE-SHE AD module describes the transport and spreading of conservative solutes in the environment by solving the advection-dispersion equations. AD consists of four components, including overland, channel, unsaturated, and saturated transport (Table 2.3). It can be coupled with other modules such as Sorption/Degradation (SD) module. MIKE-SHE SD module, which is particularly designed for simulation of behavior of pesticides, describes sorption and degradation of solutes in the unsaturated and saturated zones using equilibrium or kinetic isotherms for sorption and simple first-order method for degradation.
Table 2.3. Description of each component of water movement (WM) and advection and dispersion (AD) modules of MIKE-SHE (DHI, 2000a; DHI, 2000b).

<table>
<thead>
<tr>
<th>Module</th>
<th>Components</th>
<th>Methods or Governing equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>WM</td>
<td>Interception and Evapotranspiration</td>
<td>- Rutter model/Penman-Monteith equation or</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Kristensen-Jensen model</td>
</tr>
<tr>
<td></td>
<td>Overland and Channel flow</td>
<td>- Overland flow: 2-D diffusion wave approximation of the Saint Venant equations</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Channel flow: 1-D diffusion wave approximation of the Saint Venant equations</td>
</tr>
<tr>
<td></td>
<td>Unsaturated flow</td>
<td>- 1-D Richards’ equation</td>
</tr>
<tr>
<td></td>
<td>Ground water flow</td>
<td>- 3-D Boussinesq equation</td>
</tr>
<tr>
<td></td>
<td>Snowmelt</td>
<td>- Degree-day method or</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Energy budget method</td>
</tr>
<tr>
<td></td>
<td>Aquifer-River exchange</td>
<td>- Darcy’s law</td>
</tr>
<tr>
<td>AD</td>
<td>Overland transport</td>
<td>- 2-D advection and dispersion equation for conservative solutes</td>
</tr>
<tr>
<td></td>
<td>Channel transport</td>
<td>- 1-D advection and dispersion equation for conservative solutes</td>
</tr>
<tr>
<td></td>
<td>Unsaturated zone transport</td>
<td>- 1-D advection and dispersion equation for conservative solutes</td>
</tr>
<tr>
<td></td>
<td>Saturated zone transport</td>
<td>- 3-D advection and dispersion equation for conservative solutes</td>
</tr>
</tbody>
</table>

Selection of a Base Model

The phrase "base model" is used in this chapter to refer to any existing model selected as reference material for adopting its concepts, approaches, and equations used in a process of model development for this study. AnnAGNPS is not used as a base model due to the restrictions caused by selected curve number (CN) and Universal Soil Loss Equation (USLE) methods for simulating runoff and soil erosion components, respectively. Empirically derived CN values and USLE factors may cause difficulties in deciding parameter values according to different BMP scenarios for simulating the impacts of temporally changing BMPs on hydrology and water quality. Bouraoui (1994) reported on major limitations of the curve number method, including: 1) runoff is not related to the rainfall intensity or duration, 2) the curve number does not change with variation in vegetal cover or management practices, 3) curve numbers are not available for all areas and land uses in the United States, and 4) the curve number is not appropriate for large watersheds. Although the USLE is considered to be a good method for estimating long-term average annual soil loss from homogeneous fields, parameters have no physical meaning with respect to transport of sediments and the model cannot simulate temporal and spatial variability required by an effective planning model (Byne, 2000). In addition, AnnAGNPS uses irregularly shaped cell division, which may cause difficulties in the linkage to grid-based ground water models.
MIKE-SHE was not used as a base model because of lack of information on model components, even though the concept of MIKE-SHE is appropriate to the purpose of this research. MIKE-SHE is a commercial model and its source code is not open to the public. In addition, there is difficulty in obtaining information on BMP related model components. Application of this model is limited because it requires extensive input parameters (Bouraoui et al., 1997).

The current ANSWERS-2000 is a process-oriented, distributed-parameter, watershed-scale, continuous-simulation model and is appropriate for use in this research, except for the component dealing with the interaction of surface and ground water. Availability of source code is one important factor for selecting an appropriate NPS model for this study. Source code for ANSWERS-2000 is available in the Department of Biological Systems Engineering of Virginia Tech. As a result, ANSWERS-2000 was selected as a base model, even though it does not contain interflow and baseflow components.

Agrochemical Models

GLEAMS

Ground water Loading Effects of Agricultural Management Systems (GLEAMS) is a continuous-simulation, field-scale mathematical model developed to evaluate the effects of agricultural management systems on the movement of agricultural chemicals within and through the plant root zone (Leonard et al., 1987). The GLEAMS model was developed to consider the movement of water and chemicals through the root zone based on the CREAMS (Knisel, 1980) model. The GLEAMS model has been evolved from its original version to the current 3.0 version and has been evaluated in a number of different climatic and soil conditions. Reyes et al. (1993) modified the GLEAMS model to account for shallow water table fluctuation by replacing the evapotranspiration and percolation algorithms (GLEAMS-Water Table: GLEAMS-WT). In addition, the subsurface drainage function in the soil profile was incorporated into GLEAMS-WT by Reyes and others (1994).

The GLEAMS model considers only the root zone, which can be defined as several layers (up to five) with different soil properties. The surface soil layer has a fixed thickness of 1 cm, considering the strong correlation between pesticide concentration in runoff and pesticide concentration in the top 1 cm soil layer. Agricultural management such as planting date, cropping systems, irrigation scheduling, and tillage operations can be considered in the model. This model consists of four major components: hydrology, erosion/sediment, pesticide, and nutrient transport.
Precipitation is partitioned into infiltration and runoff, which is estimated using the modified curve number method (Williams and Nicks, 1982). Soil water redistribution within the root zone and the percolation through the root zone are based on storage-routing techniques. This approach requires capacity factors such as current soil water content, field capacity, and wilting point in each soil layer in order to simulate water movement from one layer to the next layer. Evapotranspiration is simulated using either the Penman-Monteith model (Jensen et al., 1990) or the Priestly-Taylor model (Priestly and Taylor, 1972).

Erosion in GLEAMS is represented as detachment and transport processes. Interrill detachment and rill detachment rate (Foster et al., 1980) are estimated considering kinetic energy of storm, slope, soil properties, peak runoff rate, and runoff volume. Sediment transport capacity is calculated using a modified Yalin’s equation (Foster et al., 1980). GLEAMS considers advective transport of pesticide through the soil and surface water. Up to 366 pesticides can be simulated simultaneously (GLEAMS ver. 3.0). Pesticide sorption is described by equilibrium adsorption using organic carbon-water partition coefficient (Koc) and organic matter or organic carbon content as input parameters. Pesticide degradation is described using first-order kinetics that considers temperature and water content impacts on degradation rate. Degradation half-lives can be specified for each soil horizon to take into account soil depth impacts on degradation. Pesticide losses related to plant uptake are considered by multiplying the crop transpiration rate, by the dissolved phase concentration of pesticides, and plant uptake coefficient.

**PRZM**

Pesticide Root Zone Model (PRZM) is a one-dimensional, daily time scale, management model for predicting pesticide movement within entire vadose zone. In addition to its use for pesticide registration, PRZM can consider cropping practices and agricultural management practices such as tillage. PRZM does not simulate subsurface lateral flow, macropore flow, or tile drainage. The model has evolved from PRZM-2 to the current WINPRZM (PRZM ver. 3.20 Beta, FOCUS release, August 2000). PRZM-2 links two models, PRZM and VADOFT, in order to predict pesticide fate and transport through the root zone and intermediate zone. Several features, such as soil temperature simulation, vapor phase transport in soils, microbial transformation, and irrigation simulation, are incorporated into PRZM-2. PRZM-2 simulates evapotranspiration using either Hamon formula (Hamon, 1961) or pan evaporation method (Mullins et al., 1993). PRZM-3 includes the ability to consider nitrogen cycle and nitrogen discharges from the septic tanks into soil and ground water, as well as the ability to describe pesticide degradation as a function of soil
The abilities added into WINPRZM include degradation process as a function of soil moisture, option of using Freundlich isotherm, and modified first order degradation routines for both parent and daughter compounds.

The model consists of hydrology and chemical transport components. The hydrology component includes surface runoff, evapotranspiration, and percolation. Modified curve number method (Williams and LaSeur, 1976) and modified Universal Soil Loss Equation (Williams and Berndt, 1977) are used to simulate surface runoff and erosion. Actual evapotranspiration is calculated from the daily pan evaporation, soil water availability, and stage of crop growth. Remaining water, after subtracting runoff, evapotranspiration, and interception losses from rainfall, infiltrates into the soil matrix. The routing of soil water within the unsaturated zone is based on storage-routing techniques (“tipping bucket” scheme) that consider the water holding capacity of the soil, such as field capacity and wilting point. The chemical transport component predicts dissolved, adsorbed, and vapor phase concentrations in the soil considering convection-dispersion transport, plant uptake, degradation, and foliar wash-off. Pesticide degradation is described using first-order kinetics and sorption is assumed as linear. Different degradation rates can be defined for each soil layer as well as for plant foliage. PRZM has been validated in several studies; however, most of these studies emphasize soil water distribution and the behavior of pesticides in soil.

**RZWQM**

Root Zone Water Quality Model (RZWQM) is a one-dimensional, process-based, research-level simulation model to simulate hydrologic and chemical responses of agricultural management systems (Hanson et al., 1998). The model can simulate plant growth and movement of water, nutrients, and pesticides over, within, and below the crop root zone by considering physical, chemical, and biological processes. RZWQM can be used as a tool for evaluating the impact of a variety of agricultural management practices on the behavior and movement of nitrate and pesticides to surface runoff and subsurface environment. These management practices include drainage, tillage and residue practice, crop rotations, and application (method, amount, and timing) of irrigation, fertilizer, manure, and pesticide. In addition to the simulation of a tile drainage system, the model can also simulate high and fluctuating water tables. RZWQM can also be used to estimate the potential loadings of non-point source pollutant to the ground water. RZWQM consists of six major processes: physical, plant growth, soil chemical, nutrients, pesticide, and management processes. These processes are considered at daily and hourly time scales. Hourly based processes, which are contained in physical processes, include heat.
movement, infiltration and runoff, actual evaporation and transpiration, snowpack dynamics, soil water redistribution, pesticide wash-off, plant nitrogen uptake, chemical transport, and reconsolidation of tilled soils.

The infiltration rate into the soil matrix and lateral infiltration of macropores are calculated using the Green-Ampt equation (Green and Ampt, 1911) and a modification of the Green-Ampt approach (Ahuja et al., 1995), respectively. Any surplus of the excess rainfall after infiltration into the soil matrix and macropores is considered as runoff. Soil water redistribution is described using the Richards’ equation as in LEACHM. Potential evapotranspiration is estimated using a revised version of the double-layer model of Shuttleworth and Wallace (1985). Sequential partial piston displacement and mixing approach, which is simpler than the convection and dispersion equation, is used to simulate transport of chemicals in the soil matrix. Pesticide processes include the transformations and degradation of pesticides on plant surfaces, crop residue, the soil surface, and in the soil matrix. Degradation algorithms allow for a single lumped dissipation constant or two dissipation rates that represent a quick dissipation period after the time of application until the next rainfall event and a slower dissipation period after a rainfall event. Adsorption coefficients are updated daily to consider variations in organic matter decomposition and bulk density changes (Hanson et al., 1998).

**LEACHM**

The Leaching Estimation and Chemistry Model (LEACHM) is a highly physically-based, mechanistic, finite difference, research model to simulate water flow and pesticide transport in root zone (Wagenet and Hutson, 1989). The model consists of four sub-models: 1) LEACHW, which describes soil water flow only; 2) LEACHP, which describes fate and behavior of pesticides; 3) LEACHN, which describes the transport and transformations of nitrogen; and 4) LEACHC, which describes the movement of inorganic salts. The concept of the CALF model (Addiscott, 1977; Nicholls et al., 1982) was integrated into LEACHP to describe new water and solute transport routings (LEACHA). LEACHM does not consider surface runoff and erosion components. The model considers several processes such as steady and transient water flow in the unsaturated zone, crop growth and transpiration, evaporation and soil heat flow, and changes in water table elevation. LEACHM is not effective for evaluating the long-term impacts of agricultural BMPs on ground water quality. It uses Richards' equation to predict soil moisture dynamics in the root zone. LEACHP simulates non-volatile pesticides in the unsaturated zone by considering sorption, degradation, advection, and dispersion. Pesticide movement is described
based upon the convection-dispersion equation (CDE). This module also includes the capability to predict pesticide transformation products as well as the parent pesticide compound.

Opus

Opus (Ferreira and Smith, 1992; Smith, 1992) is a comprehensive model developed to simulate the processes of sediment and chemical transport, carbon and nutrient cycles in soil microbial decay, flow of heat in soil, and growth of crops. Opus allows the user to choose between a detailed physically-based approach using breakpoint rainfall and a lumped approach using daily rainfall. Weather conditions can be simulated using a daily weather generation model (WGEN). Surface runoff and soil erosion are calculated using a modified SCS curve number approach and Modified Universal Soil Loss Equation (Williams, 1975), respectively. The model can consider the impacts of various surface boundary conditions, such as surface crusts and seals on infiltration and runoff. Opus uses a Preistly-Taylor type formula to estimate potential evapotranspiration and modification of the Ritchie model (Ritchie, 1972) to calculate plant water use in consideration of potential ET and leaf area index. Plant growth in Opus is described by a mechanistic model that considers solar radiation and availability of water, nutrients, and temperature. Water flow in the unsaturated zone is simulated by a finite difference solution of the rate-based Richards’ equation. The hydraulic characteristics of each soil layer are described using five parameters: saturated hydraulic conductivity, saturated water content, residual water content, air entry pressure, and pore-size distribution index.

Like GLEAMS, Opus does not consider dispersion of solutes. Pesticide sorption in the model is described by a linear isotherm or kinetic adsorption using parameters, such as organic carbon-water partition coefficient (Koc) and organic matter or organic carbon content. Pesticide degradation is described using first-order kinetics. Degradation rate is modified by temperature (Arrhenius equation) and water content (Walker, 1974). The ratio of organic carbon in the subsurface horizon to the top horizon is used to take into account the degradation rate as a function of depth. Like GLEAMS, pesticide losses related to plant uptake are considered by multiplying the normal crop transpiration rate by the dissolved phase concentration and plant uptake coefficient.

Selection of a Base Model

The reviewed pesticide leaching models can be classified as either rate-based or capacity-based, depending on the method in which models handle water flow and solute leaching in soil.
LEACHM uses the rate-based Richards’ equation and convection-dispersion equation (CDE) to simulate water flow and solute transport in soil, respectively. Opus and RZWQM use Richards’ equation for simulating water flow but simulate only convective solute transport. PRZM and GLEAMS use a capacity-based approach for water flow and solute transport; although, PRZM has an option to simulate solute transport using the CDE (Zacharias et al., 1999).

Rate-based models such as LEACHM and RZWQM require intensive input parameters for each soil layer to solve Richards’ and convection dispersion equations. For example, a rate-based model, LEACHMP, was judged to be a complex and difficult model due to extensive input requirement based on the comparison of five pesticide simulation models (Pennell et al., 1990). In addition, a rate-based approach requires intensive computer resources, especially when the one-dimensional vadose zone component is linked to every square grid within a watershed-scale model. MIKE-SHE identifies the homogeneous region within the modeling area and treats the homogeneous region as one representative soil column to save computational time (DHI, 2000a).

Zacharias et al. (1999) compared Opus and GLEAMS to determine if a rate-based model would predict the water flow and pesticide movement in the soil profile more accurately than a capacity-based model. Opus simulated the soil water distribution within the soil profile better than GLEAMS. However, a capacity-based model simulated depth-averaged soil water content and total pesticide mass in the root zone with reasonable accuracy using fewer parameters compared to a rate-based model (Zacharias et al., 1999). Overall, management models using capacity-based approach were considered as base models in this research.

Ground Water Models

MODFLOW and MT3D

The USGS finite difference model MODFLOW (McDonald and Harbaugh, 1984) is a modular model that simulates ground water in a three-dimensional environment. MODFLOW uses a block-centered finite difference approach to simulate ground water flow within the aquifer. Layers can be simulated as confined, unconfined, or a combination of the two. External stresses such as wells, aerial recharge, drains, evapotranspiration, and streams can be simulated using the appropriate MODFLOW packages, as well as appropriate boundary conditions developed in a conceptual model.

MT3D (Zheng, 1990) is a transport model for simulation of advection, dispersion, and chemical reactions of contaminants in ground water flow systems in either two or three dimensions. This
model was developed for use with any block-centered finite difference flow model such as MODFLOW. A flow model saves the information, which is then retrieved by MT3D. MT3D has a modular structure and make it possible to simulate advection, dispersion, source/sink, or chemical reactions independently, without reserving computer memory space.

**HST3D**

The Heat and Solute Transport Program (HST3D) simulates ground water flow, associated heat, and solute transport in saturated, three dimensional flow systems with variable density and viscosity (Kipp, 1997). The equations that are solved numerically include: 1) the saturated ground water flow equation, formed from the combination of the conservation of total fluid mass and Darcy’s Law for flow in porous media; 2) the heat transport equation from the conservation of enthalpy for the fluid and porous medium; and 3) the solute-transport equation from the conservation of mass for a single-solute species that may decay and may adsorb onto the porous medium. Finite-difference techniques are used for the spatial and temporal discretization of the equations. When appropriate boundary and initial conditions and system parameter distributions are supplied, simulation calculations can be performed to evaluate a wide variety of heat and solute transport situations.

For most applications, only the heat or the solute transport equation is solved in conjunction with ground water flow. Three-dimensional Cartesian and axially symmetric, cylindrical coordinate systems are available. The model is applicable to the study of waste injection into fresh or saline aquifers, contaminant plume movement, salt-water intrusion in coastal regions, brine disposal, freshwater storage in saline aquifers, heat storage in aquifers, liquid-phase geothermal systems, and similar transport situations.

**VS2D**

VS2D (Healy, 1990) is a two-dimensional finite difference computer model developed by the U.S. Geological Survey for solving problems of water flow and solute transport in variably saturated porous media. The finite difference method is used to approximate the flow equation, which is developed by combining the law of conservation of fluid mass with a nonlinear form of Darcy's equation, and the advection-dispersion equation. Several options for boundary conditions, which are specific to flow under unsaturated conditions, are considered. Available options are infiltration with ponding, evaporation, plant transpiration, and seepage faces.
VS2D is a useful tool in studies of water quality, ground-water contamination, waste disposal, or ground-water recharge. Program options include first-order decay, equilibrium adsorption described by Freundlich or Langmuir isotherms, and ion exchange. Boundary conditions for solute transport in VS2DT include fixed solute concentration and fixed mass flux. Simulated regions include one-dimensional columns, two-dimensional vertical cross sections, and axially symmetric, three-dimensional cylinders.

The program is written in standard Fortran 77. Extensive use of subroutines, functions, and subprograms provide a modular code that can be easily modified in order to apply the model to particular applications.

Selection of a Base Model

The MODFLOW was selected as saturated zone model in spite of a requirement of another solute transport model, such as MT3D, for simulating pesticide movement in the ground water. The main reason for selecting MODFLOW as saturated zone model is that MODFLOW has become an industry standard in ground water modeling studies and is the most widely used and supported ground water model (Anderson and Woessner, 1992). In addition, MODFLOW has the advantage that it already includes a stream-aquifer interaction module, such as River package and Streamflow Routing package (McDonald and Harbaugh, 1988; Prudic, 1989). Advantages of combined MODFLOW-MT3D approach also include: 1) separate flow simulation results in substantial savings in computer memory and 2) many different transport simulations can be executed based on the same solution of a flow model (Zheng, 1990). Impacts of pumping or land development on ground water discharge rates to streams has been simulated using MODFLOW alone (Morgan and Jones, 1995; Morgan and McFarland, 1994), and linkage between MODFLOW and existing surface models such as HSPF (Ross et al., 2005) and SWAT (Sophocleous et al., 1999) have also been developed for considering the interaction between surface water and ground water. In contrast, HST3D and VS2D are finite difference models developed to simulate both flow and solute transport in saturated zone. Their major difference is that HST3D is three-dimensional while VS2D is two-dimensional. In addition, there is a need to develop a stream-aquifer interaction module for the combined flow and solute transport models such as HST3D and VS2DT.
Summary

Three different groups of models, including 1) watershed-scale NPS models, 2) agrochemical models, and 3) ground water models, were reviewed in this chapter. An appropriate model from each group was selected as the base model for developing the proposed comprehensive modeling systems.

ANSWERS-2000 was selected as a base watershed-scale NPS model in spite of its limitations in simulating interflow and baseflow. This model is an ideal NPS model (process-oriented, distributed-parameter, and continuous-simulation model), and the availability of source code was considered as the main reason for selecting ANSWERS-2000. Capacity-based models, such as GLEAMS and PRZM, were selected as reference agrochemical models. Rate-based models including LEACHM, RZWQM, and Opus were excluded mainly due to intensive requirements of input parameter and computer resource, which does not proportionally improve the accuracy of the simulation results. MODFLOW was selected as the ground water model due to its widespread use and availability of the stream-aquifer interaction module (River package and Streamflow Routing package).

References


Chapter 3: Dynamic Agricultural Non-point Source Assessment Tool (DANSAT)

Introduction

A distributed, continuous, physically-based watershed-scale model is suggested as an ideal NPS model (Dillaha, 1990). The justification and other advantages of this type of models were mentioned in Chapter 1. The general concept and characteristics of the model should be decided before appropriate methods and equations are selected to satisfy two main criteria for the new model to be developed: 1) the model should consider temporally and spatially changing land use management practice in an agricultural watershed, and 2) interactions between surface and ground water over the entire system should be considered. The general concept and selected modeling approaches for the first criterion are described in this chapter, while the modeling approach for the second criterion is separately explained in Chapter 4.

The structure of the newly developed model is fully distributed in order to enable consideration of the impacts of spatially changing BMPs on hydrology and water quality. In vertical structure, the model needs to have multiple soil layers to consider not only plant uptake and evapotranspiration at various crop growth stages but also to evaluate the impacts of different BMPs, such as tillage and pesticide application methods, on pesticide movement in the root zone. In addition, the structure of model input files should be appropriate for considering the spatial distribution of model parameters. Spatially distributed parameters may include topographic, soil, and land use related parameters. Weather input also needs to consider spatial distribution of rainfall at the watershed-scale considering that precipitation is the major driving force behind surface runoff and contaminant transport. To evaluate the impacts of temporally changing BMPs, the model parameters should be physically-based for reflecting changes in characteristics of soil, crop, and residue cover during the simulation period.

WEPP is a physically-based water erosion prediction model designed for simulating temporal variation in plant growth, residue decomposition, and soil consolidation for various management practices, including tillage (Flanagan and Nearing, 1995). The soils component of the WEPP model simulates the impacts of tillage on various soil properties such as bulk density, total porosity, soil roughness, ridge height, and changes in erodibility parameters (Alberts et al., 1995). The plant growth component of WEPP predicts the temporal changes in plant characteristics and their impact on the hydrologic and erosion processes. The model predicts crop growth variables
for cropland and rangeland, separately. Information on plant related variables, such as canopy cover, canopy height, and biomass, are provided to other components for calculating water balance, soil detachment, and residue amount remaining on the land after management applications such as harvesting and tillage (Arnold et al., 1995). The residue decomposition component of the WEPP model simulates plant residue decomposition for different management practices such as tillage, shredding, burning, or removing residue. Residue decompositions for cropland and rangeland are considered in separate submodels (Stott et al., 1995).

A robust model should be able to provide a variety of output files for analysis of simulation results. Outputs at watershed outlets are necessary for understanding the overall impacts of implemented BMPs on surface hydrology and water quality. Model outputs at watershed outlets can be classified into two categories on the temporal scale: daily values or storm events. Spatially distributed flux outputs are necessary to analyze the BMP impacts on moisture and pollutants transport in the subsurface. For comprehensive analyses in a target area, information on temporal changes in soil moisture contents and pesticide concentrations at various soil layers is very helpful. The model should also have the ability to provide information on vertical distribution of soil moisture content and pesticide concentration in the user-defined target cells.

There are several limitations that restrict the application of distributed parameter models including 1) intensive input data or parameter requirement and 2) difficulties in analyzing the spatial simulated model results. Development of a user interface to couple GIS with hydrologic models has been the focus of many researchers since early 1990s (Borah and Bera, 2003), because data structures and conceptualizations of space and time in the current GIS are not appropriate for the internal integration of hydrological models into the GIS (Sui and Maggio, 1999; Tim, 1996). Time required to prepare input data, especially for a distributed NPS pollution model, could be significantly reduced using a GIS integrated interface. The efficiency of the interface can be optimized if the same data are utilized repeatedly. Time and labor for creating a new input file for different grid sizes and alternative management scenarios, for example, could be significantly reduced if the base spatial information, such as DEM, soil, and land use maps, exists in a GIS format.

A number of GIS interfaces have been developed for distributed hydrologic and water quality models including: GRASS-AGNPS (He et al., 1993; Line et al., 1997; Srinivasan and Engel, 1994), Arc/Info-AGNPS (Liao and Tim, 1997), Arc/View-AGNPS (He et al., 2001), GRASS-ANSWERS (Engel et al., 1993), Arc/View-ANSWERS (Zhang and Hayes, 1999), Arc/Info-
ANSWERS2000, Arc/View-ANSWERS2000 (Veith et al., 2000), GRASS-WEPP (Savabi et al., 1995), GRASS-TOPMODEL (GRASS Development Team, 2005), and GRASS-SWAT (Engel et al., 1993; Srinivasan and Arnold, 1994). GRASS was selected for a number of hydrologic models, including ANSWERS, AGNPS, TOPMODEL, SWAT, and WEPP, because of its open source code (Ogden et al., 2001). Some of those NPS pollution models have been applied as a part of decision support systems (DSS) due to complexity and variety of problems that need to be analyzed (He et al., 2001; Osmond et al., 1997). Most of these DSSs consist of an analytical model and an interface based on GIS and a spatial or attribute database as common components. The common purpose behind integration of GIS and distributed parameter models is to extract required model input parameters and to analyze and visualize the simulated results (He et al., 2001). The DSS enhances the common capability of GIS/NPS model linkage and could be used as: 1) a statistical analyzer and scenario simulator (He et al., 2001); 2) a web-based expert system to guide users in identification of water quality problems and selection of appropriate BMPs; 3) an educational tool; and 4) provide easy access to NPS related bibliography (Osmond et al., 1997).

Accordingly, the objectives of this chapter are 1) to identify the necessary characteristics and concept of the new NPS pollution simulation model capable of evaluating the effectiveness of spatially and temporally changing BMPs, 2) select appropriate approaches and methods for developing model component, and 3) develop an interface to enhance the application of the newly developed NPS pollution model.

Model Concepts

ANSWERS-2000 (Bouraoui et al., 2002) and WEPP (Flanagan and Nearing, 1995) were selected as base models for a newly developing model, Dynamic Agricultural Non-point Source Assessment Tool (DANSAT). ANSWERS-2000 was selected for considering spatial distribution of BMP applications at watershed-scales in DANSAT, while WEPP was selected for considering temporal impacts of BMPs on internal parameters of DANSAT. AnnAGNPS (Bingner and Theurer, 2001) was excluded because runoff and sediment loads are estimated based on empirical approaches such as curve number (CN) method and Revised Universal Soil Loss Equation (RUSLE), respectively. MIKE-SHE (Refsgaard and Storm, 1995) was not considered as a base model because it requires intensive input parameters and calculation time due to selected numerical methods for water and contaminant transport. In addition, the source code for ANSWERS-2000 is readily available compared to those for AnnAGNPS and MIKE-SHE. The list of recommendations for future improvement from the previous developers of ANSWERS-
2000 was considered during the stage of defining the concept, characteristics, and structure of DANSAT. Table 3.1 shows a summary of major issues considered from previous recommendations by developers for ANSWERS-2000 (Bouraoui, 1994; Byne, 2000; Zeckoski, 2002). The structure of DANSAT was designed to improve the programming efficiency by breaking the model into small size subroutines. The object oriented concept through subroutines makes it easy to add or modify a component by future model developers. The introduction of dynamic array, which is supported by Fortran90, increases the computational efficiency of DANSAT by assigning required memory based on user-defined input parameters.

Table 3.1. Summary of major issues considered from previous recommendations by developers of ANSWERS-2000.

<table>
<thead>
<tr>
<th>Limitations/Recommendations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Overland flow direction with 0-360° may cause leakage around watershed boundary cells</td>
</tr>
<tr>
<td>Solves Manning equation by a look up table requires a user input of expected peak runoff</td>
</tr>
<tr>
<td>Fixed short time-step (30 seconds) even during no runoff period</td>
</tr>
<tr>
<td>Maximum of 35000 cells</td>
</tr>
<tr>
<td>Maximum of 30 types</td>
</tr>
<tr>
<td>One soil layer</td>
</tr>
<tr>
<td>Lack of ability to simulate dynamic soil parameters</td>
</tr>
</tbody>
</table>

**Dynamic Parameters**

Spatially and temporally changing land management practices alter soil, crop, and ground surface characteristics over a watershed and influence the process of infiltration, runoff, sediment detachment and transport, and agricultural chemical leaching into ground water. A comprehensive NPS pollution model is necessary to take into account the changes in soil, crop, and residue characteristics due to the spatial and temporal changes of BMPs. A schematic representation of the impacts of spatial and temporal land use changes on crop, soil, and residue parameters is shown in Figure 3.1.
Soil, plant growth, and residue decomposition components in the WEPP model were slightly simplified and incorporated into the DANSAT to consider temporal changes of land management practices. The changes incorporated in DANSAT, which deal with the simplification of adjusting factors in WEPP, will be explained in detail later in this chapter. Temporal changes in crop variables, such as biomass, leaf area index (LAI), canopy cover, canopy height, root development, and interception, are simulated by the plant growth component. The soil component predicts both hydrology-related parameters such as effective hydraulic conductivity and soil detachment-related parameters such as interrill and rill erodibility factors. These are calculated, based on daily variable soil parameters including random roughness, ridge height, and bulk density. The residue decomposition component predicts decomposition rates of three types of residues such as flat, buried, and dead root biomasses.

The three components are interactive with each other. Daily estimated biomass is used to predict the LAI, canopy cover and height, and interception of precipitation. LAI is used in the evapotranspiration component to simulate the extraction of water from multiple soil layers in combination with the simulated root depth. The simulated canopy height and cover, as well as dead roots and live root biomass, are used to adjust the rill and interrill erodibility factors in the
soil component. Predicted random roughness, residue cover, canopy cover, and canopy height are used to simulate daily variable hydraulic conductivity, rill erodibility, and interrill erodibility. Details on the three components are explained later in this chapter.

### Input Structures

The input structure of NPS pollution models should be appropriate for considering temporally and spatially changing BMPs. DANSAT requires at least three indispensable input files such as weather, break-point rainfall, and main input files. Initial input file, which is used to define initial conditions including soil water content and pesticide concentration in soil layers, is optional. Figure 3.2 shows the necessary input files and the data structure of the main input file.

![Diagram of Input Files](image)

**Figure 3.2.** Input files for DANSAT and the data structure of the main input file.

Break-point rainfall data is separated from the weather input file. If the model reads one day of weather input and there is a rainfall event on the day, DANSAT reads break-point rainfall data from a separate break-point input file. The separation of weather data and break-point rainfall data will give more flexibility to the possible development of a daily-based hydrology component such as SCS curve number and USLE methods in the future. The hierarchical structure of “physical variable data blocks ➔ temporal variable data block (Rotation data block) ➔ spatial
variable data block (Cell data block)” was used to allow DANSAT to consider both spatial and temporal land management practices in detail.

Physical data blocks, including crop, soil, pesticide and pesticide application, tillage, and channel data blocks, define physical properties of crop, soil, agro-chemicals, and agricultural management. Physical parameters are not influenced by any spatially and temporally changing BMPs; therefore, they are not changed during the simulation period. Table 3.2 shows the physical data blocks and input parameters for each data block.

**Table 3.2. Physical variable data blocks and input parameters.**

<table>
<thead>
<tr>
<th>Data blocks</th>
<th>Parameter</th>
</tr>
</thead>
</table>
| Soil        | - Bottom depth of each layer (m)  
- Soil water characteristics (Total porosity, Field capacity, Wilting point, Residual water content)  
- Bulked density (mg/cm³)  
- Soil texture (Soil clay content(%), Soil sand content (%), Soil silt content (%), Soil organic matter content (%), Very fine sand content (%), Coarse fragment content (%))  
- Saturated hydraulic conductivity (m/h)  
- Cation exchange capacity (meq/kg) |
| Crop        | - Crop parameter for converting energy to biomass (kg/MJ)  
- Critical soil water content below which plant growth is subjected to water stress(m3/m3)  
- Base temperature (no growth occurs at or below, C), Optimum temperature (C)  
- Amount of the crop's growth period required for the crop to reach full size (NOD: 0-1)  
- Maximum Rooting Depth (m), plant canopy height (m), and Leaf Area Index  
- Root to shoot ratio (NOD:0-1)  
- Parameter for canopy cover and canopy height equation (NOD)  
- Fraction of above-ground biomass remaining after senescence  
- Fraction of canopy cover remaining after senescence (NOD:0-1)  
- Number of days between the beginning and end of leaf drop  
- Potential Heat Units to crop maturity (C)  
- Fraction of growing season when leaf area index starts declining  
- Parameter for flat residue cover equation (m²/kg) |
| Tillage     | - Random roughness immediately after tillage (m)  
- Fraction of soil surface disturbed by the tillage implement  
- Ridge height immediately after tillage (m)  
- Ridge interval (m)  
- Mean tillage depth associated with each implement (m) |
| Pesticide   | - Wash-off fraction  
- Foliar residue half-life (days) and Soil half-life (days)  
- Partitioning coefficient  
- Water solubility (mg/l)  
- Plant uptake coefficient |
| Stream      | - Channel type parameters  
- Channel type (1: Rectangle, 2: Triangle channel)  
- Channel Width (m)  
- Bank slope of channel type 2 (Triangle only)  
- Manning's n for the channel  
- Fraction of Unerodible Channel Soil, or erosion resistant for the type 1 and Maximum Erodible Depth for the type 2 |
Temporal changes of BMPs in each specific field are considered in the rotation data block by chronically combining different crop planting and harvesting, primary and secondary tillage application, and pesticide applications. Table 3.3 shows rotation data block and parameters.

Table 3.3. Temporal variable data block and parameters for DANSAT.

<table>
<thead>
<tr>
<th>Data block</th>
<th>Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rotation</td>
<td>Date (month, day, year)</td>
</tr>
<tr>
<td></td>
<td>- Agricultural management type (0: Tillage, 1: Planting, 4: Pesticide application, 8: Harvesting)</td>
</tr>
<tr>
<td></td>
<td>- Application type for each management (tillage type, crop type, pesticide type)</td>
</tr>
<tr>
<td></td>
<td>- Variables (pesticide application: application rate (kg/ha), harvesting: percent cover of residue after harvest (%))</td>
</tr>
</tbody>
</table>

Spatial distribution of rotation, soil, and topographic parameters and meteorological input are combined in the cell data block to take account of the placement of BMPs as well as spatial distribution of topographic, meteorological, and soil related variables. Table 3.4 shows input parameters for the cell data block.

Table 3.4. Spatial variable data block and parameters for DANSAT.

<table>
<thead>
<tr>
<th>Group</th>
<th>Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Topographic</td>
<td>- Surface elevation (m),</td>
</tr>
<tr>
<td></td>
<td>- Aspect from north on clockwise (Degree),</td>
</tr>
<tr>
<td></td>
<td>- Slope of surface (%)</td>
</tr>
<tr>
<td></td>
<td>- Channel type number,</td>
</tr>
<tr>
<td></td>
<td>- Slope of channel (%),</td>
</tr>
<tr>
<td></td>
<td>- Channel length for channel element</td>
</tr>
<tr>
<td></td>
<td>- Average depth to the ground water table from surface (m)</td>
</tr>
<tr>
<td>Soil</td>
<td>- Soil numbers (identification) in overland areas,</td>
</tr>
<tr>
<td></td>
<td>- Soil numbers in channel segments</td>
</tr>
<tr>
<td>Land use</td>
<td>- Rotation Number, Manning's n for bare soil (0: calculating by model),</td>
</tr>
<tr>
<td></td>
<td>Effective Depth of Interaction for overland element (m)</td>
</tr>
<tr>
<td>Weather</td>
<td>- Rain gauge number</td>
</tr>
</tbody>
</table>

Control data blocks contains directory and file name data block, flag and general input data block, and output control data block. File names as well as directory locations where input and output files are retrieved and restored, respectively, are defined in the directory and file name data block. The flag and general input data block controls the simulation environment by turning on or off components and defines number of soil layers, rain gauge stations, soil, crop, rotation, tillage, pesticide, and pesticide application types. Required dynamic arrays are defined based on the general information provided at the beginning of simulation. The output control data block defines the location of the outlet cell and user-defined cell as well as the cycles of periodic output files ranging from daily to yearly.
Multiple Soil Layers
Consideration of multiple soil layers in root zone depth is necessary to evaluate impacts of different tillage and pesticide application methods on water and pollutant transport. Determination of soil layer depth in the intermediate zone (from the bottom of root zone to the ground water table depth), considering actual characteristics of the soil profile, is also necessary for simulating water and pesticide movement through the intermediate zone to ground water table. In addition, models with multiple soil layers have the advantages of considering plant uptakes of pesticide and crop evapotranspiration at various crop growth stages in root zone. DANSAT defines multiple soil layers based on two different sources: 1) physical soil layer depth, which is usually derived from soil database (SURRGO), and 2) rotation-based soil layer depths, which are defined by combination of tillage application depths, pesticide application depths, maximum root depths of different crops, and EDI. Thereby, soil layer depths, which are defined based on different soil types and different rotation application depths, are not identical among cells. Figure 3.3 shows the concept of defining multiple soil layers in DANSAT.

Output Files
DANSAT model creates three different types of output files: 1) outlet output, 2) flux output, and 3) field-scale output. Figure 3.4 and Table 3.5 show available output files for DANSAT and spatial, temporal, and vertical density for each output type.
Table 3.5. Possible output files of the integrated modeling approach.

<table>
<thead>
<tr>
<th>Output</th>
<th>Spatial Scale</th>
<th>Temporal Scale</th>
<th>Vertical Scale</th>
<th>Components</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outlet</td>
<td>User controlled</td>
<td>Storm Event, Hydrograph</td>
<td>N/A</td>
<td>Hydrology, Sediment, Soluble and sediment bound pesticide</td>
</tr>
<tr>
<td></td>
<td>multiple outlets</td>
<td>Daily stream flow</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>hydrograph</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Field-scale</td>
<td>User controlled</td>
<td>User control (yearly,</td>
<td>Three interfaces</td>
<td>Hydrology, Soluble pesticide</td>
</tr>
<tr>
<td></td>
<td>multiple cells</td>
<td>monthly, daily)</td>
<td>(Surface to root zone, Root to intermediate zone, intermediate to saturated zone)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Daily</td>
<td>Multiple soil layer</td>
<td></td>
</tr>
</tbody>
</table>

Outlet output includes daily output and storm event output files, which provide runoff, sediment, and pesticide results at multiple user-defined outlet cells. The maximum number of outlet cells is restricted to ten in the model. Daily output files provide daily total amount of runoff, sediment load, and pesticide load at the user-defined outlets. The hydrograph and water quality results for each storm event are summarized in the storm-event output files depending on the user-defined output cycle, which should always be greater than the event time-step. The flux output files provide information about the amount of water and pesticides passing through three interfaces.
between 1) ground surface and root zone areas, 2) root zone and intermediate zone areas, and 3) intermediate zone and saturated zone areas. Flux files provide insights into BMP impacts on subsurface regime by showing the spatial distribution of predicted water and pesticide flux in each interface considering the spatially changing BMPs and different soil types. Water and pesticide fluxes in each interface are summarized for different time-scales based on the user-defined output control flag. Possible temporal-scale of flux output includes daily, monthly, yearly, total simulation period, and every user-defined number of days. Daily flux output is appropriate for research and model validation purposes, and monthly or yearly flux output can be used to evaluate the long-term BMP impacts on subsurface area. Attention should be paid when selecting daily flux time-step by considering the size of the study watershed and the selected grid resolution, because daily time-step of spatially distributed flux output creates very big output files when the size of watershed is big and the user-defined grid size is small.

Field-scale output provides vertical distribution and time series of soil water content and pesticide concentration in multiple user-defined cells. The maximum number of cells for the output is restricted to ten. The temporal-scale for the field-scale output is fixed as one day. Vertical distribution of soil water content and pesticide concentration in user-defined cells can be extracted from the output file at daily time-steps. The series of vertical distribution of pesticide concentration provides information about the pesticide movement from surface through root zone after pesticide application. Time series output provides information on daily changes in water content and pesticide concentration at a specific soil layer throughout the simulation period. Similarly, time series output of pesticide concentration can be used to evaluate the effects of different pesticide application rates, degradation rates, and user-defined transport related parameters on pesticides transport through the soils and to the ground water.

**Model Components**

DANSAT consists of a cell component and a watershed-scale component. The cell component uses interception, infiltration, percolation, and evapotranspiration to simulate water and pollutant movement in one cell. The watershed-scale component routes the water, sediment, and pesticides, which are calculated by cell components to downstream cells until they reach the watershed outlet. The watershed-scale component includes overland flow, channel flow, interflow, and baseflow sub-components. Figure 3.5 shows the field-scale and watershed-scale components of DANSAT. Surface related sub-components such as overland flow and channel flow routing simulate hydrology, sediment, and pesticide movements, while subsurface related sub-components such as
infiltration, percolation, interflow, and baseflow simulate only hydrology and pesticides. Strengths and weaknesses of available methods for basic hydrology components (infiltration and evapotranspiration) and sediment components are provided in detail by Bouraoui (1994) and Byne (2000), respectively.

Figure 3.5. Components of DANSAT Model.

Four different time-steps are possible in DANSAT, depending on the starting time of rainfall and ending time of runoff. Figure 3.6 shows the available time-steps in DANSAT, including fixed one-day Surface Water Time-step (SWT), user-defined Storm Event Time-step (SET), Before Rainfall Time-step (BRT), and After Runoff Time-step (ART). The minimum time step during storm-events (SET) was defined as one minute in DANSAT. The evapotranspiration component uses fixed one-day time-step, irrespective of rainfall events. Storm related components such as interception, infiltration, and overland flow routing components use user-defined storm event time-step during storms. Routing related components such as interflow, baseflow, and channel routing components also use user-defined storm event time-step throughout the simulation period, irrespective of the existence of storm event. Capacity-based percolation and pesticide leaching components simulate water and pesticide movement in the soil profile using variable time-steps. In the absence of rainfall, one day (1 Day) fixed time-step (SWT) is used. If there is a rainfall event, before rainfall time-step (BRT), storm event time-step (SET), and after runoff time-step (ART) are used for simulating percolation and pesticide leaching from the beginning of the day to the start time of rainfall; from the start of rainfall to the end of runoff; and from the ending time
of runoff to the end of the day, respectively. Ending time of runoff is decided in the overland routing component when the calculated minimum overland flow depth from all cells in the watershed becomes smaller than the user-defined minimum input value.

![Figure 3.6. Time-steps in the DANSAT.](image)

**Hydrology Components**

Figure 3.7 shows the flowchart of hydrology components of DANST. The flowchart consists of two main loops: During Storm Event Loop (DSEL: left side in the flowchart) and Between Storm Event Loop (BSEL: right side in the flowchart). The DSEL of hydrology components predicts water movement during storm events using user-defined storm event time-step (SET). DSEL contains interception, infiltration, percolation, interflow, baseflow, overland flow, and channel flow sub-components. Between storm events, the water moves in subsurface and channels without any supply of surface runoff from overland areas. BSEL contains percolation, interflow, baseflow, and channel flow routing sub-components.

The remaining water, which excesses the field capacity of each soil layer, is percolated down below soil layers until the percolated water reaches the ground water table. Interflow and ground water inflow, which are simulated by interflow and baseflow components, are added to channel segments as lateral flows for channel routing. Available water in the channel segment is routed to the watershed outlet by the channel routing component using a variable storage routing method, which is used by SWAT (Neitsch et al., 2002a). Routing related components such as interflow,
baseflow, and channel flow components, except for overland flow component, are commonly used in both DSEL and BSEL. Details of each hydrologic component are explained below.

Figure 3.7. Flowchart of hydrology components of DANST.

**SWT**: Surface Water Time-step  **BRT**: Before Rainfall Time-step  
**SET**: Storm Event Time-step  **ART**: After Runoff Time-step
**Interception**

Interception is the process by which precipitation is abstracted by the vegetative cover and other surfaces. Interception is the first abstractive process to be considered during a storm event. Interception losses are a function of both characteristics of storm and vegetative cover such as intensity of storm and biomass of vegetation. Light storms are more influenced by interception process compared to heavy storms. In this study, interception is described using the equation from WEPP (Savabi and Williams, 1995) as a function of above ground biomass of vegetation. Temporal changes of above ground biomass are simulated by dynamic Crop-Soil-Residue component of the model. Interception for up to five different plant types is calculated using the following equation:

\[
I = 0.001(3.7 \cdot B_{ag} - 0.00011 \cdot B_{ag}^2)
\]  

(3.1)

Where, \(I\) = precipitation interception by vegetation (m); and \(B_{ag}\) = cumulated above-ground biomass (kg/m²).

**Evapotranspiration**

Evapotranspiration (ET) is the combination of evaporation from the soil surface and transpiration through vegetation. The ET process transfers huge amounts of water from the soil back to the atmosphere. ET varies spatially and temporally in a watershed throughout the period. As a result, ET is an important component in modeling of long term water balance at a watershed-scale.

Predicting ET requires three different types of variables to be considered: atmospheric variables for the potential evapotranspiration (PET) determination and plant related and soil related variables for the actual evapotranspiration (AET) calculation. In general, potential ET is calculated based on meteorological factors and actual ET is predicted considering the current status of the plant and soil related characteristics. DANSAT predicts potential ET using one of four different methods according to the available weather data. DANSAT estimates the actual evapotranspiration (AET) in two steps based on calculated potential evapotranspiration: 1) calculates the separate actual soil evaporation and plant transpiration using Ritchie methods (Ritchie, 1972) and 2) distributes calculated soil evaporation and plant transpiration into multiple soil layers based on WEPP (Savabi and Williams, 1995).

**Potential Evapotranspiration**
Potential ET (PET) is the amount of water removed from surface under the assumption of a sufficient supply of moisture at all times. Most potential ET equations are empirical and can be classified into 1) temperature models, 2) radiation models, 3) combination models, and 4) pan-evaporation models. Even though it was known that the combination method is the best approach, temperature and radiation based models can be chosen when necessary weather input variables for the combination method are not available. In DANSAT, Hammon (Hamon, 1963), Jensen and Haise (Jensen and Haise, 1963), Priestly-Taylor (Priestley and Taylor, 1972), and pan-to-PET coefficients methods were selected as the temperature, radiation, approximated combination, and pan-evaporation models, respectively. Table 3.6 shows the selected PET methods and required weather variables for each method.

Table 3.6. Potential evapotranspiration (PET) methods used in DANSAT.

<table>
<thead>
<tr>
<th>PET method</th>
<th>Required variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hammon</td>
<td>- Air temperature</td>
</tr>
<tr>
<td></td>
<td>- Latitude of watershed</td>
</tr>
<tr>
<td>Jensen and Haise</td>
<td>- Air temperature</td>
</tr>
<tr>
<td></td>
<td>- Solar radiation</td>
</tr>
<tr>
<td>Priestly-Taylor</td>
<td>- Air temperature</td>
</tr>
<tr>
<td></td>
<td>- Solar radiation</td>
</tr>
<tr>
<td></td>
<td>- Elevation of the site</td>
</tr>
<tr>
<td>Pan-to-PET coefficient</td>
<td>- Observed daily pan evaporation</td>
</tr>
<tr>
<td></td>
<td>- Pan-to-PET coefficients</td>
</tr>
</tbody>
</table>

Even though four methods were integrated in DANSAT, only the Priestly-Taylor method is presented in detail because the model works best based on the method. In the future, other remaining methods should be validated, and it is recommended that the Penman method (Penman, 1948) be added into DANSAT as an original combination based model.

The Priestly-Taylor method was selected as a combination model. The Priestly-Taylor method is an approximation of the Penman methods. In cases where only solar radiation and temperature data are available, the Priestly-Taylor method can be used instead of the Penman method, which requires air temperature, solar radiation, humidity, and wind speed. The Priestly-Taylor method is described by:

\[
PET = 0.00128 \left( \frac{R_n}{58.3} \right) \left( \frac{\delta}{\delta + \gamma} \right)
\]

(3.2)

Where, \( R_n \) = daily net solar radiation (ly); \( \delta \) = slope of the saturated vapor pressure curve at mean air temperature; and \( \gamma \) = psychrometric constant.

48
The δ and γ are calculated by:

\[
\delta = \frac{5304}{T_k^2} \cdot e^{\left(\frac{21.25 - 5304}{T_k}\right)}
\]  

(3.3)

\[
\gamma = 6.6 \times 10^{-4} (101 - 0.0115h_e + 5.44 \times 10^{-7} h_e^2)
\]  

(3.4)

Where, \(T_k\) = daily average air temperature (Kelvin); and \(h_e\) = elevation of the site (m).

**Actual Evapotranspiration**

The Ritchie’s method (Ritchie, 1972) consists of series of equations to estimate actual ET by separately calculating soil evaporation and plant transpiration. Ritchie’s method begins with an approximation of the Penman combination equation (Priestley and Taylor, 1972) to represent PET. However, the original method for estimating PET can be replaced with one of previously mentioned PET methods. Potential soil evaporation rate below the plant canopy is determined based on the leaf area index using:

\[
PE_{so} = PET \cdot e^{(-0.4 \cdot LAI)}
\]  

(3.5)

\[
E_{pl} = PET - PE_{so}, \text{ LAI} > 3
\]  

(3.6)

\[
E_{pl} = \frac{(PET - PE_{so}) \cdot LAI}{3}, 0 \leq LAI \leq 3
\]  

(3.7)

Where, PET= potential evapotranspiration, PE_{so} = potential soil evaporation, E_{pl} = adjusted potential plant transpiration as a linear function of LAI and potential plant transpiration (ET_{p} = PET-PE_{so}), and LAI = Leaf area index defined as a ratio of plant leaf area and soil surface area.

Soil evaporation (E_{so}) is calculated in two stages. In the first stage, soil evaporation is just limited by the energy available at the soil surface and it is the same as the potential soil evaporation (e.g. E_{so1} = PE_{so}). The upper limit of stage one is determined using the equation:

\[
UE_{so1} = 0.009 \cdot (T_e - 3.0)^{0.42}
\]  

(3.8)
Where, \( U_{\text{Es}1} \) = upper limit soil evaporation of stage one (m), \( T_r \) = soil transmissivity (mm/d\(^{0.5}\)), determined by:

\[
T_r = 4.165 + 0.02456 \cdot PSand - 0.01703 \cdot PClay - 0.0004 \cdot PSand^2
\]  \( (3.9) \)

Where, \( PSand \) = percentage of sand in the bare soil, \( PClay \) = percentage of clay in the bare soil.

When the accumulated soil evaporation exceeds the upper limit of stage one, stage two begins. Stage two in soil evaporation is determined by the equation:

\[
E_{so2} = 0.001 \cdot T_r \cdot \left[ t^{0.5} - (t - 1)^{0.5} \right]
\]  \( (3.10) \)

Where, \( E_{so2} \) = stage two soil evaporation rate for a day (cm/day), and \( t \) = number of days since stage two evaporation started (days).

Stage-two of soil evaporation continues until the soil water content is at a residual moisture content below which no more soil water can be extracted from the soil layer. If there is a precipitation greater than or equal to accumulated stage-two soil evaporation, stage two reverts back to stage one.

**Distribution of Actual ET in the Root Zone**

The distribution of calculated soil evaporation (\( E_{so} \)) in the soil profile is determined by considering the maximum soil evaporation effective depth (\( D_{\text{max}} \)), which is calculated based on soil texture using the following equation (Savabi and Williams, 1995):

\[
D_{\text{max}} = 0.09 - 0.00077 \cdot PClay + 0.000006 \cdot PSand^2
\]  \( (3.11) \)

Where, \( D_{\text{max}} \) = maximum soil evaporation effective depth (m), \( PClay \) = percentage of clay in the bare soil, and \( PSand \) = percentage of sand in the bare soil.

Available soil water, which is the difference between actual soil water content and residual moisture content, will be extracted starting from the first soil layer to the maximum depth (\( D_{\text{max}} \)) until the sum of extracted water is equal to the calculated soil evaporation (\( E_{so} \)). If the available soil water within the maximum depth is not sufficient for the calculated soil evaporation (\( E_{so} \)), actual soil evaporation is restricted accordingly.
Calculated potential plant transpiration \( (E_{pl}) \) is distributed within the root depth, which is predicted daily by the model, using the equation:

\[
PE_i = \frac{E_{pl}}{1-e^{-3.065}} \left[ 1 - e^{-3.065 \left( \frac{D_i}{D_{root}} \right)} \right] - \sum_{n=1}^{i-1} AE_n
\]

(3.12)

Where, \( PE_i = \) potential water use rate by plant from layer \( i \) (m/d), \( D_i = \) depth of soil layer \( i \) (m), \( D_{root} = \) root depth (m), and \( AE = \) adjusted potential water use from the soil layer above layer \( i \) (m).

The potential water use for each soil layer \( (PE_i) \) is adjusted for water deficits to obtain the adjusted potential water use \( (AE_i) \) using the equations:

\[
AE_i = PE_i \quad SW > F_{cwc} \cdot USW
\]

(3.13)

\[
AE_i = PE_i \cdot \frac{SW}{F_{cwc} \cdot USW} \quad SW \leq F_{cwc} \cdot USW
\]

(3.14)

Where, \( SW = \) soil water content of layer \( i \) (m), \( F_{cwc} = \) critical soil water content below which plant growth is subjected to water stress (fraction by volume, m3/m3), and \( USW = \) upper limit soil water content for layer \( i \) (m).

Extractable soil water by crops, which is the difference between soil water content and moisture content at wilting point, is compared with adjusted potential plant transpiration \( (AE_i) \) for each soil layer. If the soil water is sufficient, actual plant transpiration will be equal to the adjusted potential plant transpiration \( (AE_i) \). If the soil water in each soil layer is not sufficient for the adjusted potential plant transpiration \( (AE_i) \), actual plant transpiration is reduced.

**Infiltration**

Infiltration is defined as the flux or the rate of water from the surface into the soil profile. Infiltration is an important hydrologic component that determines the amount and temporal distribution of rainfall excess available for surface runoff. The soil parameters related to the infiltration process also control the subsurface movement of water within the soil profile.

The infiltration process can be described by solving the governing differential equations in terms of physically-based soil properties. MIKE-SHE uses numerical methods to solve the one dimensional Richards’ equation (Richards, 1931), which was derived from Darcy’s law and the continuity equation. However, such an approach is rarely used in practical watershed-scale
modeling because of the intensive computational requirement, even though it is very useful to analyze the effects of various factors on the infiltration processes. The major reasons are that the numerical approach requires intensive computational time and resources and there is difficulty in obtaining necessary soil properties to solve the equation. Computational difficulty limits the options for watershed-scale modeling. In contrast, several empirical infiltration models, such as the Kostiakov (Kostiakov, 1932), Horton (Horton, 1940), and Holtan (Holtan, 1961) equations, were developed and have been used in hydrologic models. The major limitation of empirical models is that the parameters involved in empirical equations must be calibrated using experimental infiltration data.

Physically-based approximate approach including the Green-Amp (Green and Ampt, 1911) and the Philip (Philip, 1957) equations are other viable alternatives. Recently, the Green-Ampt infiltration equation has been frequently used in hydrological modeling because of the ease in its parameter’s determination and physically-based characteristics of the method. The Green-Ampt infiltration equation is an approximate model utilizing Darcy's law. The original equation was derived for the infiltration process of ponded surface. However, modifications in the original Green-Ampt equation have been applied to describe realistic infiltration process during rainfall events (Mein and Larson, 1971). In this study, the modified Green-Ampt model was selected to consider two distinct stages of unsteady rainfall: a stage with surface ponding and a stage without surface ponding. The equation is same as the Mein and Larson’s equation and is described by:

\[ K(t - t_p + t_s) = F_p - SM \cdot \ln \left(1 + \frac{F_p}{SM} \right) \]  

(3.15)

Where, \( K \) = average hydraulic conductivity of the wetted zone (m/hr), \( t_p \) = ponding time (hr), \( t_s \) = pseudo time, shift of time scale due to the effect of cumulative infiltration at the ponding time (hr), \( S \) = difference in average capillary potential before and after wetting (m), \( M \) = difference in average soil moisture before and after wetting (vol/vol), and \( F_p \) = cumulative infiltration (m). SM, the wetting front capillary potential, represents the suction gradient between the saturated zone and the unsaturated zone, which are separated by the wetting front.

Integrated method considers surface conditions using two indicators at initial and terminal time of considering time-step. The surface condition indicator at the initial time is used to check whether surface ponding occurs or not during the time-step. The indicator described by chu (1978) is selected using:
Where, $C_u =$ surface condition indicator at the initial time, \( K = \) average hydraulic conductivity of the wetted zone (m/hr), \( SM = \) the wetting front capillary potential, \( I = \) net rainfall intensity (m/h), \( P = \) cumulative rainfall (m), \( R = \) cumulative rainfall excess (m), and \( t_n \) and \( t_{n-1} = \) current and previous time-steps, respectively.

If $C_u$ is greater than zero, surface ponding occurs. If surface ponding occurs during the time-step or from the beginning of the time-step, surface condition at the terminal time is decided by comparing the calculated infiltration capacity at the end of time-step and rainfall intensity during the time-step. The infiltration capacity is calculated using the equation:

$$f_c = K + \frac{KSM}{F_p(t_n)} \quad (3.17)$$

Where, \( f_c = \) infiltration capacity (m/h) and \( F_p = \) cumulative infiltration (m)

If the constant rainfall intensity during the time-step is greater than the calculated infiltration capacity at the end of time-step, surface ponding condition continues for the next time-step.

**Percolation**

Most models developed for describing the movement of water in the unsaturated zone assume vertical and one-dimensional flow. An appropriate percolation component needs to be decided by considering the type of equations: rate-based and capacity-based models (Zacharias et al., 1999). In a capacity-based approach, water exceeding the field capacity is percolated to the below soil layer. The limitation of a capacity-based approach is that this type of model is inadequate for simulating flow in a thick vadose zone because of its assumption that drainage of the entire soil column to field capacity takes place in 1 day. Because of this limitation, GLEAMS (Leonard et al., 1987) is available only for root zone simulations, PRZM (Carsel et al., 1985) is linked to a one-dimensional vadose zone model, and VADOFT (Huyakorn and Buckley, 1987) was developed to simulate water flow and solute transport. The 1-day drainage assumption is applicable only to the specific situation such as root zone or extremely shallow ground water conditions.

Rate-based approaches such as Richard’s equation and convection dispersion equation (CDE) are usually solved using numerical methods. This approach requires extensive computer resources and computation time, especially when the model is linked to the distributed watershed-scale
model such as MIKE-SHE. In the case of MIKE-SHE, the model identifies the homogeneous region within the modeling area and this homogeneous region is lumped together and calculated as a representative column to save computation time (DHI, 1998).

The percolation component of WEPP was adapted for this study (Savabi and Williams, 1995). The percolation component of the WEPP model uses a capacity-based approach to predict one-dimensional water movement through each soil layer by considering 1) the adjusted hydraulic conductivity, which varies depending on soil water content, and 2) the effect of lower layer water content, which may restrict the water movement through a soil layer at or near saturation. The percolation of water is calculated using the equation:

\[
pe_i = (\Theta_i - FC_i) \left( 1 - e^{\left[ -\frac{\Delta t}{t_i} \right]} \right) \quad (\Theta_i > FC_i)
\]  

(3.18)

Where, \( pe_i \) = percolation rate through layer (m/day), \( \Theta_i \) = soil water content in layer i (m), \( FC_i \) = field capacity water content for layer i (m), \( \Delta t \) = time-step (sec), and \( t_i \) = travel time through layer i (sec), and is calculated by:

\[
t_i = \frac{\Theta_i - FC_i}{K_{sai}}
\]

(3.19)

Where, \( K_{sai} \) = adjusted hydraulic conductivity of layer i (m/sec), which is varied from the saturated conductivity at saturation to near zero at field capacity. Adjusted hydraulic conductivity is calculated using the equation:

\[
K_{sai} = K_{si} \left( \frac{\Theta_i}{UL_i} \right)^{-2.655} \log \left( \frac{FC_i}{UL_i} \right)
\]

(3.20)

Where, \( K_{si} \) = saturated hydraulic conductivity for layer i (m/sec), and \( UL_i \) = upper limit soil water content for layer i (m)

The effect of lower layer water content, which may restrict the water movement through a soil layer at or near saturation, is considered using the equation:

\[
pe_i = pe_{i-1} \sqrt{1 - \frac{\Theta_i}{UL_{i+1}}}
\]

(3.21)
Where, $\Theta_{i+1} = \text{soil water content in layer } i+1 \text{ (m)}$, and $UL_{i+1} = \text{upper limit soil water content for layer } i+1 \text{ (m)}$.

**Interflow**

Interflow is the movement of subsurface water, which returns to the land surface or to a stream without reaching the primary ground water body. The subsurface water usually is recharged by infiltration into the land surface and is discharged through the processes of evaporation and transpiration. Interflow occurs significantly in areas with high infiltration and sloping impeding layer at shallow soil depth. Continuous infiltration into previously wet soil sometimes causes the soil water content to be greater than its field capacity. Sloping impermeable or semi-permeable layer causes hydraulic gradients to incline from vertical to lateral direction. In soils, Darcy’s law is used to explain the water movement in porous media with a function of hydraulic head gradient. Therefore, hydraulic conductivity in soil layers, drainable soil water, slope of impeding soil layer, and depth to the impeding soil layer are important factors in considering interflow process.

DANSAT incorporates a kinematic storage model for lateral subsurface flow, which is developed by Sloan et al. (1983) and used in the SWAT model (Neitsch et al., 2002b). The equation is described by:

$$Q_{lat} = 0.024 \cdot \left( \frac{2 \cdot SW_{ly,\text{excess}} \cdot K_{sat} \cdot Slp}{\Phi_d \cdot L_{hill}} \right)$$  \hspace{1cm} (3.22)

Where, $SW_{ly,\text{excess}} = \text{drainable volume of water stored in the saturated zone of the hill slope per unit area (mm)}$, $\Phi_d = \text{drainable porosity of the soil (mm/mm) (porosity – field capacity)}$, $L_{hill} = \text{hillslope length (m)}$, $K_{sat} = \text{saturated hydraulic conductivity (mm/h)}$, and $Slp = \text{increase in elevation per unit distance}$.

As mentioned previously, interface between soil layers, which are defined by DANSAT based on physical soil layers and rotation based soil layers, are not continuously connected between adjacent cells. Depth from surface to impermeable soil layer also spatially changes according to the soil type. The number of model-interpolated soil layers between the surface and impermeable layer also can be different between adjacent cells. As a result, a lumped interflow pool approach has been selected for interflow calculation between adjacent cells instead of a layer based interflow approach. Figure 3.8 shows the representation of (a) real soil layers, (b) layer based interflow approach, and (c) lumped interflow pool approach.
Figure 3.8. Conceptual representation of (a) an actual interflow, (b) layer based interflow approach, and (c) lumped interflow pool approach.

As shown in Figure 3.8.b, the calculated layer-based interflow from one soil layer should be either distributed into multiple soil layers of the adjacent cell or calculated layer-based interflow from multiple soil layers should be lumped into one soil layer of the downstream cell, because of the different number of soil layers. In the lumped interflow approach, soil water exceeding field capacity of each soil layer are lumped into the interflow pool and interflow to the adjacent cell is calculated based on the depth of water in the pool. Same flow path with overland flow routing is assumed for interflow calculation. If lumped interflow water is not redistributed into actual soils after interflow calculation, simulated actual evapotranspiration can be underestimated because of limitation of available soil water. In the lumped pool approach, lumped water in each interflow pool is redistributed into soil layers by adding it as input to the percolation component and emptying the lumped interflow pool. If user defines a specific soil layer as impermeable in the soil layer data block of main input, DANSAT does not calculate percolation through the impermeable layer. If there is no impermeable soil layer in a cell, user-defined depth for interflow calculation, which is one of general calibration parameters, is used and percolation is considered through every soil layer. At the beginning of model simulation, depth average drainable porosity
and saturated hydraulic conductivity are estimated based on soil layer information in each cell and the average values are used for lumped interflow calculation. Another general calibration parameter related with the interflow component is anisotropic coefficient, which is ratio of horizontal saturated hydraulic conductivity to vertical saturated hydraulic conductivity, and is used for calculating average saturated hydraulic conductivity. If soil is perfectly homogeneous, an anisotropic coefficient value of 1 can be used. Many soils have stratified structures and this anisotropic characteristic makes their horizontal conductivity larger than the vertical one.

**Baseflow**

Water flux passing through the bottom layer of the intermediate zone can be used as recharge for calculating baseflow by one of several approaches, such integrated ground water approach and linked ground water approach. This chapter deals with the integrated ground water approach and chapter 4 covers linked ground water approach using existing ground water models such as MODFLOW and MT3D. Schematic comparison between integrated ground water approach and linked ground water approach is given in Figure 3.9.

![Figure 3.9. Comparison of integrated modeling approach and linked modeling approach.](image)

Baseflow is the lateral flow in a stream that originates from ground water bodies, which are recharged primarily by infiltration and percolation through the soil. In watershed modeling, the complexity of ground water component depends on the objective of the modeling and the physical nature of the ground water system that is being simulated. However, most existing watershed-scale and continuous simulation NPS models including SWAT (Arnold et al., 1998), HSPF (Bicknell et al., 1993), AnnAGNPS (Bingner and Theurer, 2001), and ANSWERS-2000
(Bouraoui et al., 2002) do not consider flow path and residence time in a saturated zone area. Aquifer, a geologic formation which contains sufficient saturated permeable material to yield significant quantities of water to wells and springs, can be divided into unconfined and confined. Unconfined aquifer has a free water table and confined aquifer has impermeable geologic formation as the upper boundary. DANSAT considers only unconfined aquifer in which recharge occurs by percolation through the watershed and ground water table is the upper boundary of the saturated zone. A similar concept used in SWAT is incorporated into the DANSAT to calculate the baseflow amount to the nearest stream segment from each overland cell (Neitsch et al., 2002b). At the beginning of simulation, DANSAT calculates distances from each overland cell to every stream cells and allocates a stream cell, which has the shortest distance from the overland cell, as a receiving stream cell. Total baseflow inflow to the stream segment is the summation of individual baseflow from several nearest overland cells. Figure 3.10 shows overall concept of baseflow component and Figure 3.11 shows the schematic procedures for baseflow calculation.

Figure 3.10. Overall concept of baseflow component.
Baseflow at a specific day ($Q_{gw,i}$) should be greater than the estimated overall threshold value ($TH_{over}$). Baseflow from individual cell can be calculated using the equation:

$$Q_{gw,i} = Q_{gw,i-1} \cdot \exp[GW_{cst}] + W_{rchrg} \cdot (1 - \exp[GW_{cst}]) \quad (3.23)$$

Where, $Q_{gw,i}$ = ground water flow into the main channel on current time-step, i (mm), $Q_{gw,i-1}$ = ground water flow into the main channel on previous time-step, i-1 (mm), $W_{rchrg}$ = amount of recharge entering the aquifer on current time-step, i (mm), and $GW_{cst}$ = baseflow recession constant.

Baseflow recession constant, a sensitivity index to changes in recharge, varies from a small value for slow response to a large value for rapid response to recharge. Baseflow recession constant is a function of saturated hydraulic conductivity and distance from current cell to the nearest stream cell. Baseflow recession constant is described using the following format:
\[ GW_{\text{cnst}} = GW_{\text{coeff}} \cdot GW_{\text{ksat}} \cdot \left( \frac{W_{\text{cell}}}{D_{\text{stream}}} \right)^{GW_{\text{power}}} \]  

(3.24)

Where, \( GW_{\text{cnst}} \)=Baseflow recession constant, \( GW_{\text{coeff}} \)= calibration parameter to control baseflow recession constant, \( GW_{\text{ksat}} \)= average saturated hydraulic conductivity in the saturated zone (m/h), \( GW_{\text{power}} \)= power coefficient for baseflow recession constant, \( W_{\text{cell}} \)= cell width (m), and \( D_{\text{stream}} \)= distance from current cell to the nearest stream cell (m).

Because the selected approach is not able to consider actual flow path between selected overland cell and stream cell, average saturated hydraulic conductivity for the overall saturated zone (\( GW_{\text{ksat}} \)) is used instead of specific hydraulic conductivity for each flow path.

It is assumed that the overall threshold baseflow (TH\text{over}) is the summation of constant minimum baseflow (TH\text{min}: green color) and variable baseflow (TH\text{var}: lite blue color), which changes according to the recharge from intermediate zone. Constant minimum baseflow (TH\text{min}) is given as input parameter for representing ground water inflows from outside of the watershed. The overall and variable baseflow threshold values are calculated based on the following equation, which converts baseflow storage volume to flow depth.

\[ TH_{\text{over}} = TH_{\text{min}} + TH_{\text{var}} = TH_{\text{min}} + GW_{\text{slp}} \cdot \log(GW_{\text{strg}}) + GW_{\text{int}} \]  

(3.25)

Where, \( TH_{\text{over}} \)= overall baseflow threshold value (mm), \( TH_{\text{min}} \)= minimum constant baseflow threshold value (mm), \( TH_{\text{var}} \)= variable baseflow threshold value according to the changes of recharges (mm), \( GW_{\text{slp}} \)= slope coefficient for converting storage volume to flow depth, \( GW_{\text{int}} \)= intercept coefficient for converting storage volume to flow depth, and \( GW_{\text{strg}} \)=baseflow storage (m\(^3\)).

When the calculated baseflow by equation (3.23) is smaller than estimated overall threshold baseflow estimated by equation (3.25), it is adjusted by replacing it with the overall threshold value.

**Overland Flow Routing**

The flow-governing equations and solution methods, especially for flow routing component, are critical to the hydrologic and water quality models. Commonly used flow-governing equations include dynamic wave equations, diffusive wave equations, kinematic wave equations, storage based equations, and curve number equations (Borah and Bera, 2003).
In DANSAT, hydraulic response in each cell is computed based on storage-based equations, which consist of the spatially uniform and temporarily variable continuity equation and a stage-discharge equation. Manning’s equation was selected as the stage-discharge equation for both overland and channel flow routing:

\[
I - O = \frac{dS}{dt} 
\]

(3.26)

Where, \(I\) = inflow rate to an element from rainfall and adjacent element, \(O\) = outflow rate, \(S\) = volume of water stored in an element, and \(t\) = time.

The discrete form of the continuity equation is:

\[
\frac{I_1 + I_2}{2} - \frac{O_1 + O_2}{2} = \frac{S_2 - S_1}{\Delta t} 
\]

(3.27)

Where, 1 indicates the beginning of the time-step and 2 indicates the end of time-step, and \(\Delta t\) = time-step (sec).

\(I_1, O_1,\) and \(S_1\) were already calculated from previous time-step. \(I_2\) is calculated during the current time-step from upslope cells. During overland flow routing, the hydraulic radius \(R_2\) can be assumed as flow depth \(D_2\). Volume of water stored in a given cell was approximated as the product of cell area and flow depth according to the uniform flow assumption of the Manning’s equation. The relationship between \(O_2\) and \(S_2\) is defined by following equations:

\[
O_2 = \frac{1}{n} \cdot R_2^{5/3} \cdot S_{lp}^{7/3} 
\]

(3.28)

\[
S_2 = D_2 \cdot \text{Area} 
\]

(3.29)

Where, \(n\) = Manning’s roughness coefficient, \(R_2\) = hydraulic radius at the end of time-step (m), \(S_{lp}\) = slope of surface or channel (m/m), \(O_2\) = outflow rate at the end of time-step (m³/s), \(S_2\) = volume of water stored in an element at the end of time-step (m³), \(D_2\) = flow depth (m), and \(\text{Area}\) = cell area (m²).

The discrete form of the continuity equation is changed to a simple equation containing only one unknown variable, \(D_2\) by combining equation (3.28) and (3.29). The simplified equation is solved using the Newton-Rapson method to calculate the storage depth \(D_2\) at the end of time-step.
Channel Flow Routing

Flow from a channel segment goes into the downstream segment as an input. One channel segment can receive water from one or more upstream channel segments as well as its own overland segment. Figure 3.12 shows the 8-D flow direction approach used in DANSAT as well as the concept of overland and channel segment connections.

![Figure 3.12. Concept of overland and channel flow routing in DANSAT.](image)

The variable storage routing method by Williams (1969), which is based on the continuity equation, was selected for channel flow routing. For a given channel segment, continuity equation can be described by:

\[
I_{lat} + \frac{I_1 + I_2}{2} - \frac{O_1 + O_2}{2} = \frac{S_2 - S_1}{\Delta t}
\]

Where, \(I_{lat}\) = lateral flow rate from overland area (m³/s), \(\Delta t\) = length of the time-step (sec), \(I_1\) = the inflow rate at the beginning of the time-step (m³/s), \(I_2\) = the inflow rate at the end of the time-step (m³/s), \(O_1\) = the outflow rate at the beginning of the time-step (m³/s), \(O_2\) = the outflow rate at the end of the time-step (m³/s), \(S_1\) = the storage volume at the beginning of the time-step (m³), and \(S_2\) = the storage volume at the end of the time-step (m³).
Travel time can be defined by dividing the volume of water in the channel by the flow rate using:

$$T = \frac{S}{O} = \frac{S_1}{O_1} = \frac{S_2}{O_2}$$

(3.31)

Where, $T$ is the travel time (sec).

By plugging $S_2 = T \cdot O_2$ and $S_1 = T \cdot O_1$ into equation (3.30), outflow rate at the end of the time-step is calculated by equation (3.32).

$$O_2 = \left( \frac{2 \Delta t}{\Delta t + 2T} \right) I_{avg} + \left( 1 - \frac{2 \Delta t}{\Delta t + 2T} \right) O_1$$

(3.32)

Where, $I_{avg}$ = the average inflow rate during the time-step and replaced by:

$$I_{avg} = I_{lat} + \left( \frac{I_1 + I_2}{2} \right)$$

(3.33)

**Sediment Component**

Figure 3.13 shows the daily flowchart of sediment components of DANST. Temporally variable soil parameters such as random roughness, ridge height, bulk density, effective hydraulic conductivity, interrill erodibility, rill erodibility, channel erodibility, and critical shear stresses in rills and streams are simulated at the beginning of simulation day using a dynamic soil component described later in this chapter. The left side of the flowchart is the During Storm Event Loop (DSEL) where the overland and channel sediment routings are calculated. No runoff occurs between storm events; therefore, only sediment routing in channels are predicted by Between Storm Events Loop (BSEL) on the right side of the flowchart. Flow rate, which is calculated in each cell by the hydrology related components prior to sediment calculation, is used for calculating the transport capacity as well as detachment by flowing water. Both overland sediment routing and channel sediment routing processes use the storm event time-step (SET), and calculation can be divided into two stages. First, detachment and transport capacity are calculated in each cell. Second, detached sediments are compared with calculated transport capacity to determine sediment outflow to the adjacent cell. Transport capacity must be calculated in order to compare possible sediment source and available transport energy. If transport capacity is greater than the available sediments, more detachment will occur by flow. If more sediments exist in flow compared to the transport capacity, sediments in flow will be deposited. In the
overland sediment process, the sediment detachment is separately calculated by interrill and rill detachment components. Interrill detachment in overland area is calculated as a function of the kinetic energy of the rainfall and flowing water, while rill detachment is a function of flowing water only. Rill detachment by overland flow does not occur unless there is excess energy available after considering energy required to transport interrill detached sediment. Daily predicted interrill and rill erodibility soil parameters are used for calculating detachment of soils from the interrill and rill areas, respectively, to enable consideration of the impact of temporally changing BMPs on soil detachment.

If a channel segment exists within a cell, available flow and sediment from overland area are added to the channel segment and channel routing process is considered. Sediment from overland areas and channel scouring are possible sediment sources in a channel segment routing. At first, channel sediment related processes calculate the sediment detachment capacity and transport capacity by channel flow. Available sediments, which come from both overland and channel, are compared with transport capacity. If the transport capacity is less than sediments from the overland area only, no sediment erosion occurs in channels and some sediments from the overland area can be partially deposited. If the transport capacity is greater than sediment from the overland area and less than the sum of sediments from the overland area and channel scouring, all sediments from the overland area will not be deposited and a portion of the detached sediment in stream will be transported to the adjacent cell. If the transport capacity is greater than the sum of sediment from the overland area and channel, all sediments are available for transportation to the neighboring cell. DANSAT considers multiple particle size classes. Washload, which is permanently suspended because of small fall velocities, is not allowed to deposit unless the flow rate is zero. In the model, particles less than 10 microns in diameter are considered as washload, similar to the current version of ANSWERS-2000 (Byne, 2000) if the particle size is not designated as washload by user.
Figure 3.13. Daily flowchart of sediment components of DANSAT.

- **SWT**: Surface Water Time-step
- **BRT**: Before Rainfall Time-step
- **SET**: Storm Event Time-step
- **ART**: After Runoff Time-step
Interrill Detachment

Interrill detachment is calculated based on the WEPP approach, which was also used in ANSWERS-2000 using the equation (Byne, 2000):

\[
D_{\text{inter}} = K_{\text{inter}} \cdot RF_{\text{int}} \cdot RN_{\text{inter}} \cdot DR_{\text{sed}} \cdot A_{\text{ratio}} \cdot Area \cdot P_{\text{soil}} \tag{3.34}
\]

Where, \(D_{\text{inter}}\) = Interrill detachment (kg/s), \(K_{\text{inter}}\) = adjusted interrill erodibility (kg-s/m\(^4\)), \(RF_{\text{int}}\) = net rainfall rate after considering interception (m/s), \(RN_{\text{inter}}\) = interrill runoff rate (m/s), \(DR_{\text{sed}}\) = sediment delivery ratio for each particle, \(A_{\text{ratio}}\) = area ratio (interrill area to total cell area), \(Area\) = total cell area, and \(P_{\text{soil}}\) = particle content of the top soil (fraction).

Estimation of interrill erodibility will be explained in the dynamic soil component in detail.

Interrill runoff rate is calculated by:

\[
RN_{\text{inter}} = \frac{Q_{\text{eff}}}{W_{\text{cell}} \cdot R_{\text{space}}} \tag{3.35}
\]

Where, \(W_{\text{cell}}\) = cell width (m), \(R_{\text{space}}\) = rill space (m), and \(Q_{\text{eff}}\) = flow rate per rill contributing area (m\(^3\)/sec) which is calculated by:

\[
Q_{\text{eff}} = \frac{FO_{12}}{N_{\text{rill}}} \tag{3.36}
\]

Where, \(FO_{12}\) = average outflow rate during the time-step (m\(^3\)/s) and \(N_{\text{rill}}\) = number of rills in a cell.

Delivery ratio depends on several factors such as surface roughness, surface slope, soil hydrologic condition, and flow length to the stream. In DANSAT, delivery ratio for each particle is estimated based on random roughness using Table 3.7.

**Table 3.7. Sediment delivery ratio for each particle size (adapted from Foster, 1982).**

<table>
<thead>
<tr>
<th>Random Roughness (mm)</th>
<th>Particle Diameter (mm)</th>
<th>D&lt; 0.002</th>
<th>0.002≤D&lt;0.05</th>
<th>0.05≤D&lt;0.25</th>
<th>0.25≤D&lt;1.0</th>
<th>1.0≤D</th>
</tr>
</thead>
<tbody>
<tr>
<td>RR &gt; 150</td>
<td>0.91</td>
<td>0.79</td>
<td>0.37</td>
<td>0.00</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>100 to 150</td>
<td>0.97</td>
<td>0.93</td>
<td>0.75</td>
<td>0.00</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>70 to 100</td>
<td>1.00</td>
<td>0.99</td>
<td>0.98</td>
<td>0.07</td>
<td>0.17</td>
<td></td>
</tr>
<tr>
<td>50 to 70</td>
<td>1.00</td>
<td>1.00</td>
<td>0.99</td>
<td>0.32</td>
<td>0.46</td>
<td></td>
</tr>
<tr>
<td>20 to 50</td>
<td>1.00</td>
<td>1.00</td>
<td>0.99</td>
<td>0.58</td>
<td>0.69</td>
<td></td>
</tr>
<tr>
<td>5 to 20</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>0.78</td>
<td>0.84</td>
<td></td>
</tr>
<tr>
<td>0 to 5</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td></td>
</tr>
</tbody>
</table>

Area ratio is calculated by:
\[ A_{\text{ratio}} = \frac{\text{Area} - \left(N_{\text{rill}} \cdot W_{\text{rill}} \cdot W_{\text{cell}}\right)}{\text{Area}} \]  

(3.37)

Where, Area = cell area (m²), \(W_{\text{cell}}\) = cell width (m), and \(W_{\text{rill}}\) = rill width (m) and calculated using the equation:

\[ W_{\text{rill}} = 1.13 \cdot Q_{\text{eff}}^{0.303} \]  

(3.38)

**Rill Detachment**

Rill detachment is calculated based on the WEPP approach, which was also used in ANSWERS-2000, using the following equation (Byne, 2000):

\[ D_{\text{rill}} = K_{\text{rill}} \cdot \left(\frac{\text{SS}_{\text{eff}} - \text{CSS}_{\text{adj}}}{N_{\text{rill}} \cdot W_{\text{rill}} \cdot W_{\text{cell}} \cdot P_{\text{soil}}}\right) \]  

(3.39)

Where, \(D_{\text{rill}}\) = rill detachment capacity (kg/s), \(K_{\text{rill}}\) = adjusted rill erodibility (kg·s/m⁴), \(\text{SS}_{\text{eff}}\) = effective shear stress (kg/m·s²), \(\text{CSS}_{\text{adj}}\) = adjusted critical shear stress (kg/m·s²), \(N_{\text{rill}}\) = number of rills in a cell, \(W_{\text{rill}}\) = rill width (m), \(W_{\text{cell}}\) = cell width (m), and \(P_{\text{soil}}\) = particle content of the top soil (fraction).

Both adjusted rill erodibility and critical shear stress are predicted daily by the dynamic soil component. Effective shear stress is calculated using following equation:

\[ \text{SS}_{\text{eff}} = 9806.65 \cdot \text{Slp} \cdot HR_{\text{rill}} \]  

(3.40)

Where, 9806.65 = specific weight of water (Kg/m²·s²), Slp = element slope (m/m), and \(HR_{\text{rill}}\) = hydraulic radius in a rill (m).

Flow depth in a rill needs to be estimated based on flow rate per rill contributing area (\(Q_{\text{cell}}\)) in order to calculate hydraulic radius in a rill (\(HR_{\text{rill}}\)). Flow depth in a rill is estimated by solving the following Darcy-Weisbach friction factor equation:

\[ DW_{\text{coef}} = \left(\frac{M_{\text{coef}}^2 \cdot 8 \cdot g}{HR_{\text{rill}}^{0.333}}\right) \]  

(3.41)

Where, \(DW_{\text{coef}}\) = Darcy-Weisbach hydraulic roughness coefficient, and \(M_{\text{coef}}\) = Manning's n friction factor, and \(HR_{\text{rill}}\) = hydraulic radius in a rill (m).
The Darcy-Weisbach friction factor equation can be transformed into the following equation by replacing two terms such as Manning’s roughness coefficient (M\text{coef}) and hydraulic radius in a rill (HR\text{rill}):

\[
f(F_{D \text{rill}}) = F_{D \text{rill}}^3 \cdot W_{\text{rill}}^3 \cdot Slp \cdot 8 \cdot 9.80665 - DW_{\text{coef}} \cdot Q_{\text{eff}}^2 \cdot 2 \cdot W_{\text{rill}} - DW_{\text{coef}} \cdot Q_{\text{eff}}^2 \cdot F_{D \text{rill}}
\]

(3.42)

Where, \(f(F_{\text{rill}})\) = flow depth function, \(F_{D \text{rill}}\) = flow depth in a rill (m), \(W_{\text{rill}}\) = rill width (m), Slp = element slope, \(DW_{\text{coef}}\) = Darcy-Weisbach hydraulic roughness coefficient, and \(Q_{\text{eff}}\) = flow rate per rill contributing area (m\(^3\)/sec).

Flow depth in a rill can be calculated by solving equation (3.42) using the modified Newton-Raphson methods for multiple roots (Chapra and Canale, 1988). Flow depth can be explained by descriptive equation:

\[
F_{D \text{rill},j} = F_{D \text{rill},j-1} - \left( \frac{f(F_{D \text{rill}}) \cdot f'(F_{D \text{rill}})}{f''(F_{D \text{rill}})} \right)
\]

(3.43)

Where, \(F_{D \text{rill},1}\) = flow depth at current iteration, \(F_{D \text{rill},j-1}\) = flow depth as previous iteration, \(f(F_{\text{rill}})\) = flow depth function, \(f'(F_{\text{rill}})\) = first derivative of the flow depth function, and \(f''(F_{\text{rill}})\) = second derivative of the flow depth function.

If the difference between flow depth from the previous iteration and newly calculated flow depth is smaller than the predefined criteria, the iteration will be stopped.

**Channel Detachment**

Channel detachment capacity is calculated using similar equations for the rill detachment capacity calculation. Detachment capacity in a channel segment is calculated by the following equation:

\[
D_{\text{chan}} = K_{\text{chan}} \cdot (SS_{\text{eff}} - CSS_{\text{adj}}) \cdot WP_{\text{chan}} \cdot L_{\text{chan}} \cdot F_{\text{erod}} \cdot P_{\text{soil}}
\]

(3.44)

Where, \(D_{\text{chan}}\) = detachment capacity in a channel segment (kg/s), \(K_{\text{chan}}\) = adjusted channel erodibility (s/m), \(SS_{\text{eff}}\) = effective shear stress (kg/m\(^2\)s\(^{-1}\)), \(CSS_{\text{adj}}\) = adjusted critical shear stress (kg/m\(^2\)s\(^{-1}\)), \(WP_{\text{chan}}\) = wetted perimeter (m), \(L_{\text{chan}}\) = channel length (m), \(F_{\text{erod}}\) = fraction of erodible area, and \(P_{\text{soil}}\) = particle content of the channel soil (fraction).
Both adjusted daily channel erodibility and critical shear stress are predicted by the dynamic soil component, which will be explained in a later section of this chapter. Effective shear stress is calculated using:

\[
SS_{\text{eff}} = 9806.65 \cdot Slp_{\text{chan}} \cdot HR_{\text{chan}}
\]  

(3.45)

Where, 9806.65 = specific weight of water (Kg/m²·s²), Slp_{chan} = channel slope (m/m), and HR_{chan} = hydraulic radius in a channel segment (m), which is calculated based on the result of channel routing component.

Hydraulic radius during the time-step is calculated using average flow depth, which is the average of flow depth at the beginning of time-step and flow depth at the end of time-step. Those flow depths are known values, which are already calculated by hydrology components.

**Transport Capacity**

Transport capacity for both rill and channel are calculated using Yalin’s equation (Yalin, 1963). Transport capacity for a particle class is estimated by:

\[
TC_i = P \cdot SG_i \cdot D_{\text{water}} \cdot ED_i \cdot S_{\text{vel}} \cdot (\text{Delta}_i / S\text{Delta}) \cdot W_{\text{cell}}
\]  

(3.46)

Where, TC_i = transport capacity for particle i (kg/m), P = nondimensional sediment transport capacity, SG_i = specific gravity of particle i, D_{water} = density of water (kg/m³), ED_i = equivalent sand diameter of particle i (m), S_{vel} = shear velocity, W_{cell} = cell width (m), S\text{Delta} = sum of Delta_i, and Delta_i is calculated by:

\[
\text{Delta}_i = \left( \frac{Y}{Y_{\text{cr},i}} \right) - 1
\]  

(3.47)

Where, \( Y_{\text{cr},i} \) = critical shear stress, and Y is calculated by:

\[
Y = \frac{S_{\text{vel}}^2}{(SG_i - 1.0) \cdot AGrav \cdot ED_i}
\]  

(3.48)

Where, SG_i = specific gravity of particle i, AGrav = acceleration of gravity (m/sec²), ED_i = equivalent sand diameter of particle (m), and S_{vel} is calculated by:
\[ S_{\text{rel}} = \sqrt{A \text{Grav} \cdot HR \cdot Slp} \]  

(3.49)

Where, HR = hydraulic radius, and Slp = slope of the energy grade line.

Non-dimensional sediment transport capacity is calculated by the following equation:

\[ P = Y_{\text{cnst}} \cdot \Delta \text{t} \cdot i \cdot 1.0 \left( 1.0 - \frac{\ln(1.0 + \Sigma_i)}{\Sigma_i} \right) \]  

(3.50)

Where, \( Y_{\text{cnst}} \) = Yalin's constant (0.635), and \( \Sigma_i \) is calculated by:

\[ \Sigma_i = 2.45 \cdot S_{\text{G}_i}^{-0.4} \cdot Y_{\text{cr},i}^{0.5} \cdot \delta \]  

(3.51)

**Sediment Routing**

The continuity equation was used to simulate movement of sediment into and out of each cell and channel element. The discrete form of the continuity equation is expressed by:

\[ \text{DetR} + \text{DetF} + \frac{I_1 + I_2}{2} - \frac{O_1 + O_2}{2} = \frac{S_2 - S_1}{\Delta t} \]  

(3.52)

Where, \( \text{DetR} \) = detachment rate by rainfall on interrill area (kg/s), \( \text{DetF} \) = detachment rate by flow in rills (kg/s), \( I_1 \) = sediment inflow rate at the beginning of time-step from the adjacent cells (kg/s), \( I_2 \) = sediment inflow rate at the end of time-step from the adjacent cells (kg/s), \( O_1 \) = sediment outflow rate to the adjacent cell at the beginning of time-step (kg/s), \( O_2 \) = sediment outflow rate to the adjacent cell at the end of time-step (kg/s), \( S_1 \) = sediment in water at the beginning of time-step, storage (kg), \( S_2 \) = sediment in water at the end of time-step (kg), \( \Delta t \) = time-step (sec).

The sediment outflow rate \( O_2 \) was assumed to be the product of the sediment concentration \( S_2 / FS_2 \) and the outflow rate \( FO_2 \) using the equation below:

\[ O_2 = S_2 \cdot \frac{FO_2}{FS_2} \]  

(3.53)

Where, \( O_2 \) = sediment outflow rate to the adjacent cell at the end of time-step (kg/s), \( S_2 \) = sediment in water at the end of time-step (kg), \( FO_2 \) = overland outflow rate to the adjacent cell at the end of time-step (m³/s), \( FS_2 \) = overland flow storage at the end of time-step (m³).
FO2 and FS2 are calculated from overland flow components. Denoting FO2/FS2 as constant K, equation (3.52) gives:

\[
DetR + DetF + \frac{I_1 + I_2}{2} - \frac{O_1}{2} + S_1 = K \left( \frac{1}{DelT} + \frac{K}{2} \right) S_2
\]

(3.54)

All the variables on the left hand side are known and can be simplified by the equation:

\[
DetR + DetF + Cnst = A \cdot S_2
\]

(3.55)

Where, \(A = \left( \frac{1}{DelT} + \frac{K}{2} \right)\) and \(Cnst = \frac{I_1 + I_2}{2} - \frac{O_1}{2} + \frac{S_1}{DelT}\)

There are four possible cases for comparing the transport capacity and total available sediments. Sediment routing in channels is similar to the overland sediment routing scheme. Sediment inflow from the overland area into the channel segment (DetO) and detached sediment rate by flow in a channel (DetC) can be replaced in the equations for DetR and DetF. The four possible cases are explained in Table 3.8.

**Table 3.8. Assumptions for the four sediment routing cases.**

<table>
<thead>
<tr>
<th>Cases</th>
<th>Overland Routing</th>
<th>Channel Routing</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>All deposition of detached sediment by rainfall and no detachment by flow</td>
<td>All deposition of sediments from the overland area and no detachment by channel flow</td>
</tr>
<tr>
<td>II</td>
<td>Partial deposition of detached sediment by rainfall and no detachment by flow</td>
<td>Partial deposition of sediments from the overland area and no detachment by channel flow</td>
</tr>
<tr>
<td>III</td>
<td>No deposition of detached sediment by rainfall and partial detachment by flow</td>
<td>No deposition of sediments from the overland area and partial detachment by channel flow</td>
</tr>
<tr>
<td>IV</td>
<td>No deposition of detached sediment by rainfall and full detachment by flow</td>
<td>No deposition of sediments from the overland area and full detachment by channel flow</td>
</tr>
</tbody>
</table>

DetR (DetO) and DetF (DetC) are assumed as zero for case I, and \(S_2\) and \(O_2\) are calculated from equation (3.55) and (3.53), respectively.

\[
S_2 = \frac{Cnst}{A}
\]

(3.56)

\[
O_2 = K \cdot S_2
\]

(3.57)

The calculated average transport capacity \(T_c\) are compared with average available sediment in the outflow \(O_{avg} = (O_1+O_2)/2\) during time-step. If the transport capacity is less than the average available sediment, sediment outflow is adjusted by the equation:
\[ O_2 = 2 \cdot T_c - O_1 \]  

(3.58)

If the transport capacity is greater than the average available sediment, case II is assumed with partial deposition of detached sediment by rainfall and no detachment by flow. The remaining sediment by rainfall detachment after considering the partial deposition (PDetR) is calculated by the following equations:

\[ O_2 = 2 \cdot T_c - O_1 \]  

(3.59)

\[ S_2 = \frac{K}{O_2} \]  

(3.60)

\[ PDetR = A \cdot S_2 - Cnst \]  

(3.61)

If the PDetR is less than the total detached sediment by rainfall (DetR), the assumption is satisfied and no adjustment is necessary. If the PDetR is greater than DetR, case III is assumed with no deposition of detached sediment by rainfall and partial detachment by flow. Partially detached sediment by flow (PDetF) is calculated by the equation below. DetR is calculated by the interrill detachment component and is a known value.

\[ PDetF = A \cdot S_2 - DetR - Cnst \]  

(3.62)

If the PDetF is less than the potential detached sediment by rill flow (DetF), the assumption is satisfied and no adjustment is necessary. If the PDetF is greater than the DetF, case IV is considered with the assumption of no deposition of detached sediment by rainfall and full detachment by flow. \( S_2 \) and \( O_2 \) are calculated directly from the equations below:

\[ S_2 = \frac{DetR + DetF + Cnst}{A} \]  

(3.63)

\[ O_2 = K \cdot S_2 \]  

(3.64)

**Pesticide Components**

The simple linear equilibrium isotherm equation and first-order pesticide degradation approach were used for simulating pesticide movement by surface runoff, interflow, and leaching in the pesticide component of DANSAT. Figure 3.14 shows a flowchart of pesticide components of DANST. At first, the model checks the rotation data block every day. If there is a pesticide
application in a specific area, the pesticide application component distributes the applied pesticide amount to foliage and soil layers, depending on the application method. DANSAT simulates daily pesticide degradation at the foliage and soils separately, using a different degradation rate. The flowchart consists of the During Storm Event Loop (DSEL) and Between Storm Events Loop (BSEL) similar to the hydrology and sediment components. During storm events, pesticide on foliage is partially washed off by rainfall and added to the first soil layer based on the wash-off fraction input parameter. Pesticide movement in soil profiles are predicted by the pesticide leaching component based on the amount of percolated water, which is already predicted by the hydrology components. Only dissolved pesticides are considered in simulating pesticide movement by interflow and baseflow components, while both dissolved and sediment-bound pesticides are simulated in the overland and channel routing components. All components in the DSEL use the storm event time-step (SET). BSEL contains pesticide leaching, interflow, baseflow, and channel flow routing components. If a channel segment exists within a cell, pesticides from overland flow, interflow, and baseflow are added to the channel segment, and the available pesticides in the channel segment are routed through the watershed outlet by the channel sediment routing component.
Figure 3.14. Flow chart of pesticide components.
**Application Methods**

GLEAMS (Leonard et al., 1987) include four application methods such as surface application, incorporation, injection, and chemigation. The method of pesticide application is usually determined according to the formulation, which is supplied by a manufacturer for improving the effectiveness of the active ingredient. Additives are added to pesticides to enhance the performance or handling of those pesticides by increasing uptake of pesticides, adherence of a chemical to a surface, and the area that a given volume of spray will cover.

DNASAT considers the impacts of four different pesticide application methods; namely, surface application, foliage application, incorporation, and injection. The pesticide losses to the atmosphere during or right after application were considered by the application efficiency factor described in the following equation:

\[ \text{Pest}_{\text{tot}} = \text{Pest}_{\text{app}} \cdot \text{Eff}_{\text{app}} \]  \hspace{1cm} (3.65)

Where, \( \text{Pest}_{\text{tot}} \) = effective amount of pesticide that reaches the ground or plants, \( \text{Pest}_{\text{app}} \) = actual amount of pesticide applied, and \( \text{Eff}_{\text{app}} \) = application efficiency factor.

Effective amount of pesticide, after considering application efficiency, can be divided into pesticide amount intercepted by plants and pesticide amount that reaches the soil surface. The distribution of effective pesticide amount between plant and soil surface for the foliage application method can be calculated based on user-defined partitioning coefficient using:

\[ \text{Pest}_{\text{foli}} = \text{Pest}_{\text{tot}} \cdot \text{Coeff}_{\text{foli}} \]  \hspace{1cm} (3.66)

\[ \text{Pest}_{\text{soil}} = \text{Pest}_{\text{tot}} \cdot (1 - \text{Coeff}_{\text{foli}}) \]  \hspace{1cm} (3.67)

Where, \( \text{Coeff}_{\text{foli}} \) = partitioning coefficient for foliage application, \( \text{Pest}_{\text{foli}} \) = amount of pesticide intercepted by plants, and \( \text{Pest}_{\text{soil}} \) = pesticide that reaches the soil.

For soil application, the separation of effective amount of pesticide (\( \text{Pest}_{\text{tot}} \)) into pesticide amount attached to foliage (\( \text{Pest}_{\text{foli}} \)) and pesticide amount that reaches the ground surface (\( \text{Pest}_{\text{soil}} \)) is calculated using canopy cover, which is a fraction of ground cover by plant. The canopy cover is internally simulated by DANSAT and the value is zero when pesticide is applied before the crop is planted. The distribution of effective pesticide amount into soil and foliage is calculated using the following equations:
\[ Pest_{foli} = Pest_{tot} \cdot C_{cover} \quad (3.68) \]
\[ Pest_{soil} = Pest_{tot} \cdot (1 - C_{cover}) \quad (3.69) \]

Where, \( C_{cover} \) = fraction of the ground that is covered by plants, \( Pest_{foli} \) = amount of pesticide intercepted by plants, and \( Pest_{soil} \) = pesticide that reaches the soil.

A graphical description of available pesticide application methods is presented in Figure 3.15.

![Total pesticide application amount](image)

With regard to soil and foliage applications, pesticides that reach the soil are distributed within the user defined soil depth and linear reduction in pesticide amount with depth is assumed. For incorporation application method, pesticides are assumed to be uniformly mixed within an assigned maximum depth of incorporation. In the case of injection, pesticides are placed in the assigned injection depth but no mixing is allowed with the soil above this depth. DANSAT does not explicitly consider difference in formulations and influence of mixed additives. As a result, input parameters should be adjusted by considering the purpose of formulation and additives.
Degradation

Pesticides are degraded or broken down at different rates by soil microorganisms and chemical reactions. Biotic breakdown processes occur mainly in the root zone and slow down considerably in deeper zones, because populations of microbes decrease rapidly below the root zone (Bollag and Liu, 1990). In addition to biological degradation, pesticides in the soil can also be dissipated through the processes of chemical reactions such as photodecomposition, hydrolysis, and oxidation (Van Den Berg and Van Den Linden, 1994). In DANSAT, pesticide degradation rate in the soil or on foliage is estimated using first-order kinetics:

\[ C_d = C_0 \cdot e^{-\left(\frac{k}{d}\right)} \]  \hspace{1cm} (3.70)

Where, \( C_d = \) soil pesticide concentration on any day \( d \), after application, \( C_0 = \) initial soil pesticide concentration at \( d = 0 \), and \( k = \) degradation rate coefficient in soil or on foliage.

With regard to the rate expressions, the half-life, which is defined as the time required for half of the applied pesticide to be completely degraded, is used as the input parameter instead of the degradation rate coefficient because it is more readily available from literatures. The major environmental factors influencing the transformation of pesticides include pH, organic matter, soil moisture status, and temperature. In the model, degradation rate for a given compound is adjusted based on different soil environments such as soil temperature and water content using the equations (Truman et al., 1998):

\[ k_s = k \cdot e^{-\left(\frac{6615}{T_s} - 22.62\right)} \]  \hspace{1cm} (3.71)

\[ k_{asm} = \frac{k}{\left[1 - (0.65 - ASM)^2\right]} \quad \text{with} \quad ASM = \left(\frac{\theta - \theta_{res}}{\theta_{sat} - \theta_{res}}\right) \]  \hspace{1cm} (3.72)

Where, \( k_s = \) adjusted dissipation rates based on soil temperature, \( k_{asm} = \) adjusted dissipation rates based on soil water content, \( k = \) base rate constant, \( T_s = \) mean daily soil temperature (K), \( ASM = \) available soil water, \( \theta = \) actual water content, \( \theta_{sat} = \) saturation water content, and \( \theta_{res} = \) residual water content.

Pesticide Adsorption and Desorption (Retention)

Retention occurs due to the interaction between the pesticide chemical and the soil particle surface. The retention process may affect the availability of pesticides for plant or microbial uptake, and biotic or abiotic transformation processes, as well as movement of pesticides (Cheng, 1990). In particular, retention is one of the most important characteristics of pesticides in
connection with their leaching potential. Pesticides that are strongly attached to soil particles are less likely to leach into ground water.

The linear isotherm process, which is a specific case of Freundlich isotherm, was selected in DANSAT because of its simplicity (Fetter, 1998). It is known that the linear approximation is acceptable at the low equilibrium concentration of solute in the dissolved phase (Truman et al., 1998). At the higher concentration, the linear equilibrium model overestimates sorption, resulting in underestimation of sediment-transported pesticides during runoff events shortly after pesticide application. In addition, this linear assumption may be invalid for certain compounds such as ionic and strongly polar compounds (Truman et al., 1998). The linear isotherm process is described with this assumption:

$$ C_s = K_d \times C_w $$

(3.73)

Where, $K_d =$ partitioning coefficient (ml/g), $C_s =$ concentration in adsorbed phase in soils (µg/g), and $C_w =$ concentration in solution phase (µg/ml).

Several partition coefficients have been used to describe sorption process in pesticide leaching models. Partition coefficient with respect to the organic carbon ($K_{oc}$) can be defined as:

$$ K_{oc} = \frac{K_d}{f_{oc}} $$

(3.74)

Where, $K_d =$ distribution coefficient of linear isotherm equation and $f_{oc} =$ fraction of organic carbon.

$K_d$ can be estimated from $K_{oc}$ (partitioning coefficient based on percent soil organic carbon) in spite of the possibilities of increased error, because $K_{oc}$ for a given pesticide is assumed to be independent of the particular soil conditions. In the DANSAT, $K_d$ is converted from $K_{oc}$ using the equation:

$$ K_d = \frac{K_{oc} \cdot OM}{1.724} $$

(3.75)

Where, $K_d =$ distribution coefficient of linear isotherm equation, $K_{oc} =$ partition coefficient with respect to the organic carbon, and $OM =$ organic matter content (fraction).
**Transport**

**Plant Uptake**

Uptake of water and pesticides by plants has a direct impact on the movement of water and pesticides through the root zone. In DANSAT, the pesticide uptake process was considered as a part of the overall transpiration process of a plant. Only dissolved pesticides in pore water were considered for the plant uptake process. Pesticide uptake from soil layers is calculated using:

\[
Pest_{uptake} = C_{pest} \cdot T_{crop} \cdot Coeff_{uptake}
\]  

(3.76)

Where, Pest\textsubscript{uptake} = pesticide uptake by plant (ug), C\textsubscript{pest} = dissolved pesticide concentration in a given soil layer (ug/l), T\textsubscript{crop} = actual water use by plant in a given soil layer (l), and Coeff\textsubscript{uptake} = pesticide uptake coefficient.

Actual amount of water use by plant has been already calculated in the evapotranspiration related component using the method by Richie (1976), which is explained in the hydrology part of this chapter. Equilibrium should be recalculated after extracting calculated pesticide uptakes from each soil layer.

**Runoff**

Accurate determination of effective depth of interaction (EDI), where soil pore water is completely mixed with runoff water, is important for the simulation of pesticide amount in runoff. Leonard et al. (1979) showed that runoff concentration over a wide range of storm conditions is strongly related with pesticide concentration in the surface top 10 mm of soil. Leonard and Wauchope (1980) considered an additional parameter, extraction ratio, which represents the effective mass ratio of the interaction from soil to runoff water and ranges from 0.05 to 0.2 for a wide range of watersheds. Wallach et al. (2001) pointed out, based on a comprehensive mathematical modeling, that the key factor on the availability of soil pesticides to the overland flow is the displacement of pesticides by infiltrating water prior to runoff initiation, and the pesticide concentration in overland flow is affected by the contact time (equilibrium time) of an overland flow with soil surface.

In DANSAT, EDI was considered as one of the spatially changing model input parameters depending on the soil type. The EDI input is defined in the cell data block of the main input. The extraction ratio, a ratio of dissolved chemical available for runoff to the total dissolved chemical in EDI, was considered as a user input for calibration. Pesticide in runoff is predicted by estimating pesticide outflow ratio using the equation below:
\[ p_{out,2} = \frac{P_{tot} \cdot R_{outflow}}{\Delta t} \] \hspace{1cm} (3.77)

Where, \( p_{out,2} \) = pesticide outflow rate at the end of time-step (ug/s), \( P_{tot} \) = total available pesticide amount (ug), \( R_{outflow} \) = ratio of pesticide outflow amount to available total pesticide amount, and \( \Delta t \) = storm event time-step (sec).

Total available pesticide is calculated by the equation:

\[ P_{tot} = P_{strg,1} + P_{in} + P_{edi} \cdot F_{dr} \] \hspace{1cm} (3.78)

Where, \( P_{strg,1} \) = pesticide amount in runoff storage at the beginning of time-step (ug), \( P_{in} \) = average pesticide inflow from adjacent cell during the time-step (ug), \( P_{edi} \) = total pesticide amount in the EDI, and \( F_{dr} \) = extraction ratio.

Pesticide outflow ratio is calculated based on hydrology output using the equation:

\[ R_{outflow} = \frac{Q_{out}}{Q_{tot}} \] \hspace{1cm} (3.79)

Where, \( Q_{out} \) = outflow amount calculated by multiplying flow rate at the end of time-step and storm event time-step (m³), and \( Q_{tot} \) = total available water for equilibrium (m³).

Outflow amount and total available water are estimated by:

\[ Q_{out} = q_{out,2} \times \Delta t \] \hspace{1cm} (3.80)

\[ Q_{tot} = Q_{rain} - Q_{infil} + Q_{strg,1} + Q_{edi} + Q_{in} \] \hspace{1cm} (3.81)

Where, \( q_{out,2} \) = flow rate at the end of time-step (m³/s), \( Q_{rain} \) = amount after considering interception, \( Q_{infil} \) = infiltrated water during the time-step, \( Q_{strg,1} \) = runoff storage at the beginning of time-step, \( Q_{edi} \) = soil water in the EDI, and \( Q_{in} \) = average inflow amount from adjacent cell.

Estimated total pesticide outflow rate (\( p_{out,2} \)) is divided into dissolved pesticide outflow rate (\( p_{out,2,dis} \)) and sediment attached pesticide outflow rate (\( p_{out,2,sed} \)) based on the fraction of the dissolved pesticide amount during the equilibrium.

\[ p_{out,2,dis} = p_{out,2} \cdot F_{P_{dis}} \] \hspace{1cm} (3.82)

\[ p_{out,2,sed} = p_{out,2} \cdot (1 - F_{P_{dis}}) \] \hspace{1cm} (3.83)

Where, \( F_{P_{dis}} \) = fraction of the dissolved pesticide amount is calculated by:
\[ FP_{dis} = \frac{C_{dis} \cdot Q_{tot}}{C_{dis} \cdot Q_{tot} + C_{sed} \cdot S_{tot}} \]  

(3.84)

Where, \( C_{dis} \) = pesticide concentration in water after equilibrium (ug/l), \( C_{sed} \) = pesticide concentration in soil after equilibrium (ug/kg), and \( S_{tot} \) = total soil amount for equilibrium (kg).

\( S_{tot}, C_{dis}, \) and \( C_{sed} \) are calculated by:

\[ S_{tot} = S_{strg,1} + S_{edi} + S_{in} \]  

(3.85)

\[ C_{dis} = \frac{P_{tot}}{Q_{tot} + K_d \cdot S_{tot}} \]  

(3.86)

\[ C_{sed} = K_d \cdot C_{dis} \]  

(3.87)

Where, \( S_{strg,1} \) = sediment amount in runoff storage at the beginning of time-step, \( S_{edi} \) = soil amount within the DEI, \( S_{in} \) = average sediment inflow from adjacent cell, \( K_d \) = partitioning coefficient (ml/g).

**Leaching**

Leaching is the movement of water and pesticides through the soil and into ground water. Pesticide leaching can be influenced by several factors such as properties of the pesticide, soil texture and organic matter, soil permeability, soil pH, pesticide application method and rate, and tillage management. Pesticide leaching models can be classified as rate-based or capacity-based, depending on the method by which the models handle water flow and solute leaching in soil (Zacharias et al., 1999). Rate-based models define the rate of change of solute concentration in terms of convection and diffusion rate processes. The capacity-based model uses a storage-routing technique to simulate movement of pesticides from layer to layer. Zacharias et al. (1999) compared two deterministic models to determine if a rate-based model (Opus) would predict the water flow and pesticide movement in the soil profile more accurately than a capacity-based model (GLEAMS). Although GLEAMS did not simulate the soil water distribution as a function of depth better than Opus, it was able to simulate depth-averaged soil water content and total pesticide mass in the root zone with reasonable accuracy, using fewer parameters compared to Opus.

In DANSAT, the capacity based approach was selected because of its simplicity. When the water content in a soil layer is greater than the field capacity the excess water moves into the next lower layer. A similar approach to the pesticide movement in runoff was used for simulating pesticide leaching. The pesticide outflow ratio to the lower layer is calculated using equation 3.88.
\[ R_{\text{outflow}} = 1 - \frac{Q_{\text{soil},2}}{Q_{\text{soil},1} + Q_{\text{ich}}} \]  

(3.88)

Where, \( R_{\text{outflow}} \) = pesticide outflow ratio to below layer, \( Q_{\text{soil},1} \) = soil water in the layer before percolation is calculated, \( Q_{\text{soil},2} \) = soil water in the layer after percolation is considered, and \( Q_{\text{ich}} \) = percolated soil water from upper soil layer during the time-step.

Only dissolved pesticide will move to a lower layer, and the fraction of dissolved pesticide amount is calculated using equations 3.82 through 3.84. For calculating equilibrium, information on total available water, pesticide, and soil amounts are necessary. Total available water is calculated by summing up the amount of existing soil water content before percolation and amount of percolated water from the upper soil layer. Total available pesticide is also calculated by adding existing pesticide in the soil layer at the beginning of time-step and the leached pesticide amount from the upper soil layer. Total available sediment amount does not change during the simulation period. Equations 3.86 and 3.87 can also be used for calculating pesticide concentrations in water and soil, respectively. Existing soil water content at the beginning of time-step and percolated soil water from the upper soil layer are simulated by the hydrology component and are known values.

**Interflow**

Pesticide movement in interflow can be simulated using a similar concept to the pesticide leaching component. Interflow from one cell to the adjacent receiving cell is calculated in the hydrology component. At first, soil water exceeding the field capacity of each soil layer are lumped into the interflow pool and then interflow to adjacent cell is calculated based on the depth of water in the pool. When exceeding soil water moves to the lumped pool, dissolved pesticide also moves and is lumped into a lumped pesticide pool. Pesticide outflow ratio from soil layer to the lumped pool is calculated by:

\[ R_{\text{outflow}} = \frac{AWC - FC}{AWC} \]  

(3.89)

Where, \( AWC \) = actual soil water content in depth (m) and \( FC \) = field capacity in depth (m).

Equations 3.82 through 3.84 can also be used to calculate the fraction of dissolved pesticide amount (FP\text{dis}) and dissolved pesticide amount moving to the lumped pool. Simple linear isotherm process was also used to calculate the dissolved pesticide concentration in each soil layer after equilibrium.
Calculation of pesticide movement from the lumped pool of current cell to a lumped pool in adjacent cell is made using the outflow ratio, which is described by the equation:

$$R_{\text{outflow}} = \frac{\text{Int}_{\text{out}}}{\text{Int}_{\text{tot}}}$$

(3.90)

Where, \(\text{Int}_{\text{out}}\) = interflow depth moving to the adjacent cell, which is calculated by hydrology components, and \(\text{Int}_{\text{tot}}\) = total water amount in depth in the lumped interflow pool.

**Ground Water**

In order to consider pesticide movement in ground water, one-dimensional transport of pesticide was assumed. Figure 3.16 shows the conceptual description of the movement of instantaneously injected pesticide in a one-dimensional flow field.

![Figure 3.16. Conceptual movement of instantaneously injected pesticide in a one-dimensional flow field.](image)

Distance from a given cell to the nearest channel cell is calculated at the beginning of simulation. Travel time, which is required for the pesticide peak concentrations to reach the nearest stream segment, is calculated based on the estimated distance, estimated retardation factor, average
saturated hydraulic conductivity, and average hydraulic gradient. Start-time, which is defined as the required time for the pesticide to reach the stream first, and end-time, which is defined as required time for the pesticide to pass through the stream cell, are calculated based on the width of plume (W in the figure), which is estimated by the equation provided below:

$$W_{\text{plume}} = 6 \cdot \sqrt{2 \cdot HD \cdot T_{\text{chan}}}$$  \hspace{1cm} (3.91)

Where, \(W_{\text{plume}}\) = plume width when peak of the plume reaches the channel cell (m), \(HD\) = hydrodynamic dispersion (m2/day), and \(T_{\text{chan}}\) = travel time for the plume peak to reach the channel cell (day).

The net pesticide flux after degradation (M in the figure), which is calculated by pesticide leaching and degradation components, is distributed during the period ranging from start-time to end-time with a simplified assumption of triangular shape pesticide mass distribution (Figure 3.16). Pesticide degradation is also considered in the baseflow storage during the estimated lag time.

**Dynamic Parameter Components**

Most of equations used for dynamic parameter components are based on the WEPP model. Soil component (Alberts et al., 1995), plant growth component (Arnold et al., 1995), and residue decomposition and management component (Stott et al., 1995) of WEPP were adapted for considering temporal impacts of BMPs on internal parameters in DANSAT.

**Soil Component**

**Random Roughness and Ridge Height**

Ridge height and random roughness is conceptually associated with depression storage and hydraulic resistance of runoff. In DANSAT, random roughness is used to predict effective hydraulic conductivity, sediment delivery ratio, and critical shear stress. Soil random roughness and ridge height immediately after soil disturbing operations, such as tillage, are estimated based upon measured average values assigned to each tillage implement. Random roughness right after tillage is estimated by:

$$RR_t = RR_0 \cdot T_{ds} + RR_{t-1} \cdot \left[1 - T_{ds}\right]$$  \hspace{1cm} (3.92)
Where, $RR_i = \text{random roughness immediately after tillage (m)}$, $RR_0 = \text{random roughness created by a tillage implement}$, $RR_{t-1} = \text{random roughness on the day previous to the tillage operation}$, and $T_{ds} = \text{fraction of the soil surface disturbed by the tillage implement}$.

Temporal decay of random roughness and ridge height after tillage is considered as a function of buried residue in the 0 to 0.15 meter soil zone and the cumulative rainfall since tillage. Temporal decay of random roughness and ridge height after tillage is calculated by:

$$RR_t = RR_i \cdot e^{-C_{br} \left[ \frac{R_c}{b} \right]^{0.6}} \quad (3.93)$$

$$RH_t = RH_0 \cdot e^{-C_{br} \left[ \frac{R_c}{b} \right]^{0.6}} \quad (3.94)$$

Where, $RR_i = \text{random roughness at time } t \text{ (m)}$, $RH_t = \text{ridge height (m) at time } t$, $RH_0 = \text{ridge height immediately after tillage (m)}$, $C_{br} = \text{adjustment factor for buried residue}$, $R_c = \text{cumulative rainfall since tillage (m)}$, and $b = \text{a coefficient}$.

$C_{br}$ and $b$ are predicted by:

$$C_{br} = 1 - 0.5 \cdot br \quad (3.95)$$

$$b = 63 + 62.7 \cdot \ln(50 \cdot \text{org}) + 1570 \cdot \text{clay} - 2500 \cdot \text{clay}^2 \quad (3.96)$$

Where, $br = \text{mass of the buried residue in the 0-to 0.15-meter soil zone (kg/m2)}$, $\text{org} = \text{soil organic matter content (0-1)}$, and $\text{clay} = \text{soil clay content (0-1)}$.

**Bulk Density and Porosity**

Temporal changing of bulk density is used to predict changes in the infiltration related parameters. Bulk density is predicted by considering the tillage effect, rainfall and weathering consolidation effects. Rainfall events after tillage application consolidate soil and increase bulk density. It is assumed that the effect of rainfall on soil consolidation reaches its maximum value after a freshly-tilled soil receives 0.1 m of rainfall. After receiving 0.1 m of rainfall in tilled soil, soil is assumed to be continuously consolidated to the upper boundary of the consolidation point.

Temporal changes of bulk density due to tillage, rainfall, and weathering is predicted by:
\[ \rho_{\text{till}t} = \rho_{\text{till}} + \Delta \rho_{\text{rf}} + \sum \Delta \rho_{\text{wt}} \]  

(3.97)

Where, \( \rho_{\text{till}t} \) = bulk density \( t \) days after tillage (kg/m\(^3\)), \( \rho_{\text{till}} \) = bulk density right after tillage (kg/m\(^3\)), \( \Delta \rho_{\text{rf}} \) = bulk density increase due to consolidation by rainfall (kg/m\(^3\)), and \( \Delta \rho_{\text{wt}} \) = daily increase in soil bulk density after 0.1m of rainfall (kg/m\(^3\)).

Bulk density right after tillage is calculated by:

\[ \rho_{\text{till}} = \rho_{\text{till}-1} - \left[ (\rho_{\text{till}-1} - 0.667 \cdot \rho_c) \cdot T_{ds} \right] \]  

(3.98)

Where, \( \rho_{\text{till}} \) = bulk density after tillage (kg/m\(^3\)), \( \rho_{\text{till}-1} \) = bulk density before tillage (kg/m\(^3\)), \( \rho_c \) = consolidated soil bulk density (kg/m\(^3\)) at 0.033 Mpa, \( T_{ds} \) = fraction of the soil surface disturbed by the tillage implement (0-1).

Increases in soil bulk density by rainfall are predicted by:

\[ \Delta \rho_{\text{rf}} = \Delta \rho_{\text{mx}} \frac{R_c}{0.01 + R_c} \]  

(3.99)

Where, \( R_c \) = cumulative rainfall since tillage (m), and \( \Delta \rho_{\text{mx}} \) = maximum increase in soil bulk density with rainfall (if \( \Delta \rho_{\text{mx}} < 0.0, \Delta \rho_{\text{mx}} = 0.0 \)), which is predicted by:

\[ \Delta \rho_{\text{mx}} = 1650 - 2900 \cdot \text{clay} + 3000 \cdot \text{clay}^2 - 0.92 \cdot \rho_{\text{till}} \]  

(3.100)

Daily change in bulk density due to weathering consolidation is calculated by:

\[ \Delta \rho_{\text{wt}} = (\rho_{\text{cnat}} - \rho_{\text{rf}0.1}) \cdot \left( 1 - e^{-0.005 \cdot \text{daycnt}} \right) \]  

(3.101)

Where, \( \Delta \rho_{\text{wt}} \) = daily increase in soil bulk density (kg/m\(^3\)) after 0.1 m of rainfall, \( \rho_{\text{cnat}} \) = naturally consolidated bulk density, \( \rho_{\text{rf}0.1} \) = soil bulk density on the day cumulative rainfall since tillage equals 0.1 m, and daycnt = counter to keep track of the number of days since the last tillage operation.

Total soil porosity is calculated from the bulk density at time \( t \) by:
Where, $\Phi_t = \text{total porosity}$ and $\rho_t = \text{bulk density (kg/m}^3\text{)}$ at time $t$.

**Green-Ampt Infiltration Parameters**

Two important parameters for Green-Ampt infiltration estimation are effective hydraulic conductivity and wetting front capillary potential. In order to consider the impacts of temporal changes of BMPs on hydrology and water quality, the model needs to dynamically predict the Green-Ampt effective hydraulic conductivity responding to temporal changes in BMPs. Two approaches are available for estimating the Green-Ampt effective hydraulic conductivity in DANSAT. The user can allow the model to calculate the parameter internally by considering the dynamic response to temporal changes in BMPs. Alternatively; the user can assign a constant value as an input parameter for the entire simulation period. Effective hydraulic conductivity is not the same as saturated hydraulic conductivity from soil survey data. If the constant value approach is selected, a value equivalent to half of the saturated hydraulic conductivity is assumed for the Green-Ampt effective hydraulic conductivity. The dynamic approach is incorporated based on WEPP (Flanagan and Nearing, 1995). At first, baseline effective hydraulic conductivity is calculated based on soil characteristics. Baseline value represents maximum effective hydraulic conductivity immediately after tillage application. This baseline value is adjusted to fallow soil condition by considering the exponential decrease of rate proportional to the kinetic energy of the rainfall and random roughness since the last tillage. Effective hydraulic conductivity for bare soil will approach the fully-crusted or final value if there is no further soil disturbance. Finally, surface cover condition according to the crop and residual management practices should be considered. It is known that increases in soil cover reduces soil crusting and increases the effective hydraulic conductivity (Alberts et al., 1995). It is also known that infiltration increases with larger storms (Alberts et al., 1995). The final adjusted effective hydraulic conductivity is calculated based on baseline value, conductivity value for bare soils, effective surface cover, and storm rainfall amount.

Baseline effective hydraulic conductivity is calculated by:

$$K_b = -0.265 + 0.0086 \cdot (100 \cdot sand)^{1.8} + 11.46 \cdot CEC^{-0.75} \quad \text{(if clay} \leq 0.4)$$  (3.103)
\[ K_b = 0.0066 \cdot e^{\frac{2.44}{\text{clay}}} \]  \hspace{1cm} \text{(if clay > 0.4)} \hspace{1cm} (3.104)

Where, \( K_b = \) baseline effective hydraulic conductivity (mm/h), CEC = cation exchange capacity (meq/100g), sand = fractions of sand, and clay = fractions of clay.

Effective hydraulic conductivity adjusted to fallow soil is calculated by:

\[ K_{\text{bare}} = K_b \cdot \left[ CF + (1 - CF) \cdot e^{-C \cdot E_a \cdot \left(1 - \frac{R_{Rt}}{0.04}\right)} \right] \]  \hspace{1cm} (3.105)

Where, \( K_{\text{bare}} = \) effective hydraulic conductivity adjusted to fallow soil (mm/h), CF = crust factor, which provides a means of considering fully-crusted hydraulic conductivity of soil surface based on the baseline value \( (K_b) \) and ranges from 0.2 to 1.0, \( C = \) Soil stability factor \((m^2/J)\), \( E_a = \) cumulative kinetic energy of the rainfall since the last tillage operation \((J/m^2)\), and \( R_{Rt} = \) random roughness of the soil surface (m).

Crust factor is estimated using the equation:

\[ CF = \frac{SC}{1 + \frac{\Psi}{100 \cdot L}} \]  \hspace{1cm} \text{(if CF <0.2, CF=0.2; if CF>1.0, CF=1.0)} \hspace{1cm} (3.106)

Where, \( SC = \) correction factor for partial saturation of the subcrust soil (0-1), \( \Psi = \) steady state capillary potential at the crust/subcrust interface, and \( L = \) wetted depth with a minimum value of crust thickness (if \( L<0.005\), \( L = 0.005\)) (m).

These parameters are calculated using the following equations:

\[ SC = 0.736 + 0.19 \cdot \text{sand} \]  \hspace{1cm} (3.107)

\[ \Psi = 45.19 - 46.68 \cdot SC \]  \hspace{1cm} (3.108)

\[ L = 0.147 - 0.15 \cdot (\text{sand})^2 - 0.0003 \cdot (\text{clay}) \cdot \rho_b \]  \hspace{1cm} (3.109)

Where, \( \rho_b = \) bulk density (kg/m³).
Soil stability factor, which represents the declining rate of effective hydraulic conductivity from baseline to fully-crusted value, is calculated using the equation with the minimum and maximum values of 0.0001 and 0.01, respectively (Alberts et al., 1995):

\[ C = -0.0028 + 0.0113 \cdot \text{sand} + 0.125 \cdot \left( \frac{\text{clay}}{\text{CEC}} \right) \]  
(3.110)

Where, CEC = cation exchange capacity (CEC>1.0 meq/100g), sand = fractions of sand (0-1), and clay = fractions of clay.

Effective hydraulic conductivity (mm/h) is finally computed by:

\[ K_e = K_{bare} (1 - s_{cov\text{ef}}) + (0.0534 + 0.01179 \cdot K_h)(\text{coeff}_{\text{rain}})(s_{cov\text{ef}}) \]  
(3.111)

Where, \( K_e \) = effective hydraulic conductivity (mm/h), \( K_{bare} \) = storm rainfall amount (mm), \( s_{cov\text{ef}} \) = effective surface cover, and \( \text{coeff}_{\text{rain}} \) = rainfall adjustment factor.

The total effective surface cover is calculated by:

\[ s_{cov\text{ef}} = c_{cov\text{ef}} + \text{res}_{cov} - (c_{cov\text{ef}})(\text{res}_{cov}) \]  
(3.112)

Where, \( \text{res}_{cov} \) = residue cover and \( c_{cov\text{ef}} \) = effective canopy cover, which is computed by equation (3.113).

\( \text{Coeff}_{\text{rain}} \) in equation (3.111) is not originally included in the equation for the WEPP model. \( \text{Coeff}_{\text{rain}} \) is given by the user as a general calibration parameter for considering the impacts of rainfall amount on effective hydraulic conductivity. If the infiltration is overestimated for big storm events, the user can change the coefficient within the range of 0 to 1.

\[ c_{cov\text{ef}} = c_{\text{cov\text{ef}}} \cdot C_h \]  
(3.113)

Where, \( C_h \) = correction factor for canopy height effectiveness, which is calculated by:

\[ C_h = e^{\left( -0.33 \cdot \frac{h}{2} \right)} \]  
(3.114)

Wetting front capillary potential for Green-Ampt infiltration calculation is internally calculated by DANSAT based on soil types using the following equation:
Where, $S_f =$ wetting front capillary potential (m), $\text{Por}_\text{con} =$ total porosity of the consolidated soil, $\text{Sand} =$ percent sand content (%), and $\text{Clay} =$ percent clay content (%).

Erodibility

DANSAT predicts three different erodibility parameters such as interrill erodibility, rill erodibility, and channel erodibility. These three erodibility parameters are estimated based on WEPP, while excluding some adjustment factors.

Interrill erodibility is a measure of sediment delivery rate to rills as a function of rainfall intensity and runoff rate. Interrill erodibility is calculated by multiplying the baseline interrill erodibility, which represents a loose, unconsolidated soil condition immediately after tillage practices, and several adjusting factors. Baseline interrill erodibility needs to be adjusted for influencing factors such as canopy, ground cover, live and dead root, sealing and crusting, interrill slope, and soil freezing and thawing. The slope and freeze and thaw adjustment factors were not considered in the model. Equations for predicting temporally adjusted interrill erodibility are as follow:

$$K_{\text{adj}} = K_{\text{ib}} \cdot CK_{\text{ican}} \cdot CK_{\text{igc}} \cdot CK_{\text{idr}} \cdot CK_{\text{ir}} \cdot CK_{\text{isc}}$$  \hspace{1cm} (3.116)

Where, $K_{\text{adj}} =$ adjusted interrill erodibility (s/m), $K_{\text{ib}} =$ baseline interrill erodibility (s/m), $CK_{\text{ican}} =$ adjustment factor for canopy effects, $CK_{\text{igc}} =$ adjustment factor for ground cover, $CK_{\text{idr}} =$ adjustment factor for dead root biomass, $CK_{\text{ir}} =$ adjustment factor for live root biomass, and $CK_{\text{isc}} =$ adjustment factor for sealing and crusting.

The experimental equation derived by Elliot et al. (1989) was selected to calculate baseline interrill erodibility. If the constant approach for baseline interrill erodibility is selected, the DANSAT model uses a default value of 5,300,000 kg·s/m³, which is recommended by the WEPP documentation. The equations are:

$$K_{\text{ib}} = 2728000 + 19210000 \cdot vfs \quad \text{if} \quad \text{sand} \geq 0.3$$  \hspace{1cm} (3.117)
\[ K_{ib} = 6054000 - 5513000 \cdot \text{clay} \quad \text{(if sand < 0.3)} \quad (3.118) \]

Where, sand = fraction of sand in the surface soil, vfs = fraction of very fine sand in the surface soil (if vfs > 0.4, vfs = 0.4), and clay = fraction of clay in the surface soil (if clay < 0.1, clay = 0.1).

Adjustment factors are calculated by:

\[
CK_{ican} = 1 - 2.941 \frac{\text{can cov}}{h} \left[ 1 - e^{-0.344h} \right] 
\]

\[
CK_{igc} = e^{-2.5 \cdot \text{inrcov}} 
\]

\[
CK_{idr} = e^{-0.56 \cdot \text{dr}} 
\]

\[
CK_{adr} = e^{-0.56 \cdot \text{lr}} 
\]

\[
CK_{isc} = \frac{K_{icons}}{K_{ib}} \left[ 1 - \frac{K_{icons}}{K_{ib}} \right] e^{-\rho_{c} \cdot \text{daydis}} 
\]

Where, cancov = canopy cover, h = canopy height (m), inrcov = interrill cover (0-1), dr = mass of dead roots (kg/m²), lr = mass of living roots (kg/m²) within the 0- to 0.15-m soil zone, K_{ib} = baseline interrill soil erodibility, \( \rho_{c} \) = consolidated soil bulk density at 0.033 Mpa (kg/m³), daydis = number of days since disturbance, and K_{icons} = consolidated interrill erodibility and is predicted by:

\[
K_{icons} = 10^3 \cdot (3042 - 3166 \cdot \text{sand} - 8816 \cdot \text{org} - 2477 \cdot \theta_{cf}) \quad (3.124) \]

Where, org = organic matter content, sand = sand content, and \( \theta_{cf} \) = Soil water content at 0.033 Mpa by volume.

Rill erodibility (\( K_{r} \)) is a measure of soil susceptibility to detachment by concentrated flow, and is often defined as the increase in soil detachment per unit increase in shear stress of clear water flow. Rill erodibility is calculated by multiplying the baseline rill erodibility, which is characteristic of a freshly-tilled soil, and several adjusting factors. Freeze and thaw adjustment was not considered in the calculation of rill erodibility in DANSAT. The experimental equation derived by Elliot et al.(1989) was used to calculate baseline rill erodibility. If the constant
approach for baseline rill erodibility is selected, the DANSAT uses a default value of 0.0115 s/m, which is recommended by the WEPP documentation. The equations are:

\[ K_{rb} = 0.00197 + 0.030 \cdot vfs + 0.03863 \cdot e^{-184 \cdot \text{org}} \quad (\text{if } \text{sand} \geq 0.3) \]  
(3.125)

\[ K_{rb} = 0.0069 + 0.134 \cdot e^{-20 \cdot \text{clay}} \quad (\text{if } \text{sand} < 0.3) \]  
(3.126)

Where, \( K_{rb} \) = baseline rill erodibility (s/m), \( \text{sand} \) = fraction of sand in the surface soil, \( vfs \) = fraction of very fine sand in the surface soil (if \( vfs < 0.4, vfs = 0.4 \)), \( \text{org} \) = fraction of organic matter in the surface soil (if \( \text{org} < 0.0035, \text{org} = 0.0035 \)), and \( \text{clay} \) = fraction of clay in the surface soil (if \( \text{clay} > 0.4, \text{clay} = 0.4; \text{if } \text{clay} < 0.1, \text{clay} = 0.1 \)).

Temporally adjusted rill erodibility is predicted by:

\[ K_{radj} = K_{rb} \cdot CK_{rbr} \cdot CK_{rdr} \cdot CK_{rlr} \cdot CK_{rsc} \]  
(3.127)

Where, \( K_{radj} \) = adjusted rill erodibility (s/m), \( K_{rb} \) = baseline rill erodibility (s/m), \( CK_{rbr} \) = adjustment factor for buried residue, \( CK_{rdr} \) = adjustment factor for dead roots, \( CK_{rlr} \) = adjustment factor for live roots, and \( CK_{rsc} \) = adjustment factor for sealing and crusting.

Adjustment factors to account for temporally changing rill erodibility and predicting adjusted rill erodibility on a simulation day are calculated by:

\[ CK_{rbr} = e^{-0.4 \cdot br} \]  
(3.128)

\[ CK_{rdr} = e^{-2.2 \cdot dr} \]  
(3.129)

\[ CK_{rlr} = e^{-3.5 \cdot lr} \]  
(3.130)

\[ CK_{rsc} = \frac{K_{rcons}}{K_{r}} + \left[1 - \frac{K_{rcons}}{K_{r}}\right] \cdot e^{-\rho C \cdot \text{daydis}} \]  
(3.131)

Where, \( br \) = mass of buried residue (kg/m²) within the 0- to 0.15-m soil zone, \( dr \) = mass of dead roots (kg/m²), \( lr \) = mass of living roots (kg/m²) within the 0- to 0.15-m soil zone, \( K_{r} \) = rill soil
erodibility (s/m), \( \rho_c \) = Consolidated soil bulk density at 0.033 Mpa (kg/m\(^3\)), \( \text{daydis} \) = number of days since disturbance, and \( K_{\text{cons}} \) = consolidated rill erodibility and is predicted by:

\[
K_{\text{cons}} = 0.00035 - 0.0014 \cdot \theta_{cf} + 0.00068 \cdot \text{silt} + 0.0049 \cdot M_{cf}
\]  

(3.132)

Where, \( M_{cf} \) = Coarse fragment content by weight, \( \text{silt} \) = silt content, and \( \theta_{cf} \) = Soil water content at 0.033 Mpa by volume.

In a channel, it was assumed that there is no soil disturbance. Therefore, the channel erodibility is calculated using the same equation for the consolidated rill erodibility calculation (3.132).

**Critical Hydraulic Shear**

DANSAT needs to predict critical shear stress for rill and channel to calculate sediment detachment. An experimental equation derived by Elliot et al.(1989) was used to calculate baseline critical shear stress in a rill. If the constant approach for critical shear stress is selected, the DANSAT model uses a default value of 3.1. Baseline critical shear stress is calculated using:

\[
\tau_{rb} = 2.67 + 6.5 \cdot \text{Clay} - 5.8 \cdot \text{vfs} \quad \text{(if sand} \geq 0.3) \]

\[
\tau_{rb} = 3.5 \quad \text{(if sand} < 0.3) \]  

(3.133)

(3.134)

Where, \( \tau_{rb} \) = baseline critical shear stress in a rill, \( \text{vfs} \) = fraction of very fine sand in the surface soil (if \( \text{vfs} < 0.4 \), \( \text{vfs} = 0.4 \)), and \( \text{clay} \) = fraction of clay (if \( \text{clay} > 0.4 \), \( \text{clay} = 0.4 \)).

Temporally adjusted critical shear stress value is calculated using the below equation by multiplying the baseline critical shear stress and a set of adjustment factors. Freeze and thaw adjustment was not considered in the calculation of critical shear stress.

\[
\tau_{\text{adj}} = \tau_{rb} \cdot C_{\tau_{rr}} \cdot C_{\tau_{sc}}
\]  

(3.135)

Where, \( \tau_{\text{adj}} \) = adjusted critical shear stress value in a rill, \( \tau_{rb} \) = baseline critical shear stress in a rill, \( C_{\tau_{rr}} \) = adjustment factor for random roughness, and \( C_{\tau_{sc}} \) = adjustment factor for sealing and crusting. Adjustment factors are calculated by:

\[
C_{\tau_{rr}} = 1.0 + 8.0 \cdot (RR_t - 0.006)
\]  

(3.136)
\[ C \tau_{sc} = \frac{\tau_{cons}}{\tau_{rb}} + \left(1 - \frac{\tau_{cons}}{\tau_{rb}}\right) \cdot e^{-0.02 \cdot \text{days} \cdot \tau_{rb}} \quad (3.137) \]

Where, \( R_{R_s} \) = random roughness of the surface soil (mm) and \( \tau_{cons} \) = consolidated critical shear and is calculated using the equation:

\[ \tau_{cons} = 8.37 - 11.8 \cdot \theta_{fc} - 4.9 \cdot \text{Sand} \quad (3.138) \]

Where, \( \theta_{fc} \) = Soil water content at 0.033 MPa by volume and Sand = sand content (%).

Similar to the channel erodibility, critical shear stress in a channel was assumed as consolidated critical shear stress, which is calculated by Equation (3.138).

**Plant Growth Component**

Even though eight different plant types are selected for DANSAT, only five plant types are defined in the code. Table 3.9 shows the list of selected and defined plant types in DANSAT.

**Table 3.9. List of selected and defined plant types in DANSAT.**

<table>
<thead>
<tr>
<th>Plant group</th>
<th>Selected plant types</th>
<th>Flag No.</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Annual</td>
<td>Warm season annual</td>
<td>1</td>
<td>Defined</td>
</tr>
<tr>
<td></td>
<td>Cold season annual</td>
<td>2</td>
<td>Defined</td>
</tr>
<tr>
<td></td>
<td>Warm season annual-legume</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Cold season annual-legume</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>Perennial</td>
<td>Perennial</td>
<td>5</td>
<td>Defined</td>
</tr>
<tr>
<td></td>
<td>Perennial-legume</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>Tree</td>
<td>Conifer</td>
<td>7</td>
<td>Defined</td>
</tr>
<tr>
<td></td>
<td>Deciduous or Mixed</td>
<td>8</td>
<td>Defined</td>
</tr>
</tbody>
</table>

Temporal changes in crop variables such as canopy cover, canopy height, root development, and biomass are simulated by the plant growth component. The simulated canopy height and cover is used in the soil erosion component for predicting detachment parameters of interrill. Leaf area index, calculated based on biomass produced by plant, is used in the evapotranspiration component to simulate the extraction of water from multiple soil layers in combination with the simulated root growth.

**Root depth**

Constant root depth was assumed for perennial crops and trees. The maximum root depth input from Crop data block are used to control the constant root depth. Root depth for annual crop is predicted by Borg and Grimes (1986).
\[ R_d = R_{ds} \left[ 0.5 + 0.5 \cdot \sin \left( 3.03 \left[ \frac{D_p}{D_m} \right] - 1.47 \right) \right] \]  

(3.139)

Where, \( R_d \) = root depth (cm), \( R_{ds} \) = maximum root depth (cm), \( D_m \) = number of days to reach maturity, and \( D_p \) = number of days after planting.

**Leaf Area Index**

Leaf Area Index (LAI) for annual crop is calculated using the equations:

\[
LAI = \frac{LAI_{max} \cdot B_{ag}}{B_{ag} + 0.552 \cdot e^{-6.8B_{ag}}} \quad \text{(if } HUI_i < F_{LAI} \text{)} \tag{3.140}
\]

\[
LAI = LAI_{d} \left[ \frac{1 - HUI_i}{1 - F_{LAI}} \right] \quad \text{(if } HUI_i > F_{LAI} \text{)} \tag{3.141}
\]

Where, \( LAI_{max} \) = maximum leaf area index potential, \( LAI_d \) = leaf area index value when LAI starts declining, \( F_{LAI} \) = fraction of growing season when leaf area index starts declining, \( HUI_i \) = heat unit of current day, and \( B_{ag} \) = above-ground vegetative biomass (kg/m²).

With regard to the perennial crops, hay cut and pasture grazing management are considered in DANSAT. Starting time of hay cut and pasture grazing is automatically decided by DANSAT based on the heat unit ratio (HUR), which is the ratio of current cumulative heat unit to potential heat units to crop maturity. The user is able to define the starting point of cutting and grazing using the heat unit ratio as an input parameter. When the heat unit ratio (HUR) is the same or greater than user-defined ratio, hay cut or pasture grazing occurs. If there is hay cut in a specific day, LAI value is set to minimum LAI value. In the case of pasture grazing, LAI linearly decreases based on the user-defined grazing period. Constant LAI value is used during the dormancy period of perennial crops. Constant LAI value is defined in the minimum LAI of crop data block. After the dormancy period ends, perennial crop starts to grow. The same equation is used to simulate increase of LAI for both hay and pasture:

\[
LAI = LAI_{min} + \left( \frac{LAI_{max} - LAI_{min}}{B_{ag}} \right) \cdot \frac{B_{ag}}{B_{ag} + 0.276 \cdot e^{-13.6B_{ag}}} \tag{3.142}
\]

Where, \( LAI_{min} \) = minimum leaf area index.
Linear decrease in LAI for pasture grazing is considered by:

\[
LAI = LAI_d - (LAI_d - LAI_{\text{min}}) \cdot \frac{(Day_c - Day_d)}{Grz_{\text{period}}}
\]  

(3.143)

Where, \( LAI_d \) = leaf area index value when grazing starts, \( LAI_{\text{min}} \) = minimum leaf area index, \( Day_c \) = Julian day of current date (day), \( Day_d \) = Julian day when LAI starts declining by grazing (day), and \( Grz_{\text{period}} \) = grazing period as a user input (day).

For conifer plants, a constant LAI value is assumed for the entire simulation period. The constant value is defined by the maximum LAI input from the crop data block of the main input file. The same methods as those used for perennial crop are used for calculating LAI of deciduous or mixed trees. During the dormancy period, constant LAI is used based on a minimum LAI input parameter by which a fraction of deciduous trees in mixed area can be considered. If there are no conifer trees, a minimum LAI of zero can be used. The user can increase or decrease the minimum LAI value between zero and the user-defined minimum LAI according to the fraction of conifer trees within the mixed trees. The same equation (3.142) is used to simulate the increase in LAI during growing season. Linear decrease of LAI is considered by:

\[
LAI = LAI_d - (LAI_d - LAI_{\text{min}}) \cdot \frac{(Day_c - Day_d)}{(Dorm_{\text{begin}} - Day_d)}
\]  

(3.144)

Where, \( LAI_d \) = leaf area index value when LAI starts declining, \( LAI_{\text{min}} \) = minimum leaf area index, \( Dorm_{\text{begin}} \) = Julian day when dormancy period begins (day), \( Day_c \) = Julian day of current date (day), and \( Day_d \) = Julian day when LAI starts declining (day).

**Above-ground and Root Biomass**

Photosynthetic active radiation is calculated by:

\[
PAR = 0.02092 \cdot RA \cdot \left(1.0 - e^{-0.65LAI}\right)
\]  

(3.145)

Where, \( PAR \) = photosynthetic active radiation (MJ/m²), \( RA \) = solar radiation (Ly), and \( LAI \) = leaf area index.

Adjusted daily potential change in total biomass (kg/m²) is predicted by:
\[ \Delta B = 0.0001 \cdot BE \cdot PAR \cdot REG \quad (3.146) \]

Where, \( BE \) = crop parameter for converting energy to biomass for crop (kg/MJ) and \( REG \) = Growth regulating factor (minimum of the water and temperature factors).

Water stress factor (WS) is calculated by:

\[
WS = \sum_{l=1}^{nl} \frac{u_l}{E_p} \quad (3.147)
\]

Where, \( u_l \) = plant water use in soil layer \( l \) (mm), \( nl \) = number of soil layers, and \( E_p \) = potential plant evaporation (mm).

Temperature stress factor (TS) is calculated by:

\[
TS = \sin \left[ \pi \frac{T_a - T_b}{2 \left( T_o - T_b \right)} \right] \quad (3.148)
\]

Where, \( T_a \) = average daily temperature (°C), \( T_b \) = base temperature for the crop (°C), and \( T_o \) = optimum temperature for the crop (°C).

For annual crops, the following equations are used to simulate increases in above-ground and root biomass when heat unit ratio (HUR) is less or equal to one. Above-ground and root biomass is calculated using the root to shoot ratio (\( R_{sr} \)).

\[
\Delta B_{ag} = \Delta B \cdot (1.0 - R_{sr}) \quad (3.149)
\]

\[
\Delta B_{rt} = \Delta B \cdot R_{sr} \quad (3.150)
\]

Where, \( \Delta B_{ag} \) = daily change in above-ground biomass (kg/m²), \( \Delta B_{rt} \) = daily change in total root biomass (kg/m²), and \( R_{sr} \) = root to shoot ratio.

Total above-ground biomass is calculated by:

\[
B_{ag(i)} = B_{ag(i-1)} + \Delta B_{ag} \quad (3.151)
\]
Where, $B_{ag(i)} =$ total above-ground biomass at day i (kg/m$^2$) and $B_{ag(i-1)} =$ total above-ground biomass at day i-1 (kg/m$^2$).

Total root biomass in the 0 to 0.15m soil zone is calculated by:

\[
B_{rtl(i)} = B_{rtl(i-1)} + \Delta B_{rt} \quad \text{(if root depth is < 0.15 m)} \tag{3.152}
\]

\[
B_{rtl(i)} = B_{rtl(i-1)} + (0.6 \cdot \Delta B_{rt}) \quad \text{(if root depth is > 0.15 m and <0.3 m)} \tag{3.153}
\]

\[
B_{rtl(i)} = B_{rtl(i-1)} + (0.45 \cdot \Delta B_{rt}) \quad \text{(if root depth is > 0.3 m and <0.6 m)} \tag{3.154}
\]

\[
B_{rtl(i)} = B_{rtl(i-1)} + (0.42 \cdot \Delta B_{rt}) \quad \text{(if root depth is > 0.6 m)} \tag{3.155}
\]

Where, $B_{rtl(i)} =$ root biomass in the 0- to 0.15-m soil zone at day i (kg/m$^2$) and $B_{rtl(i-1)} =$ root biomass in the 0- to 0.15-m soil zone at day i-1 (kg/m$^2$).

If heat unit ratio (HUR) becomes greater than one, senescence of annual crop, which is the phenomenon where plant loses the ability to grow, starts. Senescence continues during the user-given senescence period, which is the number of days between the beginning and end of leaf drop. Decreased above-ground biomass by senescence is converted to the flat residue biomass during senescence period. Decrease of biomass is calculated by the following equation:

\[
B_{ag,i} = B_{ag,i-1} - B_{ag,mat} \cdot \frac{(1-F_{bs})}{S_{period}} \tag{3.156}
\]

Where, $B_{ag,i} =$ cumulated above-ground biomass at day i (kg/m$^2$), $B_{ag,i-1} =$ cumulated above-ground biomass at day i-1 (kg/m$^2$), $B_{ag,mat} =$ cumulated above-ground biomass at crop maturity (kg/m$^2$), $F_{bs} =$ fraction of above-ground biomass remaining after senescence, and $S_{period} =$ number of days between the beginning and end of leaf drop.

Equations (3.149) to (3.156) were used to simulate increases in above-ground biomass for perennial crops. If there is a hay cut, above-ground biomass is set to minimum biomass, which is defined in the daily initial data block of main input. In the case of pasture grazing, decrease in above-biomass is considered using the following equation:
\[ B_{ag,i} = B_{ag,mat} - (B_{ag,mat} - B_{ag,min}) \left( \frac{Day_c - Day_d}{Grz_{period}} \right) \]  \hspace{1cm} (3.157)

Where, \( B_{ag,i} \) = cumulated above-ground biomass at day \( i \) (kg/m\(^2\)), \( B_{ag,mat} \) = cumulated above-ground biomass at crop maturity (kg/m\(^2\)), \( Day_c \) = Julian day of current date (day), \( Day_d \) = Julian day when above-ground biomass starts decrease by grazing (day), and \( Grz_{period} \) = grazing period (day).

For conifer trees, constant above-ground biomass was assumed during the simulation period. The constant value is defined in the daily variable initial data block of the main input file. The same assumption as that for the perennial crop is used for deciduous or mixed trees. During the dormancy period, constant minimum above-ground biomass is used. The user can increase or decrease the minimum above-ground biomass according to the percent of the conifer trees. Decreased above-ground biomass by dropped leaves is converted to the flat residue biomass. Linear decrease in above-ground biomass per day is estimated by:

\[ B_{ag,i} = B_{ag,i-1} - \frac{B_{ag,mat} - B_{ag,min}}{Dorm_{begin} - Day_d} \]  \hspace{1cm} (3.158)

Where, \( B_{ag,i} \) = cumulated above-ground biomass at day \( i \) (kg/m\(^2\)), \( B_{ag,i-1} \) = cumulated above-ground biomass at day \( i-1 \) (kg/m\(^2\)), \( B_{ag,mat} \) = cumulated above-ground biomass at crop maturity (kg/m\(^2\)), \( B_{ag,min} \) = minimum cumulated above-ground biomass during dormancy period (kg/m\(^2\)), \( Dorm_{begin} \) = Julian day when dormancy period begins (day), and \( Day_d \) = Julian day when above-ground biomass starts to decrease (day).

**Canopy Cover and Height**

Canopy cover for all plant types is calculated by the following equation based on simulated above-ground biomass (Arnold et al., 1995):

\[ C_c = 1 - e^{-\beta_c B_{ag}} \]  \hspace{1cm} (3.159)

Where, \( C_c \) = canopy cover (0-1), \( \beta_c \) = parameter for canopy cover equation as an input parameter, and \( B_{ag} \) = cumulated above-ground biomass.
The temporal changes in canopy height for annual crops are estimated by the following equation. All other plant types are assumed to have constant canopy height during simulation period.

\[
H_c = \left[1 - e^{-\beta_h B_{ag}} \right] H_{cm}
\]

(3.160)

Where, \(H_c\) = canopy height, \(H_{cm}\) = maximum canopy height (m), \(\beta_h\) = parameter for canopy height equation as an input parameter, and \(B_{ag}\) = cumulated above-ground biomass.

**Residue Decomposition Component**

The WEPP approach for crop residue decomposition (Stott et al., 1995) was simplified in the DANSAT. Even though WEPP simulates four different crop residue types such as standing, flat, buried, and dead root, DANSAT does not consider the standing biomass after harvest. In addition, no difference was considered in the decomposition process of last and all prior harvested crop residues. Only annual crops and deciduous trees are considered for the decomposition of flat residue. Decomposition process of buried and dead root residue is considered for annual crops, while for all other plants constant residues values, which are defined in the initial data block, are used. All live root biomass are assumed to be converted to dead root biomass after the harvesting date. Flat residue and dead root biomass are converted to buried-residue based upon tillage intensity and depth at tillage application date.

Residue decomposition rates are affected by environmental factors such as water content and temperature. Environmental factor (ENVIND) is defined as the minimum value of temperature and water factors described by the following equations. The temperature factor (TFC) and water factor (WFC) are normalized values between 0 and 1.

The temperature factor for flat residues is calculated by:

\[
TFC = \frac{2(T_{avg} + T_{min})^2 \cdot (T_{max} + T_{min})^2 - (T_{avg} + T_{min})^4}{(T_{max} + A)^4}
\]

(3.161)

Where, \(TFC\) = Temperature factor (If \(T_{avg}\ < -6.1\) or \(T_{avg}\ > 49.2\), \(TFC=0\)), \(T_{avg}\) = average daily air temperature (°C), \(T_{max}\) = maximum temperature for the function (°C), and \(T_{min}\) = minimum temperature for the function (°C).

Water factor for flat residues is calculated by:
\[ WFC = \frac{\theta_{\text{till}}}{\theta_{\text{opt}}} \quad \text{(if } \theta_{\text{opt}} > \theta_{\text{till}}) \] (3.162)

\[ WFC = \frac{\theta_{\text{opt}}}{\theta_{\text{till}}} \quad \text{(if } \theta_{\text{opt}} \leq \theta_{\text{till}}) \] (3.163)

Where, \( \theta_{\text{till}} \) = water content of the surface tilled zone of the soil and \( \theta_{\text{opt}} \) = water content of the surface soil that would be considered optimum for microbial activity.

Decomposition of flat residues is calculated by:

\[ M_t = M_{t-1} \cdot e^{\text{ENVIND-ORATE}} \] (3.164)

Where, \( M_t \) = residue biomass per unit area remaining (kg/m\(^2\)), \( M_{t-1} \) = biomass per unit area remaining the previous day (kg/m\(^2\)), ORATE = optimum decomposition rate (kg/m\(^2\)-d), and \( \text{ENVIND} \) = environmental index used to determine residue decomposition.

Remaining flat biomass after harvest (kg/m\(^2\)) is calculated using user-defined residue cover input by:

\[ M_f = -\frac{\ln(1-C_{rf})}{c_f} \] (3.165)

Where, \( M_f \) = flat residue biomass (kg/m\(^2\)), \( C_{rf} \) = fraction of the soil surface covered by the flat residue after harvesting as a user input, and \( c_f \) = crop specific constant.

During the tillage management, conversion from flat residue to buried biomass is calculated as a function of tillage intensity. Conversion from dead root biomass to buried biomass is calculated considering tillage depth. Decomposition of buried and dead root residues is calculated using the same equations used for flat residue decomposition.

**Model Interface**

User-friendly interface has become an indispensable component in preparing data set for distributed, watershed-scale NPS models that require intensive spatial, physical, and management input data. Most interfaces, especially interfaces for the distributed parameter models, utilize the GIS functionalities in order to treat intensive spatial data. The three coupling approaches of GIS and models, namely loose, close, and tight couplings (Liao and Tim, 1997), can be subdivided
into two groups according to the location of the major interface. Figure 3.17 shows reclassified coupling approaches of GIS and models.

Figure 3.17. Approaches for GIS and model coupling: (a) GIS-based loose coupling; (b) model-based loose coupling; (c) GIS-based close coupling; (d) model-based close coupling; (e) GIS-based tight coupling; and (f) model-based tight coupling.

In the loose coupling approach (Figure 3.17.a and b), GIS and the model have separate user interface and ASCII or binary files are used to transport data between GIS and the model. Loose coupling approach, which may be the most realistic method for developing GIS-model interface, requires minimum modification of GIS software and hydrologic models. Loose coupling can be divided into GIS-based loose coupling and model-based loose coupling based on the location of
interface, which controls the conversion of data structure and transfer of model input and output data. GRASS-AGNPS (Line et al., 1997; Srinivasan and Engel, 1994) uses the model-based loose coupling approach. The model interface use GIS map layers which are separately generated by GRASS to extract data and create model input file.

The close coupling approach uses a single common interface for both GIS and the model. This approach can be subdivided into GIS-based close coupling (Figure 3.17.c) and model-based close coupling (Figure 3.17.d) depending on the location of the interface. GIS and the model exist independently in spite of the common interface. One example of GIS-based close coupling is Arc/View-AGNPS developed based on Arc/View GIS extension (He et al., 2001). AGNPS interface was plugged into the Arc/View GIS menu as the hydrology extension. Both spatial data manipulation and generation of the model input data are performed in the Arc/View environment. QUESTIONS (Veith et al., 2000) and Watershed Modeling System (WMS) (Environmental Modeling Research Laboratory, 1998) can be classified as model-based close coupling.

QUESTIONS, the interface for the ANSWERS-2000, was developed using Visual Basic to generate input files for the model. However, functionalities of Arc/View are plugged into the interface to manipulate spatial data. WMS was developed to provide interface for several lumped and distributed parameter models such as HEC-1, TR-20, TR-55, and HSPF. WMS can be used without any commercial GIS software, because it contains its own mapping tool, which is compatible with different GIS data structures (Ogden et al., 2001).

Tight coupling, which is also referred to the integrated approach, provides common user interface for both GIS and the model. Both the functionality of GIS and processes of the model rely on a single system; thus, there is no need to transfer data between GIS and the model. In tight coupling, GIS and the model rely on a single data manager and share data with computer memory rather than ASCII/Binary files. This approach requires a significant amount of time and money for development. In tight coupling approach, hydrologic modeling functions can be embedded on top of existing GIS software (GIS-based tight coupling) or GIS functionalities can be embedded in hydrological modeling package (model-based tight coupling). GIS-based tight coupling approach is able to use full built-in GIS functionalities but hydrologic modeling capabilities are restricted in GIS software. A simple surface runoff model based on the curve number was incorporated into the Arc/Info environment in order to simplify the transfers of inputs and outputs between GIS and the model (Yu et al., 2001). Model-based tight coupling use GIS as a mapping tool, which may
not be comparable to commercial GIS data structures, but the programming environment for the development of hydrological models can be maximized (Sui and Maggio, 1999).

Model-based loose coupling was selected for the DANSAT interface. The loose or close coupling approach has been frequently applied in linking GIS and models because of the significant amount of programming efforts required for developing a tightly coupled system (Sui and Maggio, 1999). However, GIS-based loose and close coupling approaches can be dependent on selected GIS software for manipulating spatial data. For example, a number of GIS-AGNPS interfaces, including GRASS-AGNPS, Arc/Info-AGNPS, and Arc/View-AGNPS, have been developed for the same model, AGNPS, using popular GIS softwares such as GRASS, Arc/Info, and Arc/View. In addition, functionalities of an interface as a pre-processor for a distributed model can be subdivided into two stages. One is to manipulate spatial data using GIS and the other is to manage non-spatial databases and create model input files based on both spatial and non-spatial data. If both functionalities are necessary to be included in the GIS, according to the selected GIS software (GIS based loose or close coupling), later functionality of an interface must be repeatedly coded in a different GIS environment. Several spatial data manipulation procedures, including watershed and channel network delineation, can be commonly used for different hydrologic models. If GIS functionalities are embedded into an interface for a specific model in the model-based close coupling, the common GIS functionalities should be repeated in other interfaces. If the GIS functionalities are separated from the interface, this independency will improve the efficiency in developing an interface and provides users with flexibility in selecting not only the GIS software but also the operating system.

The overall concept and major functions of the interface are described in Figure 3.18. Three different types of data, namely spatial, meteorological, and physical or managerial data, were used as input to the interface, which creates input files for the DANSAT.
Spatially variable information, such as surface elevation, slope, aspect, stream network, soils, rain gauge number and rotation number, is extracted from Arc/View ASCII format, which can be independently exported by other GIS software as well as Arc/View. Cell data block interface assists with extracting the spatially distributed parameters from user-supplied Arc/View ASCII files. Management and physical information are restored and extracted using a predefined MS Access database file (Input DB in Figure 3.18), which is accessed and manipulated by the interface. The interface uses non-spatial databases of existing hydrologic models to add information into the input database of the interface. The existing databases include SSURGO from NRCS, crop and tillage databases from WEPP, and pesticide database from GLEAMS. General and layer-specific soil parameters for DANSAT can be easily generated from SSURGO using the interface, and the detail assumption and equations used are explained in Appendix A. Meteorological input requires general weather file and break-point rainfall input file, which is created by the interface based on HAS format of the Biological Systems Engineering Dept. at Virginia Tech (Carr et al., 1988). The post-processor component was coded for reading output files of DANSAT and saves the results into pre-defined MS Access database file (Result DB in Figure 3.18), which can be accessed by Microsoft Excel for further analysis using VBA. The
post-processor, however, was not validated and is not used in this research due to the speed limitation in copying results from output files to the MS Access database file.

**Summary**

DANSAT was developed using Fortran90 to evaluate the spatial and temporal impacts of BMPs on hydrology, sediment, and pesticide losses in agricultural watersheds. An interface was developed for DANSAT using Visual Basic to create intensive model input files. The source codes for DANSAT and the interface are available only in the electric form of the dissertation (Appendix F). DANSAT’s hydrology components include interception, evapotranspiration, infiltration and percolation, overland flow, channel flow, interflow, and baseflow components. The sediment component include interrill detachment, rill detachment, channel detachment, transport capacity, overland routing, and channel routing related sub-routines. The pesticide component consists of pesticide application, degradation, equilibrium, plant uptake, pesticide leaching, interflow pesticide, and ground water pesticide related sub-routines.

The overall sequence of components and selected time-step for the components are described in Figure 3.19. There are two different loops in the flowchart: During Storm Event Loop (DSEL) and Between Storm Events Loop (BSEL). Infiltration, overland flow, overland sediment, and overland pesticide routing components are used only for the DSEL. Channel routing related components and subsurface related component such as percolation, pesticide leaching, interflow, and baseflow components are commonly used for both DSEL and BSEL. Table 3.10 shows a summary of characteristics of DANSAT based on the criteria defined by Borah and Bera (2003).
Figure 3.19. The flowchart for DANSAT Model and time-steps used for various components.
Table 3.10. A summary of DANSAT’s characteristics.

<table>
<thead>
<tr>
<th>Criteria</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model component / capabilities</td>
<td>- Continuous, distributed, physically-based, and watershed-scale NPS model&lt;br&gt;- Simulates hydrology, sediment, and pesticide.&lt;br&gt;- Temporal and spatial changes in BMPs can be considered by dynamic variable components and hierarchical structure of main input.&lt;br&gt;- Different types of output files are available including outlet, flux, and field-scale output files.</td>
</tr>
<tr>
<td>Temporal scale</td>
<td>- Continuous simulation model.&lt;br&gt;- Different time-steps are used.</td>
</tr>
<tr>
<td>Watershed representation</td>
<td>- Three-dimensional watershed representation using regular grids and multiple soil layers.</td>
</tr>
<tr>
<td>Rainfall excess on overland / water balance</td>
<td>- Excess rainfall for overland flow is separated based on Green-Ampt equation (Green and Ampt, 1911).&lt;br&gt;- Potential evapotranspiration is estimated based on Priestley-Taylor method (Priestley and Taylor, 1972).&lt;br&gt;- Actual evaporation and transpiration are separately calculated based on Richie’s method (Ritchie, 1972).</td>
</tr>
<tr>
<td>Runoff on overland and channel</td>
<td>- Eight flow directions are used.&lt;br&gt;- Overland flow routing is calculated by combined continuity equation and Manning’s equation.&lt;br&gt;- Channel flow routing is variable storage routing method (Williams, 1969).</td>
</tr>
<tr>
<td>Runoff in channel</td>
<td>- Two different channel shapes can be simulated: rectangle and triangle.&lt;br&gt;- Channel routing is calculated using variable storage routing method.</td>
</tr>
<tr>
<td>Flow in reservoir</td>
<td>- Not considered.</td>
</tr>
<tr>
<td>Overland sediment</td>
<td>- Multiple particle sizes can be considered.&lt;br&gt;- Rill and interrill erodibility are separately calculated based on the WEPP approach (Alberts et al., 1995).&lt;br&gt;- Transport capacity is estimated based on Yalin’s equation (Yalin, 1963).&lt;br&gt;- Sediment routing is considered based on continuity equation (Byne, 2000).</td>
</tr>
<tr>
<td>Channel sediment</td>
<td>- Channel erodibility is calculated based on the simplified rill erodibility approach in WEPP.&lt;br&gt;- Transport capacity is based on Yalin’s equation.&lt;br&gt;- Bank erosion is not included.</td>
</tr>
<tr>
<td>Reservoir sediment</td>
<td>- Not considered.</td>
</tr>
<tr>
<td>Chemical simulation</td>
<td>- Multiple pesticides can be considered in one simulation.&lt;br&gt;- Different application methods can be considered.&lt;br&gt;- Degradation is based on the first-order kinetics equation by adjusting based on soil temperature and water content (Truman et al., 1998).&lt;br&gt;- Equilibrium is based on the linear isotherm equation.&lt;br&gt;- Overland pesticide routing is calculated based on hydrology output and pesticide concentration by linear isotherm equation.&lt;br&gt;- Pesticide movement in ground water is considered based on distance to a nearest stream segment and average velocity of pesticide movement.&lt;br&gt;- Pesticide movement by plant uptake, leaching, and interflow are considered.</td>
</tr>
<tr>
<td>BMP evaluation</td>
<td>- Dynamic crop rotations can be considered.&lt;br&gt;- Different tillage applications can be considered.&lt;br&gt;- Different pesticide application methods can be considered.&lt;br&gt;- Residue management can be considered.&lt;br&gt;- Structural BMPs are not included.</td>
</tr>
<tr>
<td>Interface</td>
<td>- Model-based loose coupling interface developed by Visual Basic. &lt;br&gt;- Most of functionalities are to create model input files.</td>
</tr>
</tbody>
</table>
References


Dillaha, T.A. 1990. Role of Best management practices in restoring the health of the Chesapeake Bay. In Perspectives on the Chesapeake Bay: 1990. Advances in Estuarine Sciences. Chesapeake Bay Program, CBP/TRS41/90. USEPA, WASHINGTON, DC.


Chapter 4: Surface and Ground Water Interactions

Introduction

Both monitoring and modeling approaches could be used for conjunctive investigation of surface water and ground water. Mathematical models such as linear Boussinesq equation, and non-linear Boussinesq equation were used to simulate stream-aquifer interaction in an unconfined aquifer (Serrano and Workman, 1998; Workman et al., 1997). These mathematical models can be solved analytically based upon simplifications such as assumptions of homogeneity and one- or two-dimensional flow. Numerical solutions have been widely used in practical applications because of disadvantages of mathematical models. Numerical solutions are more versatile and easier to use than analytical solutions due to widespread use of computers. Through the numerical modeling approach, interaction between surface water and ground water can be investigated by: (1) using relevant modules of existing ground water models, (2) linkage of a ground water model and a surface hydrology model, and (3) developing an integrated surface-subsurface model.

Existing ground water models: Existing ground water models can be used for considering aquifer-stream interactions. MODFLOW (McDonald and Harbaugh, 1988) has been widely used in ground water modeling studies. The River package of MODFLOW considers a constant stage in a stream and computes the flow between ground water and surface water systems. The stream stages can be either specified by the user or calculated by Manning’s equation within MODFLOW. In addition to variable stream stages, the stream routing can be conducted in the Streamflow Routing package (Prudic, 1989).

Linking ground water model and surface hydrology model: Swain (1994) developed MODBRANCH for simulation of stream-aquifer interactions. The model links BRANCH (Schaffranek et al., 1981), which is a one-dimensional numerical model designed to simulate unsteady flow in open-channel networks, to MODFLOW. In MODBRANCH, streams are simulated more realistically than in the River and Stream Packages of MODFLOW.

Havard and others (1995) linked a newly developed one-dimensional unsaturated flow model to an existing ground water model, MODFLOW, to calculate the movement of water during various water table management practices. The linked model, LINKFLOW, was validated against observed data and the simulated results showed good agreement with measured values (Havard et al., 1997). Li (1993) developed a linked system by linking PRZM (Carsel et al., 1985), VADOFT
(Huyakorn and Buckley, 1987), and SUTRA (Voss, 1984) for simulating pesticide transport in the root zone, intermediate zone, and saturated zone, respectively. The capability of the linked system for providing spatial distribution of pesticide concentrations at any desired depth in the unsaturated zone and saturated zone was demonstrated in the research.

Sophocleous and others (1999) replaced the ground water component of SWAT with MODFLOW in order to evaluate long-term water management strategies. Daily and monthly time steps were used for SWAT and MODFLOW simulation, respectively. A weighted average, calculated over all hydrologic response units (HRUs) in SWAT, was used as input to MODLOW for each aquifer time step. As a result, the linked system (SWATMOD) cannot represent the variations of stream-aquifer interactions on a daily basis. Sophocleous and Perkins (2000) applied SWATMOD to three different watersheds in Kansas. In this study, the integrated model successfully demonstrated two-way interactions between surface and ground water. Watershed heterogeneities were considered using the hydrologic response unit (HRU) concept.

Ramireddygar and others (2000) showed the flexibility of a linked approach in handling stream-aquifer interaction by substituting POTYLD (Koelliker, 1994) for SWAT in linkage to the existing ground water model, MODFLOW. Cho and others (2001) evaluated the impact of land use activities on the surface and subsurface flow regimes by using the HSPF simulation results as inputs to MODFLOW. The ground water recharge output from HSPF was used as the input to the transient MODFLOW simulation. Differences in spatial and temporal scales provided challenges when linking a lumped surface hydrology model with a distributed ground water model.

**Integrated surface-subsurface model:** MIKE-SHE is one of the very few currently available integrated, physically-based, and fully distributed modeling tools suitable for long-term simulation of the effectiveness of BMPs that consider the interaction between surface water and ground water. Jayatilaka et al. (1998) simulated hydrology in a small experimental irrigation site using MIKE-SHE to quantify the effects of flow processes on surface drainage and shallow ground water level. The simulated results showed general consistency with the observed data despite deficiency in simulating rapid flow through macropores. Andersen et al. (2001) modified the MIKE-SHE model to simplify the movement of water in the subsurface zone. In this model, water movement in the unsaturated zone is estimated based upon gravity, and the soil profile is represented by a number of computational nodes in the vertical direction. The subsurface zone was represented by interconnections between a number of interflow and ground water storages. In
addition, horizontal and vertical movement of percolating water through the root zone is considered.

Heng and Nikolaidis (1998) developed the Watershed Nutrient Transport and Transformation (NTT-Watershed) model to simulate water and nutrient transport at the watershed-scale. This model is a physically-based, distributed-parameter model, which can be used for predicting the fate and transport of nitrogen in surface, unsaturated, and saturated zones. This model consists of four submodels: (1) hydrologic and energy budget submodel, (2) transport submodel, (3) chemical reaction submodel, and (4) stream routing and transport submodel. The hydrology component simulates overland flow, vadose zone flow, stream flow, and ground water flow. A two-dimensional unconfined ground water flow equation is used to describe the movement of ground water. The solute transport submodel simulates the transport of nitrogen in surface, unsaturated, and saturated zones. A one-dimensional convection dispersion equation (CDE), and a two-dimensional CDE are used to describe chemical transport in the vadose zone and saturated zone, respectively. Ground water seepage into or out of the stream is calculated using Darcy’s Law. NTT-Watershed model performed well in simulating hydrology and nitrogen dynamics in the Muddy Brook watershed in Connecticut (Heng and Nikolaidis, 1998).

Yu and Schwartz (1998) developed a physically-based, distributed-parameter model, Basin-Scale Hydrologic Model (BSHM), to simulate hydrologic responses on a basin-scale considering water movement in both surface and subsurface areas. The model consists of four modules including Digital Elevation Generator (DEG), Versatile Soil-Moisture Budget (VB) Model, Surface-Runoff Delay-Time Model (RDTM), and Ground-water Flow Model (GFM). DEG was developed for generating digital landscape for watersheds where existing data are unavailable. VB calculates vertical soil water flow, evapotranspiration, and infiltration. RDTM simulates overland and channel flow routing. The Muskingum routing procedure was used for simulating channel routing. GFM simulates ground water flow using a two-dimensional finite-difference numerical equation derived using Darcy’s equation together with a law of mass conservation. The interaction between steam and ground water is considered based on Darcy’s equation with assumptions of rectangular channel geometry and a hydraulic conductivity of stream bed that is smaller than the aquifer.
Selection of an Appropriate Approach for Surface and Ground Water Interactions

The selection of an appropriate approach for considering interactions between surface and ground water depends on the acceptable assumptions and available data required for simulations. As mentioned previously, an ideal modeling system should be able to simulate the impacts of land use changes on hydrology and water quality of surface and subsurface areas. Possible approaches for considering the interactions between surface water and ground water include: (1) use of existing ground water models, (2) linkage of ground water model and surface hydrology model, and (3) developing an integrated surface-subsurface model. Among the three possible approaches, use of an existing ground water model is not appropriate for this study because most of these models do not consider the impacts of BMPs, which are usually applied to overland area, on ground water. The integrated modeling approach can be more efficient than the linked model approach in terms of its application. The integrated modeling approach can minimize the size of the model by incorporating only necessary algorithms or functions into the integrated model. The integrated approach uses computer memory to consider both the surface-to-ground water and ground water-to-stream interactions, rather than saving and retrieving a data file. As a result, this approach may decrease the computation time and increase the efficiency of the model application. In addition, this integrated modeling approach has the advantage of a smaller input data requirement, compared to the linked approach. However, an integrated approach would be less reliable than a linked model approach from the model developer’s point of view because the integrated approach requires modification of most existing model components and verification of the newly developed components. In contrast to the integrated approach, the approach of linking existing ground water and surface water models has the flexibility of exchanging a component of one model with an appropriate component from another model. For example, the SWAT component of SWATMOD can be substituted by another surface hydrology model, such as POTYLRD, without modifying the original source code of SWAT, POTYLRD, or MODFLOW. Developing a new interface module or modifying an existing interface module for a linked system is easier and more reliable than developing a new integrated surface-ground water modeling system because individual models in a linked system have been widely used and are already verified. As a result, only a verification process for the interface module is necessary. However, the major disadvantage of the linked approach is in its input data requirement because some input data can be overlapped between individual surface and ground water models. Users also need to be familiar with all individual models.
In this research, more importance was given to the flexibility and reliability rather than the efficiency of the model, considering the fast growth of computer hardware. As a result, the linked modeling approach was selected to consider the interaction between surface and ground water. MODFLOW (McDonald and Harbaugh, 1988) and MT3D (Zheng, 1990) were selected as ground water models for the linked approach with DANSAT, used to simulate water and pesticide movement in the saturated zone, respectively. Figure 4.1 shows the conceptual model of the selected linked approach. The Recharge package of MODFLOW was selected to simulate the hydrologic impact of agricultural BMPs on the ground water system. The Streamflow Routing package was selected to represent the stream and consider stream-aquifer interactions.

The linked approach should have the ability to consider two-way interactions between surface and ground water. Both interactive influences of surface water on ground water (surface-to-aquifer interaction) and ground water on surface water (aquifer-to-stream interaction) should be considered. For example, changes in the ground water table resulting from recharge should be reflected in the ground water simulation by changing the input data for the ground water model. Similarly, the changes in the ground water table and calculated discharge from aquifer to the stream segment should be considered in the surface model simulation to consider interactive interactions between two systems.

The major difficulty in linking a surface water model with a ground water model is derived from the differences in their temporal and spatial scales. If the surface and ground water models use different spatial scales, the recharges and pesticide loads from surface water should be lumped or

![Figure 4.1. Conceptual model of linked approach used in this study.](image-url)
subdivided into the various discrete cells of the ground water model. Specifically, linkage between a lumped or semi-lumped surface model and a distributed ground water model, such as HSPF-MODFLOW or SWAT-MODFLOW, has difficulties in taking into account the location of land use changes that could have significant impacts on streamflow and hydraulic head in ground water. With regard to the spatial scale, smaller grid size is recommended for the distributed parameter NPS pollution model to satisfy the assumption that all properties, such as soil, vegetation, surface condition, crop management, and climate, are homogeneous within each grid (Dillaha, 1990). Although a smaller grid size can be used for local ground water simulation, larger cell sizes (> 10 ha) are typically used in most watershed-scale ground water modeling. When a smaller cell size for the surface model and a larger cell size for the ground water model are used, fluxes such as recharges and pollutant loads from several surface cells should be spatially lumped into the underlying ground water cell. Using the same larger cell size for both the surface and ground water models can violate the homogeneous assumption of the surface model. In this research, the same smaller grid size for both the surface and ground water model are selected to avoid inefficiency at the expense of computational time.

The surface and ground water models also operate on different time scales. The difference in time step is appropriate considering that surface runoff occurs more quickly than ground water flow. DANSAT uses varying time steps with a minimum 1-minute time step during rainfall events and a daily time step between rainfall events. An appropriate time step for the ground water model needs to be decided based on the characteristics of ground water flow. A shorter time step will be necessary if the ground water table significantly fluctuates during a small period of time. Considering the variable time-step of ground water model, user can decide the ground water time-step (GWT) as an input parameter, which should be equal to or greater than surface water time-step (SWT), as shown in figure 4.2.
In representing the dynamic surface-to-aquifer interactions, the daily recharge input option in the Recharge module of MODFLOW was used to prevent the daily predicted recharge and pesticide loads from DANSAT being lumped into the larger time step of MODFLOW. The simulated discharge to the stream segments by MODFLOW also should be updated at each time step of the surface components of DANSAT to consider aquifer-to-stream interactions.

In this study, a Dual-Simulation approach (DSA) was developed to consider surface-to-aquifer and aquifer-to-stream interactions (Cho and Mostaghimi, 2004). Figure 4.3 shows the flowchart of the DSA. DSA consists of three major procedures. First, Virtual Simulations (VS) predict the daily recharges and pesticide fluxes to the ground water using temporal arrays of the surface model. The recharge input file of MODFLOW (*.rch) and the sink and source mixing input file of MT3D (*.ssm) are updated based on temporally calculated daily recharges and pesticide fluxes. Second, ground water models are run at the transient mode using updated input data to predict the daily discharges from aquifer to stream segments. Third, Actual Simulation (AS) predicts the final results for hydrology, sediment, and pesticides considering the input from the ground water models. The VS and AS use the exact same values for the simulations.
The Linked model approach has several advantages and disadvantages compared to the integrated approach. DSA requires calculating surface related components of DANSAT twice, once for virtual simulation and again for the actual simulation. This approach dramatically increases the required calculation time, which can be a restricting factor for using the linked system. Moreover, input parameters and observed data for the calibration and validation of ground water models are difficult to obtain. However, the advantages of the linked system include the fact that the system is able to provide the spatial distribution and temporal changes in ground water table elevation.
and pesticide concentration in ground water. Figure 4.4 shows the temporal, spatial, and vertical scale of ground water output by the linked approach and additional output files by the integrated approach discussed in Chapter 3.

The linked modeling approach is recommended when the major concern in a watershed is to evaluate the impacts of agricultural BMPs on spatial distribution and movement of water and contaminant in a saturated zone rather than impacts on overall total runoff and pollutant loads in a stream. Furthermore, the linked approach is appropriate for considering the ground water related managements such as pumping.

In summary, the modeling procedure for the linked approach consists of three steps: 1) calibrating DANSAT using an integrated ground water approach; 2) calibrating the ground water models in a steady-state condition; and 3) running the linked system with the transient simulation of ground water models to solve time-dependent problems. Details of each step will be explained in the validation chapter.

**Summary**

The linked modeling approach, which links a newly developed surface model, DANSAT, with existing ground water models, MODFLOW and MT3D, was selected to consider surface and ground water interactions. DANSAT predicts the movement of water and pesticides in runoff and in leachate at a watershed-scale. MODFLOW and MT3D simulate ground water and pesticide
movement in the saturated zone, respectively. The same spatial scale was used for both surface and ground water models, but different time scales were used because surface runoff occurs more quickly than ground water flow. The Dual-Simulation (DS) approach was introduced to resolve the problems occurring by the different temporal scale between DANSAT and MODFLOW/MT3D. Virtual Simulations (VS) predict the daily recharges and pesticide fluxes to the ground water using temporal arrays. Ground water models predict the daily discharges from aquifer to stream segments using updated input data by VS. Then, the Actual Simulation (AS) predicts the final results for hydrology, sediment, and pesticides by considering the discharge input from the ground water models. Acquiring input parameters and observed data for the calibration and validation of ground water models can be a significant problem when using the linked system. Use of the linked approach is recommended if the spatial and temporal changes in the ground water zone due to implementation of management practices on surface and subsurface are of major concern.

References


Dillaha, T.A. 1990. Role of Best management practices in restoring the health of the Chesapeake Bay. In Perspectives on the Chesapeake Bay. 1990: Advances in Estuarine Sciences. Chesapeake Bay Program, CBP/TRS41/90. WASHINGTON, DC: USEPA.,


Chapter 5: Model Evaluation

Introduction

The eleven steps in the modeling protocol, ranging from definition of purpose to post-audit, were presented by Refsgaard (1997). Among these eleven steps, parameterization, calibration and validation procedures have been the focus of investigations with regard to the application of hydrologic and water quality models (Refsgaard, 1997). The common idea behind calibration and validation in modeling process is 1) to evaluate and refine the model parameters in order to improve accuracy of model results with iterative procedure of comparing simulated and observed values and 2) to assure and demonstrate that the calibrated set of parameters are appropriate for predicting the field observations, which are never used for calibration, respectively. However, verification process, which determines that model algorithms, solution techniques, and equations are accurately represented in the model according to the developer’s conceptual description, should be included in the procedures because DANSAT is a newly developed model. The “evaluation” term in this chapter is used to describe the overall procedures including verification, calibration, and validation.

In spite of the physically-based parameters, which are related directly to the physical characteristics of watershed, physically-based and spatially distributed models still require some form of model calibration due to a lack of data to characterize the spatial variability of watershed and the difficulties in representation of real processes and measurement in models. Model calibration procedure can be generalized into 1) temporal-, 2) spatial-, and 3) component-aspects. With regard to the temporal aspect, calibration involves successive adjustments of relevant hydrologic and water quality parameters from long term to short term, in the following order: 1) annual, 2) seasonal or monthly, 3) daily, and 4) storm hydrograph (Donigian, 2002; Im et al., 2003). Model performance also should be evaluated based on sufficient years of observed data in order to consider variety of climatic, soil water, and water quality conditions (Donigian, 2002). For the spatial aspect, if the model is able to predict spatial distributions and multiple monitoring stations are available in a watershed, the multi-site calibration, which starts upland in the sub-watersheds and follows to the outlet of the watershed, are recommended for spatially distributed predictions and understanding of the behavior of individual sub-systems (Neitsch et al., 2002). Finally, calibration should be performed by hierarchical process, beginning with hydrology,
followed by sediment, and finally pollutant transport, because errors in the current component will be transferred and magnified in all the following components (Donigian, 2002).

Even though several approaches are available for assessing the predictive capability of a model, the split-sample approach, which uses only a portion of the observed records for calibration and remaining period of observed records for validation, is commonly used and recommended (Donigian, 2002). Recently, concerns have been raised about the potential impacts of land use changes and development in ungaged watershed. Split-sample approach with a traditional lumped conceptual hydrologic model has limitations in providing acceptable basis to decision makers for predicting the impact of land use changes (O'Connell and Todini, 1996).

As an extension of the split-sample approach, Klemes (1986) proposed a hierarchical scheme for validation of hydrologic models. The hierarchical scheme is classified into four categories according to the watersheds used for validation and changes in climate, land use, and other watershed characteristics. The model can be validated in the same watershed used for calibration or in other ungaged watersheds. In each case, watershed characteristics can be considered as unchanged (stationary) or changed (nonstationary). Three different types of models ranging from lumped conceptual to distributed physically-based models were validated on three watersheds in Zimbabwe using four cases by Klemes (1986) and two additional modified cases (Refsgaard and Knudsen, 1996). It was concluded that a distributed model performed better than a lumped model for ungaged watersheds. Liew et al. (2003) compared the performance of SWAT and HSPF for varying climatic conditions using eight nested subwatersheds and two adjacent agricultural watersheds. Each model was calibrated on two subwatersheds and validated on six other subwatersheds and two adjacent watersheds.

Ewen and Parkin (1996) developed a blind validation technique for assessing a capability of models to predict impacts of future changes in land use and climate. In the blind validation approach, the modeler is not allowed to see the output data from the watershed and cannot calibrate the model for the watershed in order to clearly test the model’s ability to predict the hypothetical watershed.

The predictive capability of the model is restricted to watersheds where measured data are available and significant land use changes have not occurred when model parameters are not directly linked to the physical conditions of a watershed (Refsgaard and Knudsen, 1996). Therefore, physically-based models have been recognized as potentially useful tools for predicting the impacts of possible future changes in land use and climate. The blind validation
procedure was selected to validate the capability of the physically-based and spatially distributed model, SHETRAN, for predicting the impacts of land use and climate changes on watershed response (Bathurst et al., 2004).

Refsgaard (1997) discussed various requirements for lumped and distributed models in relation to parameterization, calibration, and validation procedures. In his study, establishment of conceptual model, as well as model parameterization, was emphasized for the successful calibration and validation of distributed models. Minimizing the number of free parameters, which are subject to adjustments during subsequent calibration, was suggested as a means to avoid the over-parameterization problem in applications of distributed models.

Non-unique parameterization in both lumped and distributed models is another problem. A large number of alternative parameterizations techniques can produce similar results in terms of an integrated measure of system response, such as a watershed. This problem has been referred to as non-uniqueness or equifinality in parameter estimation (Beven, 1996). For example, evaluation of PRZM-2 by four different users using the same data shows that different users may create parameters set in very different ways in spite of using exactly the same data. The subjectivity in choosing input parameters can lead to very different model outputs (Trevisan et al., 2000). Anderton et al. (2002) also showed that parameter optima occurred in different parts of the parameter space for different responses including discharge, soil moisture reserve, and ground water surface level when applying a physically-based and spatially distributed model. The possibility of non-uniqueness in parameterizations of a physically-based and spatially distributed model can be greatly reduced by increasing the dimensionality of the measurement space (O’Connell and Todini, 1996). A good validation procedure needs to consider internal consistency of the distributed results on subwatershed or on specific simulation unit (Ambroise et al., 1995).

Multi-site, multi-response, and multi-criteria calibration and validation have been recommended for understanding the behavior of individual sub-systems and for minimizing the possibility of the presence of compensating errors within the model by reducing uncertainty in parameter estimation (Andersen et al., 2001; Anderton et al., 2002; Guntner et al., 1999; Refsgaard, 1997).

Useful criteria for evaluating the “goodness-of-fit” of watershed models are suggested by several researchers (ASCE task committee on definition of criteria for evaluation of watershed models of the watershed management committee, 1993; Legates and McCabe, 1999b). The performance criteria also should be decided prior to the first model run based on the data availability and reliability, limitation of the model, specific hydrologic conditions, and the purpose of the study.
Refsgaard, 1997). The criteria should not be established based on model results. Heatwole et al. (1991) suggested that good hydrologic assessment models should be accurate to within a factor of 2 of observed values if model parameters are measured on-site or calibrated. This guideline was selected by the recent model developer for ANSWERS-2000 (Bouraoui, 1994; Byne, 2000; Zeckoski, 2002). Criteria established by HSPEXP (Lumb et al., 1994) have been used for the hydrologic calibration of HSPF. The criteria consider seasonal variations by considering error in total volume, error in low flow recession, error in 50% lowest flows, error in 10% highest flows, error in storm volumes, seasonal volume error, and summer storm volume error. Less than 10% error in total volume is recommended in the criteria (Lumb et al., 1994). Ramanarayanan and others (1997) suggested greater than 0.6 and 0.5 values for the coefficient of determination ($R^2$) and Nash-Sutcliffe efficiency index (E) values for the acceptable or satisfactory model prediction, respectively. These values are not absolute but should be adjustable based on the full understanding of monitored data, model characteristics, and purpose of the research. For example, hydrologic performance of a model could be evaluated using both graphical comparison and statistical tests based on sufficient observed data, while accurate statistical evaluation of model performance for water quality components is often restricted by inadequate frequency of observed data. Even though calibration is conducted, criteria that are decided before the model run cannot always be satisfied. If the criteria cannot be met, a justifying explanation should be given.

The overall goal of this chapter is to validate the newly developed model components and to evaluate the capability of DANSAT to simulate temporal and spatial changes in BMPs by applying the model to actual watersheds in Virginia using the following specific objective:

1) to discuss the procedures for defining the conceptual model and for preparing spatially and temporally changing input parameters; 2) to evaluate the predictive capability of DANSAT to consider temporal changes in agricultural BMPs at the watershed scale; 3) to evaluate how DANSAT is able to appropriately simulate spatial distributions of sub-watershed with a minimum calibration; 4) to evaluate the linked approach for considering interaction between surface water and ground water; and finally, 5) to discuss the strengths and weaknesses of the model.

**Methods**

**Evaluation Strategy**

In addition to the common purpose of calibration and validation processes mentioned previously, another purpose of the calibration and validation in this study is to find possible errors in model
algorithms, solution techniques, and equations. It is necessary to confirm that model equations appropriately simulate real world conditions and that the employed numerical techniques accurately solve the model equation. If the algorithms and solution techniques are not appropriate to simulate the real world conditions or if the equations in the code contain critical errors, the simulated results will not agree with the observed data.

Specific situations were considered to isolate the relevant model components and narrow down the scope of analysis. The responses of the model to the specific situation were investigated by comparing differences between model predictions and field observation. Model verification was conducted by considering possible errors in observed data and uncertainties in model input parameters for each specific situation. The four steps of verification procedures and relevant components as well as data sources are shown in Figure 5.1.

![Figure 5.1. The four steps of model verification procedure used in DANSET.](image)

First, the model was applied to a field plot in the Nomini Creek (NC) watershed located in the Coastal Plain region of Virginia to validate most of the cell components. The cell components include evapotranspiration, infiltration, percolation, interception, rill and interrill sediment detachment, pesticide application, pesticide degradation, pesticide equilibrium, and pesticide leaching. Routing related components for simulating overland flow and sediment and pesticide
movement in runoff were treated as cell components because only one cell was used for representing the plot.

Secondly, the watershed-scale components, except for the baseflow component, were validated using the observed data from Owl Run watershed. The validated components include the overland flow routing component, channel flow routing component, and interflow routing component. The Owl Run watershed was selected because surface runoff dominates the total stream flow in the watershed. Only the hydrology component and sediment component were validated due to the lack of pesticide observed data. The internal validation approach, in which the model is first calibrated to the overall watershed and then validated on subwatersheds, was selected for this study (Ambroise et al., 1995). At first, sensitive parameters are calibrated at the watershed outlet for the simulation period (1990-1993) by excluding pre-BMP and BMP implementation periods. Then two subwatersheds are used for the internal validation over the same simulation period without further calibration or with minimum calibration. The internal validation approach was selected to evaluate how the model simulates internal consistency of spatially distributed results on sub-watersheds according to the spatial variation of watershed characteristics without any intensive calibration of data sets from the sub-watersheds.

Finally, both the integrated baseflow component and the linked interface component for the interactions between surface water (SW) and ground water (GW) were evaluated on the Nomini Creek (NC) watershed. Baseflow was estimated by two different approaches: the integrated ground water approach and the linked ground water approach, which were described in chapter 3 and 4. The NC watershed is an ideal watershed for evaluating baseflow related components because over 85 percent of total runoff in the watershed is due to ground water discharge. In the integrated ground water approach, split-sample validation process is used to evaluate how the model simulates the temporal changes in land use at the watershed scale. DANSAT was calibrated using the observed data from pre-BMP implementation period (1987 through 1990) and validated on post-BMP period (1991 through 1992). The hydrology, sediment, and pesticide components were evaluated on the NC watershed.

For the linked approach, the performance can be evaluated using observed data from the surface and saturated zone. For example, both runoff discharges at watershed outlets and spatial distribution of ground water table elevation can be used for the validation of the model. The advantages of multi-criteria calibration is that increased calibration target from both surface and ground water enhances the reliability of model results. The pesticide components were not
simulated in the linked application due to lack of parameter information for the MT3D simulation, even though the code for the linked simulation of pesticide components (interface code for the interaction between DANSAT and MT3D) was incorporated in the newly developed model.

**Quantitative Model Performance Measures**

Both qualitative and quantitative measures were used for comparison of observed data and predicted values. Graphical analysis such as scatter-plot and time-series plot were used to instinctively identify general trends, potential sources of error, and differences between measured and predicted values. Percent error (Err) was selected as a general quantitative measure for the comparison of observed and simulated total runoff, sediment load, and pesticide load for the entire simulation period. Normalized Objective Function (Pennell et al., 1990) and Nash-Sutcliffe Efficiency Index (Nash and Sutcliffe, 1970) were selected as an error statistics and a correlation related statistics for the daily and monthly output, respectively. Normalized Objective Function (NOF) is a better criterion than the Root Mean Square Error (RMSE) for the comparison of model performance among subwatersheds because RMSE is only normalized with the number of observations, but NOF is normalized for the overall mean, as well. Likewise, Nash-Sutcliffe Coefficient of Efficiency (E) was suggested as a better criterion for measuring the fit between observed and simulated data compared to the Coefficient of Determination ($R^2$) because E is sensitive to differences in the observed and simulated means and variances (Legates and McCabe, 1999a).

NOF and Index of Agreement (D) (Willmott, 1981) were respectively selected as an error statistics and a correlation related statistics for comparison of the vertical distribution of soil water content and pesticide amount in soil profile in the field-scale validation. Mean Normalized Objective Function (NOF$_{avg}$) and Mean Index of Agreement (D$_{avg}$) were used for comparison of overall performance of the model for simulating the movement of infiltrated water and applied pesticide in soil profile. Nash-Sutcliffe Efficiency Index (E) is negative in some cases, while the index of agreement varies between 0 and 1. A value of 1 indicates perfect fit and smaller values indicate less agreement between the observed and simulated data in both Nash-Sutcliffe Efficiency Index (E) and Index of Agreement (D). Index of Agreement (D) was selected as correlation related criteria for subsurface comparison in field-scale validation instead of Nash-Sutcliffe Efficiency Index (E) because the range of index of agreement (0 to 1) seems more reasonable for the averaging procedure to calculate overall performance. The overall objectives of model calibration are 1) to decrease the error statistics such as NOF and NOF$_{avg}$ and 2) to increase
the correlation related statistics such as E, D, and Davg. The criteria used in this research were calculated using the following relationships:

\[ Err = \left( \frac{P_{tot} - O_{tot}}{O_{tot}} \right) \times 100 \] (5.1)

Where, \( Err \) = percent error of a prediction (%), \( P_{tot} \) = simulated total for the entire simulation period, and \( O_{tot} \) = observed total for the entire simulation period.

\[ NOF = \frac{\text{RMSE}}{\bar{O}} = \sqrt{\frac{1}{t} \sum_{i=1}^{t} (O_i - P_i)^2} \] (5.2)

\[ NOF_{avg} = \frac{1}{n} \sum_{j=1}^{n} NOF_j \] (5.3)

Where, \( NOF \) = Normalized objective function, \( O_i \) = observed value of an event i, \( P_i \) = predicted value of an event i, \( t \) = number of observed values, \( \bar{o} \) = average observed value, \( NOF_{avg} \) = mean normalized objective function, and \( n \) = number of calculated normalized objective function.

\[ E = 1 - \frac{\sum_{i=1}^{t} (O_i - P_i)^2}{\sum_{i=1}^{t} (O_i - \bar{O})^2} \] (5.4)

Where, \( E \) = Nash-Sutcliffe Efficiency Index, \( O_i \) = observed value of an event i, \( P_i \) = predicted value of an event i, \( \bar{o} \) = average observed value.

\[ D = 1.0 - \frac{\sum_{i=1}^{t} (O_i - P_i)^2}{\sum_{i=1}^{t} (|P_i - \bar{O}| + |O_i - \bar{O}|)^2} \] (5.5)

\[ D_{avg} = \frac{1}{n} \sum_{j=1}^{n} D_j \] (5.6)
Where, $D$ = index of agreement, $O_i$ = observed value of an event $i$, $P_i$ = predicted value of an event $i$, $t$ = number of observed values, $\bar{O}$ = average observed value, $n$ = number of calculated index of agreement, and $D_{avg}$ = average index of agreement.

Average observed value is calculated by:

$$\bar{O} = \frac{1}{t} \sum_{i=1}^{t} O_i$$  \hspace{1cm} (5.7)

Multiple criteria based on different time-scales, including simulation total, monthly criteria, and daily criteria were selected for evaluating the performance of DANSAT in both field-scale and watershed-scale validations. Table 5.1 and Table 5.2 list a summary of the selected quantitative criteria for the field-scale and watershed-scale validations, respectively. As mentioned previously, subsurface components were validated by comparing the observed and simulated vertical distribution of soil water and pesticide amount in field-scale validation, while surface components were validated on the smallest temporal-scale by comparing the shape of single hydrograph and sedigraph for each selected storm event in watershed-scale validation.

**Table 5.1. Selected quantitative criteria for field-scale validation of DANSAT.**

<table>
<thead>
<tr>
<th>Temporal scale</th>
<th>Hydrology</th>
<th>Components</th>
<th>Sediment</th>
<th>Pesticide</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Surface</td>
<td>Subsurface</td>
<td>Surface</td>
<td>Subsurface</td>
</tr>
<tr>
<td>Simulation total</td>
<td>Err</td>
<td>Err</td>
<td>Err</td>
<td>Err</td>
</tr>
<tr>
<td>Monthly</td>
<td>NOF, E</td>
<td>NOF, E</td>
<td>NOF, E</td>
<td>NOF, E</td>
</tr>
<tr>
<td>Daily</td>
<td>NOF, E</td>
<td>NOF, E</td>
<td>NOF, E</td>
<td>NOF, E</td>
</tr>
<tr>
<td>Observed date</td>
<td>NOF, NOFavg, D, D_{avg}</td>
<td>NOF, NOF_{avg}, D, D_{avg}</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Note: criteria were calculated based on daily pesticide load only when samples existed.
- Err: percent error
- NOF: normalized objective function
- E: Nash-Sutcliffe model efficiency
- D: index of agreement
- NOF_{avg}: mean normalized objective function
- D_{avg}: average index of agreement
Table 5.2. Selected qualitative and quantitative criteria for the watershed-scale validations of DANSET.

<table>
<thead>
<tr>
<th>Temporal scale</th>
<th>Hydrology</th>
<th>Components</th>
<th>Sediment</th>
<th>Pesticide</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simulation total</td>
<td>Err</td>
<td>Err</td>
<td>Err</td>
<td></td>
</tr>
<tr>
<td>Monthly</td>
<td>NOF, E</td>
<td>NOF, E</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Daily</td>
<td>NOF, E</td>
<td>NOF†, E†</td>
<td>NOF†, E†</td>
<td></td>
</tr>
</tbody>
</table>

- †: criteria was calculated based on estimated daily sediment or pesticide load only when samples exist.
- Err: percent error
- NOF: normalized objective function
- E: Nash-Sutcliffe model efficiency
- Davg: average index of agreement

In the watershed-scale validation, quantitative criteria for different time-scale should be selected considering the quality of data sets, which are used for calculating the criteria. The data sets for calculating criteria can be measured values or estimated values based on the original data set. If the used data set for calculating criterion is derived from the other original observed data set, the selected method for manipulating original data is an important factor to be considered. The used data sets for both Owl Run and Nomini Creek watersheds are estimated values, which were derived based on original data set of HAS format (Carr et al., 1988). For the hydrology component, the smallest time-step for criterion calculation is one day, but the time-step of original observed data in HAS is smaller than one day. Moreover, observed data exist for every simulation day. As a result, the quality of daily runoff data for both watersheds is high and reliable. For the sediment data, several water quality samples were collected during a storm event using the auto sampler and a grab sample was collected during baseflow based on pre-defined time-step, which is greater than a week. If there were no samples in a specific day, daily sediment load was interpolated based on the existing observed data around the sampled day. As a result, interpolated daily sediment loads may contain higher error, and the estimated values can be changed according to the selected interpolating method. Daily sediment load was selected for calculating the criteria (NOF and E) in Table 5.2 only when samples existed in a given day. Pesticide samples were collected less frequently compared to sediment samples. As a result, only daily NOF and E and total percent error (Err) were calculated based on daily pesticide loads, which are directly estimated using observed data without interpolation.
Plot-scale Evaluation

Study Area
A plot-scale monitoring study was conducted to characterize the fate and transport of atrazine, metolachlor, and bromide using two filed plots in the Nomini Creek watershed located in the Coastal Plain region of Virginia (Heatwole et al., 1992). One plot (QNB) was plowed and disked and the other plot (QNA) was remained no-till with a heavy soybean-wheat residue before corn was planted and pesticides were applied. Corn was planted on April 23 and harvested on October 9, 1990. Atrazine, metolachlor, and bromide (tracer) were applied on April 25, 1990. Forty hours after pesticide application, 37 mm of rainfall was applied to the plots in one hour using a rainfall simulator. Water quantity and quality in surface runoff were measured during the five-month corn growing season, from April 25 (day 115) to September 29 (day 272). The soil is a Suffolk sandy loam, characterized as deep and well-drained. The soil cores were sampled up to 1.5 m depth, 6 times after pesticide application, on 118, 128, 145, 167, 209, and 272 Julian days.

DANSAT has limitations when applied to no-till plot where preferential flows might be dominant. Therefore, DANSAT was applied to the tilled plot (QNB) to validate cell-based components. Figure 5.2 shows the location and layout of the plot. The tilled plot (18m x 27m) was treated as one cell in DANSAT considering only the overland flow component, because it was assumed that the area of the plot is small enough to ignore interflow, baseflow, and channel flow. Simulation of DANSAT requires the initial values, which are difficult to measure. The model was simulated from January 1 to December 31, 1990, to minimize the impacts of initial values on hydrology and water quality before the starting day of sampling. Validation process using a different period of data set was not considered because of the short monitored period of less than 1 year. Simulated water and pesticide movement in the soil profile as well as surface hydrology, sediment yields, and pesticide loads were compared with the observed data.
Development of Input Parameters

Spatial distribution of crop rotations, soil types, and topographic parameters were ignored because the tilled plot was considered as one cell in the simulation. Among parameters in the cell data block, values of surface slope, Manning’s roughness coefficient, surface elevation, effective depth of interaction, and average depth to the ground water table were necessary for the one cell simulation. A 0.01 m effective depth of interaction for overland element was assumed as the default value based on the result by Leonard and others (1979). Surface slope and surface elevation were 2.0% and 34.3m, respectively, based on survey and 30 m DEM. The Manning’s roughness coefficient was assumed to be 0.08 based on Kilgore’s research (1997). Tillage related input parameters were estimated using the information for the Chisel Plow and Disk applications within the WEPP database. Tillage database for WEPP was imported to the user interface for DANSAT and parameter values from WEPP database were considered as default values in DANSAT. Crop and pesticide parameters were also imported to the user interface for DANSAT based on WEPP and GLEAMS database, respectively. The physically-based parameters for tillage, crop, and pesticide characteristics used in the simulations were explained in Chapter 3. Pesticide application rates used in the simulation were measured in the plot using filter papers (Heatwole et al., 1992). Atrazine was applied to the plots on April 25, 1990, at the application
rate of 2.24kg/ha, with an application efficiency of 0.55. The corresponding values for Metolachlor were 1.69kg/ha and 0.40, respectively. Surface application method with 0.01m of application depth was selected for both atrazine and metolachlor in DANSAT. Temporal changes of crops, tillage, and pesticide application were combined in the rotation data block. Figure 5.3 shows the structure and description of rotation data block.

![Application Type Diagram](image)

**Figure 5.3.** Structure and description of the rotation data block of main input file for plot-scale application.

Five soil particle size classes were defined and used in this research based on the USDA soil classification. The selected five particle classes include clay (<0.002 mm), silt (0.002-0.05 mm), very fine sand (0.05-0.1 mm), fine and medium sand (0.1-0.5 mm), and coarse and very coarse sand (0.5-0.2 mm). Soil aggregates were not considered in the model even though soil aggregates are probably an important soil property governing soil erodibility on soil surface and transportation in runoff. The breakdown of soil aggregates by raindrop may affect infiltration and soil detachment by surface sealing. Thus, the model may over-predict the sediment loads in clay soil by underestimating the possible sediment deposition due to the increased weight of aggregates. The main input file for the field application is included in Appendix C. The file shows the structure of main input file and the selected parameters for the field-scale application.

Break-point rainfall data from PN5 rain gauge station (Figure 5.2), which is the nearest station from the plot, was used for the simulation because rainfall data recorded at the LN3 weather station, which is approximately 500 m from the plot, were not complete. Only daily rainfall amount values measured at LN3 are available from the previous reports (Zacharias, 1998). Total
amount of rainfall at PN5 was adjusted to be the same as the total rainfall at LN3 without considering temporal variations in rainfall intensity. Other meteorological data such as solar radiation and air temperature data were also obtained from PN5 instead of LN3.

Parameters impacting the infiltration process were selected for the calibration of runoff. Green-Ampt infiltration calculation can be affected by two major factors. One is the magnitude of effective hydraulic conductivity ($K_e$), and the other is the soil moisture content in a representative soil layer. Selected parameters affecting $K_e$ are soil texture (clay silt and sand contents) and rainfall adjustment factor ($\text{Coeff}_{\text{rain}}$ in equation 3.110). An increase or decrease in the soil moisture content changes overall infiltration amount throughout the simulation period without considering temporal variations, while $\text{Coeff}_{\text{rain}}$ is used to control temporal variations in $K_e$, based on the rainfall amount. Selected parameters affecting soil moisture content are effective soil depth for infiltration calculation ($\text{InfilDep}$) and saturated hydraulic conductivity ($K_s$) of each soil layer within the soil profile. Increased $K_s$ values increases percolation, reduces soil moisture content in soil layers, and consequently increases the infiltration.

For the calibration of sediment yield, parameters affecting sediment detachment in overland areas are selected because channel is not considered in the field-scale validation. Rill space ($R_{\text{space}}$) has a significant impact on total sediment yields during the simulation period. Reduced rill space increases the number of rills in a cell and reduces the flow rate per rill since the total flow rate remains constant. As a result, sediment detachments are reduced with the decrease in rill space. Other sensitive parameters for sediment detachment in overland areas are rill and interrill erodibilities. However, it was difficult to calibrate temporal variation of sediment yield based on the variable approach for estimating the rill and interrill erodibility. Thus, the constant approach, which uses a constant value without considering the temporal impacts of BMPs such as tillage, was selected for estimating the rill and interrill erodibilities. After calibrating the hydrology and sediment yields, parameters defining pesticide characteristics were used for pesticide calibration. Selected parameters included the partitioning coefficient ($K_{oc}$) and half-life of pesticide. A best set of parameters was decided for satisfying hydrology and water quality from both surface and subsurface areas. Increased runoff and pesticide yields in surface runoff decreases soil moisture contents and pesticide amount reaching the lower soil layers.
Results and Discussion

Hydrology

Observed and predicted daily and monthly runoff amounts over the monitoring periods, along with performance criteria, are given in Table 5.3. The 348.49 mm of rainfall amounts from events on May 26 (154.52 mm), May 29 (104.14 mm), and August 23 (89.83 mm) resulted in 129.73 mm and 157.93 mm of observed and simulated total runoff, respectively. The runoff from the rainfall event on May 29 was slightly underestimated with -2.2% error, while runoff events of May 26 and August 23 were overestimated by 29.2% and 57.7% error, respectively. The differences in daily total runoff for the three significant rainfall events can possibly be attributed to the spatial distribution of rainfall amount and intensity within the watershed. As mentioned, break-point rainfall data from the nearest rain gauge (PN5) were used for the simulation instead of that recorded by the rain gauge (LN3) closest to the plot used by Zacharias (1998). For example, the measured total rainfall amounts on May 26 were 155 mm and 104 mm in PN5 and LN3, respectively. Overall, the total runoff during the monitoring period was well simulated by the model with -1.52% of relative error. The monthly and daily Nash-Sutcliffe efficiency indexes (E) were 0.87 and 0.97, respectively. Both values are greater than 0.5, which is the suggested lower range value for acceptable model prediction by Ramanarayanan and others (1997). The overall result (higher EI values and low total percent error) shows that DANSAT reasonably predicts surface runoff in the field plots with calibration. Figure 5.4 shows the time-series of observed and simulated daily runoff. Scatter-plot of observed and simulated monthly runoff is shown in Figure 5.5.
Table 5.3. Observed and predicted daily and monthly runoff over the monitoring period from QNB plot.

<table>
<thead>
<tr>
<th>Month</th>
<th>Date</th>
<th>Rainfall (mm)</th>
<th>Daily runoff</th>
<th>Monthly runoff</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Observed</td>
<td>Simulated</td>
</tr>
<tr>
<td>April</td>
<td>4/27</td>
<td>36.48</td>
<td>0.37</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>4/29</td>
<td>20.23</td>
<td>0.19</td>
<td>0.00</td>
</tr>
<tr>
<td>May</td>
<td>5/4</td>
<td>16.38</td>
<td>6.38</td>
<td>3.96</td>
</tr>
<tr>
<td></td>
<td>5/5</td>
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<td>0.00</td>
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<tr>
<td></td>
<td>5/9</td>
<td>2.54</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>5/10</td>
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<td>14.88</td>
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</tr>
<tr>
<td></td>
<td>5/21</td>
<td>5.82</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>5/22</td>
<td>2.52</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>5/25</td>
<td>0.50</td>
<td>0.00</td>
<td>0.00</td>
</tr>
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<td></td>
<td>5/26</td>
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<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>5/29</td>
<td>104.14</td>
<td>55.43</td>
<td>54.19</td>
</tr>
<tr>
<td>June</td>
<td>6/3</td>
<td>1.51</td>
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<td>0.00</td>
</tr>
<tr>
<td></td>
<td>6/9</td>
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<td>7.23</td>
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<td>July</td>
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</tr>
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<td>7/29</td>
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<td>0.00</td>
</tr>
<tr>
<td>August</td>
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<td>3.51</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
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<td>0.45</td>
<td>0.00</td>
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<td>14.85</td>
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<tr>
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<td>1.51</td>
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<td>0.00</td>
</tr>
<tr>
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<td>8/20</td>
<td>8.85</td>
<td>0.00</td>
<td>0.00</td>
</tr>
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<td></td>
<td>8/22</td>
<td>13.19</td>
<td>0.00</td>
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</tr>
<tr>
<td></td>
<td>8/23</td>
<td>89.83</td>
<td>27.21</td>
<td>42.90</td>
</tr>
<tr>
<td></td>
<td>8/24</td>
<td>4.04</td>
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<td>0.00</td>
</tr>
<tr>
<td></td>
<td>8/29</td>
<td>27.94</td>
<td>6.76</td>
<td>7.76</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>736.99</td>
<td>172.67</td>
<td>170.04</td>
</tr>
<tr>
<td>Percent Error</td>
<td></td>
<td>-1.52</td>
<td>-1.52</td>
<td>-1.52</td>
</tr>
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<td></td>
<td>0.93</td>
<td>0.24</td>
<td>0.24</td>
</tr>
<tr>
<td>E</td>
<td></td>
<td>0.87</td>
<td>0.97</td>
<td>0.97</td>
</tr>
</tbody>
</table>

- NOF: normalized objective function (unit is mm/watershed)
- E: Nash-Sutcliffe model efficiency
Figure 5.4. Time-series of observed and simulated daily runoff for QNB plot.

Figure 5.5. Scatter-plot of observed and simulated monthly runoff for QNB plot.
The amount of infiltrated water, which is estimated after subtracting the interception by plant from the precipitation, was estimated using subsurface components of DANSAT. The observed and simulated soil water contents in soil layers (0 – 0.9 m) on the field sampling dates are shown in Table 5.4, along with normalized objective function (NOF) and index of agreement (D). The index of agreement (D), which is calculated based on the depth-wise distribution of soil water content on each sampling date, shows that DANSAT reasonably predicted the movement of infiltrated water through the soil profile on days 128, 145, and 209, with the minimum value of 0.75 on day 209. The NOF values increased as Julian day increased, ranging from 0.2 on day 118 to 0.78 on day 272. The poorest prediction occurred on day 272, with 0.78 and 0.08 values of NOF and D values, respectively. The mean normalized objective function (NOF$_\text{avg}$) and mean index of agreement (D$_\text{avg}$) were 0.35 and 0.57, respectively. NOF$_\text{avg}$ and D$_\text{avg}$ values, which are average of NOF and D values on sampling dates, were used for comparison of overall performance of the model for simulating the movement of infiltrated water in soil profile. Better model performance can be expected by decreases in NOF$_\text{avg}$ (error statistics) and increases in D$_\text{avg}$ (correlation related statistics) values. NOF$_\text{avg}$ was decreased to 0.26 and D$_\text{avg}$ was increased to 0.67 when excluding the poorest simulation on day 272. The depth-wise distributions of observed and simulated soil water content in each of the soil layers on the field sampling dates (118, 128, 145, 167, 209, and 272) are shown in Figure 5.6. Vertical distributions on days 118, 128, 145 and 167 showed a similar trend to each other with the overestimation occurring at 0 – 0.6 m soil depth. The biggest difference in observed and simulated soil water content on day 209 occurred within the 0.15 - 0.3 m of soil layer depth, while the biggest difference in observed and simulated soil water content on day 272 occurred within the deeper soil layers (0.3-0.9 m).
Table 5.4. The depth-wise distributions of observed and simulated soil water content in soil layers (0 - 0.9m) on the field sampling dates for QNB plot.

<table>
<thead>
<tr>
<th>Date (Julian)</th>
<th>Depth (cm)</th>
<th>Soil water content</th>
<th>NOF</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Observed</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Simulated</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4/28 (118)</td>
<td>0-15</td>
<td>17.7</td>
<td>23.8</td>
<td></td>
</tr>
<tr>
<td></td>
<td>15-30</td>
<td>23.5</td>
<td>27.1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>30-45</td>
<td>24.0</td>
<td>26.5</td>
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</tr>
<tr>
<td></td>
<td>45-60</td>
<td>22.9</td>
<td>22.6</td>
<td></td>
</tr>
<tr>
<td></td>
<td>60-90</td>
<td>21.0</td>
<td>15.2</td>
<td></td>
</tr>
<tr>
<td>5/8 (128)</td>
<td>0-15</td>
<td>12.9</td>
<td>15.9</td>
<td></td>
</tr>
<tr>
<td></td>
<td>15-30</td>
<td>19.8</td>
<td>26.3</td>
<td></td>
</tr>
<tr>
<td></td>
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<td>22.6</td>
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<td>0.21</td>
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<td>45-60</td>
<td>22.8</td>
<td>24.8</td>
<td></td>
</tr>
<tr>
<td></td>
<td>60-90</td>
<td>17.4</td>
<td>17.1</td>
<td></td>
</tr>
<tr>
<td>5/25 (145)</td>
<td>0-15</td>
<td>11.3</td>
<td>14.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>15-30</td>
<td>18.4</td>
<td>24.6</td>
<td></td>
</tr>
<tr>
<td></td>
<td>30-45</td>
<td>21.5</td>
<td>26.6</td>
<td>0.22</td>
</tr>
<tr>
<td></td>
<td>45-60</td>
<td>21.3</td>
<td>23.9</td>
<td></td>
</tr>
<tr>
<td></td>
<td>60-90</td>
<td>17.9</td>
<td>16.6</td>
<td></td>
</tr>
<tr>
<td>6/16 (167)</td>
<td>0-15</td>
<td>13.0</td>
<td>15.9</td>
<td></td>
</tr>
<tr>
<td></td>
<td>15-30</td>
<td>15.6</td>
<td>22.5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>30-45</td>
<td>17.7</td>
<td>26.3</td>
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<td>19.6</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>60-90</td>
<td>16.9</td>
<td>17.0</td>
<td></td>
</tr>
<tr>
<td>7/28 (209)</td>
<td>0-15</td>
<td>4.8</td>
<td>5.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>15-30</td>
<td>8.5</td>
<td>1.2</td>
<td></td>
</tr>
<tr>
<td></td>
<td>30-45</td>
<td>11.1</td>
<td>10.3</td>
<td>0.35</td>
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<td>12.4</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>60-90</td>
<td>11.3</td>
<td>9.5</td>
<td></td>
</tr>
<tr>
<td>9/29 (272)</td>
<td>0-15</td>
<td>11.3</td>
<td>15.1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>15-30</td>
<td>16.8</td>
<td>13.0</td>
<td></td>
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<tr>
<td></td>
<td>30-45</td>
<td>20.1</td>
<td>1.2</td>
<td>0.78</td>
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<td>45-60</td>
<td>21.5</td>
<td>3.3</td>
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<td>60-90</td>
<td>18.6</td>
<td>3.4</td>
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</tr>
<tr>
<td>Mean</td>
<td></td>
<td></td>
<td>0.35</td>
<td>0.57</td>
</tr>
</tbody>
</table>

- NOF: normalized objective function (unit is mm/watershed)
- D: Index of agreement
Figure 5.6. The depth-wise distributions of observed and simulated soil water content in soil layers (0 - 0.9m) on the field sampling dates for QNB plot: a) day 118, b) day 128, c) day 145, d) day 167, e) day 209 and f) day 272.
The observed and simulated depth-averaged soil water contents in the top 0.9 m soil depth on various sampling dates, along with measured daily rainfalls, are shown in Figure 5.7. The predicted daily fluctuations in the depth-average soil water content are also shown in Figure 5.7. Depth-average soil water content increased rapidly after rainfall events on May 26 and May 29 and decreased during the growing season. Predicted values were lower than the observed average values on all dates except on day 272. The simulated depth-average soil water contents on all field sampling dates were close to the observed ones. Overall, the movement of infiltrated water through soil layers was well predicted by the plot-scale subsurface components of DANSAT.

![Figure 5.7. Observed and simulated depth-averaged soil water content in the top 0.9 m soil depth on sampling dates for QNB plot.](image)

**Sediment**

The observed and predicted daily and monthly sediment loads during the monitoring period are given in Table 5.5. Figure 5.8 shows the time-series of observed and simulated daily sediment load, while Figure 5.9 shows the scatter-plot of observed and simulated monthly sediment load. As mentioned earlier, variable erodibility approach has difficulty in simulating temporal variation of sediment yield. Results were obtained based on the constant erodibility approach in which rill and interrill erodibility parameters do not change during simulation period as user input.
The four rainfall events on May 26, May 29, August 23, and August 29, resulted in 846 kg/ha of observed sediment yield (87% of total sediment yields for the monitoring period), while these rainfall events resulted in 51.1% of total rainfall and 79% of total runoff amounts during the simulation period (Table 5.5). The largest sediment yield (384.2 kg/ha) resulted (39.5% of total sediment yield) from the storm that occurred on August 23, which only produced 15.8% of total surface runoff. DANSAT underestimated the sediment yield and overestimated surface runoff volume from the August 23 storm with -22.8% and 57.7% errors, respectively. Total sediment load during the monitoring period was well reproduced by the model with only 2.90% in relative error. Monthly sediment yields were overestimated during May and underestimated during August with 84.7% and -40.7% of relative error, respectively. As a result, monthly and daily Nash-Sutcliffe efficiency indexes (E) were 0.48 and 0.38, respectively. Both values are smaller than the lower range value for acceptable model prediction suggested by Ramanarayanan et al. (1997). The overall result shows that DANSAT needs to realistically consider temporal changes in erodibility factors by considering characteristics of rainfall and surface cover, which could be impacted by various management practices.
Table 5.5. Observed and predicted daily and monthly sediment yield over the monitoring period for QNB plot.

<table>
<thead>
<tr>
<th>Month</th>
<th>Date</th>
<th>Rainfall (mm)</th>
<th>Daily sediment loss (kg/ha)</th>
<th>Monthly sediment loss (kg/ha)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Observed</td>
<td>Simulated</td>
</tr>
<tr>
<td>April</td>
<td>4/27</td>
<td>36.48</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>4/29</td>
<td>20.23</td>
<td>2.5</td>
<td>0.0</td>
</tr>
<tr>
<td>May</td>
<td>5/4</td>
<td>16.38</td>
<td>23.0</td>
<td>27.3</td>
</tr>
<tr>
<td></td>
<td>5/5</td>
<td>3.52</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>5/9</td>
<td>2.54</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>5/10</td>
<td>42.90</td>
<td>68.5</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>5/21</td>
<td>5.82</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>5/22</td>
<td>2.52</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>5/25</td>
<td>0.50</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>5/26</td>
<td>154.52</td>
<td>73.0</td>
<td>375.0</td>
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<td></td>
<td>5/27</td>
<td>4.73</td>
<td>0.0</td>
<td>0.0</td>
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<tr>
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<td>5/28</td>
<td>6.53</td>
<td>0.0</td>
<td>0.0</td>
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<td></td>
<td>5/29</td>
<td>104.14</td>
<td>188.5</td>
<td>249.5</td>
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<tr>
<td>June</td>
<td>6/3</td>
<td>1.51</td>
<td>0.0</td>
<td>0.0</td>
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<tr>
<td></td>
<td>6/9</td>
<td>4.79</td>
<td>0.6</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>6/15</td>
<td>22.11</td>
<td>8.0</td>
<td>0.0</td>
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<td></td>
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</tr>
<tr>
<td></td>
<td>6/27</td>
<td>7.23</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>July</td>
<td>7/1</td>
<td>12.82</td>
<td>2.1</td>
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<td></td>
<td>7/14</td>
<td>10.10</td>
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<td></td>
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<td>3.74</td>
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<td></td>
<td>7/21</td>
<td>20.39</td>
<td>12.6</td>
<td>0.3</td>
</tr>
<tr>
<td></td>
<td>7/28</td>
<td>0.50</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>7/29</td>
<td>5.01</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>August</td>
<td>8/6</td>
<td>3.51</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>8/9</td>
<td>40.00</td>
<td>1.2</td>
<td>0.0</td>
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<tr>
<td></td>
<td>8/10</td>
<td>14.85</td>
<td>1.7</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>8/11</td>
<td>1.51</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>8/20</td>
<td>8.85</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>8/22</td>
<td>13.19</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>8/23</td>
<td>89.83</td>
<td>384.2</td>
<td>296.6</td>
</tr>
<tr>
<td></td>
<td>8/24</td>
<td>4.04</td>
<td>1.5</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>8/29</td>
<td>27.94</td>
<td>199.9</td>
<td>52.4</td>
</tr>
<tr>
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<td></td>
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<td>972.8</td>
<td>1001.0</td>
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<tr>
<td>Percent Error</td>
<td></td>
<td>2.90</td>
<td>2.90</td>
<td></td>
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<tr>
<td>NOF</td>
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<tr>
<td>E</td>
<td>0.38</td>
<td>0.48</td>
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</tr>
</tbody>
</table>

- NOF: normalized objective function (unit is kg/ha)
- E: Nash-Sutcliffe model efficient
Figure 5.8. Time-series of observed and simulated daily sediment load for QNB plot.

Figure 5.9. Scatter-plot of observed and simulated monthly sediment load for QNB plot.
**Pesticides**

Observed and predicted daily and monthly atrazine loads over the monitoring periods are given in Table 5.6. Over 96% of total atrazine in runoff occurred during May. The highest atrazine mass in runoff was expected during an artificial application of 36.5 mm of rainfall, forty hours after pesticide was applied to the plots. However, the highest atrazine mass in runoff was measured after 16.38 mm of natural rainfall occurred on May 4. The observed runoff and pesticide loss on April 27 was 0.37 mm and 0.26 g/ha, while the corresponding figures for May 4 were 6.38 mm and 6.34 g/ha, respectively. The smaller atrazine loss measured on April 27, compared with May 4, could be attributed to the smaller runoff volume resulting from the April 27 storm. During May, atrazine losses were due to major storm events on May 4, May 10, May 26, and May 29. Atrazine masses in runoff on May 26 and May 29 were smaller than those on May 4 and May 10, even though both rainfall and runoff amounts were greater on May 26 and May 29.

Total atrazine losses were predicted fairly well by DANSAT with a total error of -2.75%. Atrazine loss during the storm on May 4 was overestimated by the model (80.3% error), while the losses were underestimated during the remaining storm events, which occurred on May 10, May 26, and May 29. Figure 5.10 shows a time-series comparison of observed and simulated daily atrazine mass in runoff during the simulation period. DANSAT predicted 96.9% of the simulated total atrazine loss during the first major storm after the atrazine application. Rate of atrazine extraction by runoff should be reduced to improve the temporal trend of daily atrazine loads in Figure 5.10. Decreases in daily atrazine load on May 4 and increase in atrazine load on May 10 will improve the simulation results. Gradual extraction of atrazine by runoff could be simulated by increasing the half-life in soil (HLsoil) and partitioning coefficient (Koc) parameters in DANSAT. However, changes in HLsoil and Koc also impact the atrazine movement in the subsurface zone, which will be described in a later part of this section. Therefore, the pesticide component was calibrated by considering both pesticide in runoff and pesticide in soil layers. Figure 5.11 shows a time-series comparison of observed and simulated monthly atrazine mass in runoff. Atrazine loss in May was well simulated by the model with the monthly Nash-Sutcliffe efficiency indexes (E) of 1.0. Overall, DANSAT reasonably predicted monthly and total atrazine losses in runoff but gradual extraction of atrazine by runoff should be considered in daily simulations.
Table 5.6. Observed and predicted daily and monthly atrazine losses in runoff over the monitoring period for QNB plot.

<table>
<thead>
<tr>
<th>Month</th>
<th>Date</th>
<th>Rainfall (mm)</th>
<th>Daily atrazine loss (g/ha)</th>
<th>Monthly atrazine loss (g/ha)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Observed</td>
<td>Simulated</td>
</tr>
<tr>
<td>April</td>
<td>4/27</td>
<td>36.48</td>
<td>0.26</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>4/29</td>
<td>20.23</td>
<td>0.11</td>
<td>0.00</td>
</tr>
<tr>
<td>May</td>
<td>5/4</td>
<td>16.38</td>
<td>6.34</td>
<td>12.88</td>
</tr>
<tr>
<td></td>
<td>5/5</td>
<td>3.52</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>5/9</td>
<td>2.54</td>
<td>0.00</td>
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</tr>
<tr>
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<td>42.90</td>
<td>2.71</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>5/21</td>
<td>5.82</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>5/22</td>
<td>2.52</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>5/25</td>
<td>0.50</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
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<td>5/26</td>
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</tr>
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Percent Error

- NOF: normalized objective function (unit is g/ha)
- E: Nash-Sutcliffe model efficient
Figure 5.10. Time-series of observed and simulated daily atrazine load for QNB plot.

Figure 5.11. Monthly comparison of observed and simulated monthly atrazine load for QNB plot.
The observed and simulated atrazine amounts in soil layers on various sampling dates are shown in Table 5.7. Index of agreement (D) value, which is calculated based on the distribution of atrazine amount at different depths on each sampling date, shows that DANSAT predicts the movement of atrazine through the soil profile fairly well between the Julian days of 118 and 145, with a minimum D value of 0.89 on day 118. However, D value decreased rapidly between days 145 and 167. The poorest prediction occurred on day 167, with the largest NOF (3.67) and smallest D (0.41) values. The poor prediction on day 167 can be attributed to the underestimation of measured atrazine mass in soil layers on that day. The measured total atrazine mass on day 167 seems to be underestimated because total atrazine mass within the soil profile on day 167 is smaller than that of day 209. In Table 5.7, the total measured atrazine masses within the top 0.9m of soil depth were 11.08 g and 27.58 g on days 167 and 209, respectively. Measured total atrazine mass should be reduced as time goes on because no atrazine was applied after the first pesticide application on April 25, 1990. In addition, measured atrazine mass in top soil layers (0.01 - 0.15 m and 0.15 - 0.3 m) on day 272 seems to be overestimated because the pesticide mass in the top two soil layers increased compared to the previous sampling dates (209), with no further atrazine application between the two sampling dates. The depth distributions of measured and simulated atrazine amount in each of the soil layers on the field sampling dates are shown in Figure 5.12. Vertical distributions of simulated atrazine in soil layers on day 118, 128, and 145 showed a similar trend to the observed one. DANSAT seems to consistently overpredict peak atrazine mass within soil layers except for day 272. The mean normalized objective function (NOF_{avg}) and mean index of agreement (D_{avg}) values were 1.44 and 0.69, respectively.
Table 5.7. Observed and simulated atrazine amounts in the top 0.9 m soil depth on the field sampling dates for QNB plot.

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<tr>
<th>Date (Julian days)</th>
<th>Depth</th>
<th>Atrazine amount (g)</th>
<th>NOF</th>
<th>D</th>
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<td>Simulated</td>
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<tr>
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<td>1.82</td>
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<tr>
<td></td>
<td>90-120</td>
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Figure 5.12. The depth distributions of measured and simulated atrazine amounts in the top 0.9 m soil depth on the field sampling dates: a) day 118, b) day 128, c) day 145, d) day 167, e) day 209 and f) day 272.
Figure 5.13 shows a comparison of observed and simulated depth-averaged atrazine mass in the top 0.9 depth of the soil profile. DANSAT predicted that the depth-averaged atrazine mass consistently decreased with time, whereas the measured atrazine mass reduced very slowly between days 128 and 145 and between days 209 and 272. The slow reduction in atrazine mass between days 128 and 145 may be attributed to incomplete recovery of atrazine from the soil on day 118. The slow decrease in atrazine mass between days 209 and 272 can be attributed to the possible error in measurement of atrazine mass on day 272. A comparison of the distributions of measured atrazine amounts in various soil layers on days 209 (Figure 5.12.(e)) and 272 (Figure 5.12. (f)) shows that atrazine mass in the top soil layers increased on day 272 without any further atrazine application between these dates. As a result, depth-averaged observed atrazine mass may have been overestimated on day 272. In addition, a rapid decrease in depth-averaged atrazine mass was measured between days 128 and 145. The rapid decrease may be attributed to the leaching loss below the root zone, degradation, extraction by runoff, and plant uptake. Except for the first and last sampling dates, DANSAT accurately predicted the depth-averaged atrazine mass in the top 0.9 m depth during the growing season.

Figure 5.14 shows the simulated temporal changes in atrazine mass in several pools of pesticide components and simulated atrazine losses during the simulation period. Considered pesticide pools in DANSAT include pesticide on foliage, pesticide in soil profile, and plant uptake. Simulated pesticide losses include degradation, harvest, pesticide in runoff, and pesticide leaching below the root zone. Most of the applied atrazine disappeared through the degradation, which accounted for over 90% (41.44 g/ha) of atrazine losses predicted by DANSAT. The minor atrazine losses by runoff, plant uptake, and leaching below the root zone were negligible, accounting for a total loss of 0.64 g/ha. About 2.86 g/ha of atrazine remained in the soil profile at the end of simulation period. DANSAT simulated the atrazine mass balance correctly because the amount of pesticide applied was equal to the sum of simulated pesticide amounts in all considered pesticide pools and losses.
Figure 5.13. Measured and simulated depth-averaged atrazine mass in the top 0.9 m of the soil profile on various sampling dates.

Figure 5.14. Simulated temporal changes in atrazine mass in storage and losses during the simulation period.

Observed and predicted daily and monthly metolachlor load over the monitoring period are given in Table 5.8. Similar to the atrazine, over 95% of total metolachlor mass in runoff was lost by four major storm events during May, and the highest metolachlor mass in runoff was measured
during 16.38 mm of rainfall, which resulted in 6.38 mm of runoff and 4.42 g/ha of metolachlor on May 4.

The total metolachlor loss was well predicted by DANSAT with 4.15% error. Total measured and predicted metolachlor in runoff over the monitoring period were 11.30 g/ha and 11.34 g/ha, respectively. Metolachlor mass in runoff was overestimated on May 4 with 153% error, while the model underpredicted metolachlor mass in runoff from the remaining storm events. DANSAT predicted 98.7% of the simulated total metolachlor loss during the first major storm on May 4. Figure 5.15 shows a comparison of measured and simulated daily metolachlor mass in runoff during the simulation period. Slower extraction of metolachlor from effective depth of soil to runoff can be simulated by changing sensitive parameters, which do not impact the hydrology and sediment results. However, changes in sensitive pesticide related parameters such as half-life in soil (HLsoil) and partitioning coefficient (Koc) also impact the metolachlor movement in the soil profile. Parameter values were determined by considering metolachlor mass both in runoff and in soil profile. Figure 5.16 shows a comparison of observed and simulated monthly metolachlor mass in runoff. The metolachlor losses during the month of May were well simulated by the model, resulting in monthly Nash-Sutcliffe efficiency indexes (E) of 1.0. Overall, DANSAT reasonably predicted the monthly and total metolachlor losses in runoff. To enhance the predictive capability of DANSAT, the gradual extraction of metolachlor by runoff should be considered in the daily simulations.
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<th>Monthly metolachlor loss (g/ha)</th>
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<td></td>
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<td>Simulated</td>
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<tr>
<td></td>
<td>7/29</td>
<td>5.01</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>August</td>
<td>8/6</td>
<td>3.51</td>
<td>0.00</td>
<td>0.00</td>
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<td></td>
<td>8/9</td>
<td>40.00</td>
<td>0.00</td>
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<tr>
<td></td>
<td>8/10</td>
<td>14.85</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>8/11</td>
<td>1.51</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>8/20</td>
<td>8.85</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>8/22</td>
<td>13.19</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>8/23</td>
<td>89.83</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>8/24</td>
<td>4.04</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>8/29</td>
<td>27.94</td>
<td>0.01</td>
<td>0.00</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>736.99</td>
<td>11.30</td>
<td>11.34</td>
</tr>
</tbody>
</table>

Percent Error

| - NOF: normalized objective function (unit is g/ha)
| - E: Nash-Sutcliffe model efficient |
Figure 5.15. Time-series of observed and simulated daily metolachlor load for QNB plot.

Figure 5.16. Monthly comparison of observed and simulated Metolachlor load for QNB2 plot.
Observed and simulated metolachlor amounts in the soil profile on the sampling dates are shown in Table 5.1. Selected model performance criteria such as normalized objective function (NOF) and index of agreement (D) are also indicated. Index of agreement value for each sampling date shows that DANSAT predicts the movement of metolachlor through the soil profile well throughout the simulation period except for day 272. The index of agreement (D) value on day 272 was 0.48, while the D values on remaining sampling days were greater than 0.8. The mean normalized objective function (NOFavg) and mean index of agreement (Davg) were 1.02 and 0.82, respectively. The depth distributions of observed and simulated metolachlor amount in each of the soil layers on days 118, 128, 145, and 167 are shown in Figure 5.17. Results show that DANSAT consistently overpredicted peak metolachlor mass in the second soil layer (0.1 – 0.15 m) and underpredicted metolachlor mass in the remaining layers. The depth distributions of observed and simulated metolachlor amount on day 272 (Figure 5.17.e) showed that DANSAT failed to accurately simulate the remaining metolachlor in the second soil layer (0.1 – 0.15 m). Figure 5.18 shows a comparison of observed and simulated depth-averaged metolachlor mass in the top 0.9 m soil depth. DANSAT accurately predicted the trend in the depth-averaged metolachlor mass to constantly decrease with time. The maximum difference in depth averaged metolachlor mass occurred on day 167. Overall, the movement of metolachlor through soil profile was well predicted by the DANSAT.
Table 5.9. Measured and simulated metolachlor amounts in the top 0.9m soil profile on the field sampling dates for QNB plot.

<table>
<thead>
<tr>
<th>Date</th>
<th>Depth</th>
<th>Metolachlor amount (g)</th>
<th>NOF</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Observed</td>
<td>Simulated</td>
<td></td>
</tr>
<tr>
<td>4/28 (118)</td>
<td>0-1</td>
<td>9.25</td>
<td>15.55</td>
<td>54</td>
</tr>
<tr>
<td></td>
<td>1-15</td>
<td>28.63</td>
<td>33.82</td>
<td></td>
</tr>
<tr>
<td></td>
<td>15-30</td>
<td>2.19</td>
<td>0.27</td>
<td></td>
</tr>
<tr>
<td></td>
<td>30-45</td>
<td>0.98</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td></td>
<td>45-60</td>
<td>1.04</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td></td>
<td>60-90</td>
<td>2.05</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td></td>
<td>90-120</td>
<td>5.02</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Total</td>
<td>49.14</td>
<td>49.65</td>
<td></td>
</tr>
<tr>
<td>5/8 (128)</td>
<td>0-1</td>
<td>5.06</td>
<td>1.04</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1-15</td>
<td>25.75</td>
<td>33.33</td>
<td></td>
</tr>
<tr>
<td></td>
<td>15-30</td>
<td>2.80</td>
<td>1.34</td>
<td></td>
</tr>
<tr>
<td></td>
<td>30-45</td>
<td>2.44</td>
<td>0.13</td>
<td>62</td>
</tr>
<tr>
<td></td>
<td>45-60</td>
<td>0.92</td>
<td>0.01</td>
<td></td>
</tr>
<tr>
<td></td>
<td>60-90</td>
<td>0.91</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td></td>
<td>90-120</td>
<td>1.14</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Total</td>
<td>39.03</td>
<td>35.86</td>
<td></td>
</tr>
<tr>
<td>5/25 (145)</td>
<td>0-1</td>
<td>3.19</td>
<td>0.08</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1-15</td>
<td>12.05</td>
<td>21.83</td>
<td></td>
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<tr>
<td></td>
<td>15-30</td>
<td>1.46</td>
<td>2.53</td>
<td></td>
</tr>
<tr>
<td></td>
<td>30-45</td>
<td>0.85</td>
<td>0.45</td>
<td></td>
</tr>
<tr>
<td></td>
<td>45-60</td>
<td>1.04</td>
<td>0.07</td>
<td>28</td>
</tr>
<tr>
<td></td>
<td>60-90</td>
<td>2.28</td>
<td>0.02</td>
<td></td>
</tr>
<tr>
<td></td>
<td>90-120</td>
<td>1.14</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td></td>
<td>120-150</td>
<td>2.05</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Total</td>
<td>24.06</td>
<td>24.99</td>
<td></td>
</tr>
<tr>
<td>6/16 (167)</td>
<td>0-1</td>
<td>0.96</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1-15</td>
<td>4.86</td>
<td>7.80</td>
<td></td>
</tr>
<tr>
<td></td>
<td>15-30</td>
<td>0.97</td>
<td>4.60</td>
<td></td>
</tr>
<tr>
<td></td>
<td>30-45</td>
<td>0.61</td>
<td>1.84</td>
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<tr>
<td></td>
<td>45-60</td>
<td>0.92</td>
<td>0.62</td>
<td>33</td>
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<tr>
<td></td>
<td>60-90</td>
<td>0.68</td>
<td>0.37</td>
<td></td>
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<tr>
<td></td>
<td>90-120</td>
<td>1.14</td>
<td>0.08</td>
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<td></td>
<td>120-150</td>
<td>0.68</td>
<td>0.01</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Total</td>
<td>10.84</td>
<td>15.32</td>
<td></td>
</tr>
<tr>
<td>7/28 (209)</td>
<td>0-1</td>
<td>0.21</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1-15</td>
<td>1.88</td>
<td>1.76</td>
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<td>0.23</td>
<td>0.11</td>
<td>67</td>
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<td>60-90</td>
<td>0.91</td>
<td>0.07</td>
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<tr>
<td></td>
<td>90-120</td>
<td>0.23</td>
<td>0.02</td>
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<td>120-150</td>
<td>0.68</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>Total</td>
<td>5.97</td>
<td>3.19</td>
<td></td>
</tr>
<tr>
<td>9/29 (272)</td>
<td>1-15</td>
<td>1.44</td>
<td>0.22</td>
<td></td>
</tr>
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<td></td>
<td>15-30</td>
<td>0.49</td>
<td>0.24</td>
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<td>30-45</td>
<td>0.00</td>
<td>0.07</td>
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<td></td>
<td>45-60</td>
<td>0.00</td>
<td>0.02</td>
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<td></td>
<td>60-90</td>
<td>0.00</td>
<td>0.01</td>
<td>70</td>
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<td>90-120</td>
<td>0.00</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td></td>
<td>120-150</td>
<td>0.00</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Total</td>
<td>1.92</td>
<td>0.61</td>
<td></td>
</tr>
</tbody>
</table>

Average | 1.02 | 0.82 |
Figure 5.17. The depth-wise distributions of observed and simulated metolachlor amount in soil layers (0 - 0.9m) on the field sampling dates: a) day 118, b) day 128, c) day 145, d) day 167, e) day 209 and f) day 272.
Figure 5.18. Observed and simulated depth-averaged metolachlor mass in the top 0.9 m soil depth on different sampling dates.
Watershed-scale Evaluation without Considerable Baseflow

Study Area

The Owl Run watershed is located in Fauquier County, Virginia (Figure 5.19). The Owl Run Watershed/Water Quality Monitoring project was initiated to evaluate the impact of land use changes and agronomic/cultural practices on downstream water quality. Meteorologic, hydrologic, biological, soil and water quality, and land use information were monitored at several locations within the watershed over a 10-year study period (Mostaghimi et al., 1989a).

Eight precipitation monitoring stations (POA through POH) were installed to characterize the spatial distribution of rainfall. Additional meteorological data, including evaporation, wind direction and speed, air temperature, and relative humidity, were measured at station POH. Surface runoff and water quality were measured at four stream monitoring stations to study the watershed response to BMP implementations. Figure 5.19 shows the location and the monitoring network of Owl Run watershed.

A pre- versus post-BMP monitoring design was implemented in the watershed. The pre-BMP implementation phase of the monitoring project was started in 1986 and ended in 1988. A combination of structural and managerial BMPs were installed in June 1988 and continued over
approximately two years. The BMPs implemented in the watershed include no-till, grassed waterway, vegetative filter strips, conservation reserve program, animal waste storage facilities, fencing, and stripping cropping.

Corn production with conventional and no-till practices covers about 26% of the watershed area, and about 50% of the corn follows a rye cover or small grain rotation. Most of the hay fields remain as grass for three to four years followed by one year of corn production. The soils on the watershed are mostly shallow (0.3-0.6 m) silt loams. Penn, Bucks and Montalto associations are the major soil accounting for approximately 72% of the soil series within the watershed. These soils are shallow and excessively drained.

**Development of Input Parameters**

Only hydrology and sediment related components of the model were validated due to the lack of pesticide observed data from this watershed. Watershed-scale components, except for the baseflow component, were validated using the observed data from the Owl Run watershed. The components validated included overland flow, channel flow, and interflow routing components. The detailed soil survey data for the watershed show that impermeable bedrock exists within one meter of the top soil depth, approximately covering 78.9 percent of the watershed (Petro, 1956). Figure 5.20 shows the spatial distribution of impermeable soil layers in the Owl Run watershed, and Figure 5.21 shows the measured average monthly runoff to rainfall ratio for the watershed based on observed data during the simulation period (1990-1993). The highest runoff/rainfall ratio was measured during the month of January (with a ratio exceeding 1.0) because most of rainfall remains in the soil due to the negligible percolation through the impermeable soil layer and minimum soil water extraction by evapotranspiration. The ratio decreased from January through June and then increased again from October to January (Figure 5.20). This trend is likely the result of higher evaporation and transpiration during the crop growing season.
In the distributed modeling application, structural parameters including grid size and time-step should be selected before the preparation of functional parameters, which represent general model
input parameters for model calibration. Different input parameters, including topographic and rainfall inputs, can be derived according to the user-selected grid size and time-step. The minimum time-step of one minute and a grid size of one ha (100m × 100m) were selected for this study. Larger time-steps, which still satisfy the required assumptions for the overland routing approach, can be chosen based on the time-step analysis presented later in this study. Finer grid size is recommended for distributed parameter models to satisfy the assumption that all properties such as soil, vegetation, surface condition, crop management, and climate are homogeneous within each grid. DANSAT requires intensive computational resources due to the small time-step. A one hectare grid size was selected to decrease the computational time based on professional judgment. According to the preliminary grid size sensitivity analysis, accuracy of GIS processes to represent spatial distribution of input parameters such as topographic, soil related, and land use related parameters was not guaranteed in larger than one ha grid size. Grid size sensitivity analysis will be discussed in Chapter 6.

Data collected at three watershed outlets, including QOA, QOC, and QOD, were selected to evaluate the response of DANSAT to spatial distribution of input parameters. Spatially distributed parameters can be generally classified into four categories. The four input data categories include topographic, soil related, land use related, and rainfall related input parameters, which can be combined in the cell data block. Only the procedures for considering the spatial distribution of input parameter will be considered in this section because manipulation of the physically-based parameters such as crop, tillage, and pesticide characteristics were explained in the previous section. Arc/View GIS software was used to manipulate spatially distributed parameters according to the selected grid size of 1 ha. Table 5.10 shows the data source and the derived spatially distributed input parameters for the four different data categories.
Table 5.10. Data source and derived spatially distributed input parameters for the Owl Run watershed.

<table>
<thead>
<tr>
<th>Source</th>
<th>Data source</th>
<th>Derived GIS layers</th>
</tr>
</thead>
<tbody>
<tr>
<td>Topography</td>
<td>30 m DEM</td>
<td>Boundary</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cell number</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Flow direction based on 8-direction approach</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Flow accumulation</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Elevation value based on filled DEM</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Channel related parameters (channel type, length, slope, soil type)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Surface slope</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Surface aspect</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Depth to ground water table</td>
</tr>
<tr>
<td>Soil</td>
<td>SSURGO soil database</td>
<td>Soil type</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Effective depth of interaction</td>
</tr>
<tr>
<td>Land use</td>
<td>Surveyed GIS data</td>
<td>Rotation type</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Manning’s roughness coefficient</td>
</tr>
<tr>
<td>Rainfall</td>
<td>Location of rain gauge stations</td>
<td>Thiessen polygon</td>
</tr>
</tbody>
</table>

**Topographic Inputs**

Topographical properties for the model input include watershed boundary, surface elevation, channel network, flow direction, surface slope, and surface aspect. Topographic parameters can be easily extracted from existing digital elevation model (DEM) using any GIS software. DEM of 30 m grid resolution, which is distributed by the U.S. Geologic Survey (USGS), was downloaded and re-sampled into 100 m DEM for the terrain analysis using Arc/View GIS software (ESRI, 1992). The ANSWERS extension for Arc/View, which is included in the interface for ANSWERS-2000 (Veith et al., 2000), was used to provide standard functions for removing sinks, calculating slope and aspect, deriving flow direction and flow accumulation, and delineating watershed boundary and stream network based on a single flow direction algorithm. The cell number map, which defines the order of overland and channel flow routing calculation, was generated by the DANSAT interface using a flow accumulation map as an input. The delineated watershed boundary was used for clipping other grid files in order to exclude the areas outside of the boundary. Figure 5.22 shows the original DEM of 30 m grid resolution for the Owl Run watershed.
Figure 5.22. DEM of 30 m grid resolution for the Owl Run watershed.

Figure 5.23 shows the spatial distribution of the stream after terrain analysis and the shapes of stream cross section assigned for each stream type. Two different stream shape types, including rectangular and triangular streams, can be simulated in the DANSAT to consider the appropriate cross section of each stream. Stream cross section shape and dimensions were determined based on field trips to the watershed and professional judgments. A high value of FUES parameter, which represents a fraction of unerodible channel soil, was assigned to each channel type in Owl Run because of heavy armoring and the presence of exposed shale (Byne, 2000). This parameter was used for sediment calibration. Manning’s roughness coefficient of 0.06 was used for both stream section 1 and 2 and 0.05 was assigned for stream section 3 based on Kilgore’s (1997) data (Figure 5.23).
Soil Data Input
Soil GIS data layer was developed based on detailed soil survey maps (Petro and et al., 1954) because Soil Survey Geographic (SSURGO) database, which is the most detailed county scale soil mapping database, is not yet developed for the Fauquier County. First, the detailed soil survey map was scanned and four points with known coordinates in the scanned image were selected and registered in the UTM coordinate system. The registered map was digitized on the screen using Arc/View GIS software. Finally the attribute of soil series name was assigned to each polygon to consider spatial distribution of input parameters. A spatial distribution of major soil types in the watershed is given in Figure 5.24.
In addition to the spatial distribution of soil types, engineering, physical, and chemical properties of soil layers in a specific soil type are required as model input. Some engineering, physical, and chemical soil properties were derived from the tabular SSURGO data (VA061, Fauquier County, Virginia), which was downloaded from NRCS soil database (http://soildatamart.nrcs.usda.gov/). The properties include soil layer depth, clay percent, bulk density, available water capacity (AWC), organic matter content, saturated hydraulic conductivity, and effective cation exchange capacity. The other required soil properties such as total porosity, wilting point, field capacity, sand percent, silt percent, very fine sand percent, and percent coarse fragment were assumed or estimated based on existing soil properties. Procedural details are provided in Appendix D.

**Land Use**

Land use related and spatially distributed input parameters include crop rotation type and Manning’s roughness coefficient. Land use related parameters were derived based on series of yearly land use GIS data for simulation period from 1990 to 1993. GIS database consists of spatial map and attribute files containing the unique field number and land use activities for each year. Each year of land use activity data was represented by two land use periods: 1st: April-October and 2nd: November-March (Mostaghami et al., 1999a). Four years of land use data from 1990 to 1993 were combined into one GIS database using Union geoprocessing functionality in...
Arc/View (ESRI, 1992). Figure 5.25 shows the spatial distribution of land use activities during the first period of 1992.

![Spatial distribution of land use activities](image)

**Figure 5.25.** Spatial distribution of representative land uses in the Owl Run watershed in 1992 (April through October).

The land use codes used in Figure 5.25 were replaced by the six typical rotation categories such as crop, pasture, hay, forest, and low density and high density developed areas. For example, CO (corn), NTC (no-till corn), NTB (no-till soybean), and OAT (oat) were replaced by Crop. The most frequently occurred rotation type in each combined sequence of land use activities was assigned as representative rotation type. Table 5.11 gives the typical rotation information for crop area in the Owl Run watershed. Corn/Small grain rotation was assigned to the entire crop area.

**Table 5.11.** Typical rotation information for crop areas in the Owl Run watershed.

<table>
<thead>
<tr>
<th>Application date</th>
<th>Application type</th>
<th>Description</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>4/20/01</td>
<td>Planting</td>
<td>Corn</td>
<td></td>
</tr>
<tr>
<td>8/30/01</td>
<td>Harvesting</td>
<td>Corn</td>
<td>30% residue cover</td>
</tr>
<tr>
<td>9/1/01</td>
<td>Tillage</td>
<td>Disc</td>
<td></td>
</tr>
<tr>
<td>10/1/01</td>
<td>Planting</td>
<td>Winter wheat</td>
<td></td>
</tr>
<tr>
<td>6/30/02</td>
<td>Harvesting</td>
<td>Winter wheat</td>
<td>30% residue cover</td>
</tr>
<tr>
<td>10/1/02</td>
<td>Tillage</td>
<td>Chisel plow</td>
<td></td>
</tr>
</tbody>
</table>

The DANSAT model simulates overland flow using a constant Manning’s roughness coefficient throughout the simulation period without considering the relationship between temporally...
changing surface condition and the Manning’s roughness coefficient. The land use data were used to estimate the average Manning’s roughness coefficient for the overland area. Kilgore (1997) estimated Manning’s roughness coefficients for the specific land uses found in Owl Run watershed through literature review and through making a number of assumptions. The roughness coefficients used in this research for different land use type are summarized in Table 5.12. The average temporal value of Manning’s roughness coefficient was calculated using a weighted linear interpolation of smoothness (a reciprocal of roughness) rather than roughness (Liong et al., 1989). The temporal average of Manning’s roughness coefficient is calculated by Equation (5.8).

\[
\frac{1}{n_{avg}} = \frac{1}{N} \left( \frac{1}{n_1} + \frac{1}{n_2} + \ldots + \frac{1}{n_N} \right)
\]  

(5.8)

Where, \( n_{avg} = \) temporal average of the Manning’s roughness coefficient in a specific rotation (sequence of land use changes), \( N = \) number of land use categories in a specific rotation, and \( n_{1:N} = \) Manning’s roughness coefficient for each land use category in a specific rotation.
Table 5.12. Summary of the Owl Run land uses and Manning’s roughness coefficients, (adapted from Kilgore, 1997).

<table>
<thead>
<tr>
<th>Land use</th>
<th>Crop</th>
<th>Residue</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>n</td>
<td>Note/Sources</td>
</tr>
<tr>
<td>Full season beans</td>
<td>0.04</td>
<td>Normal, mature field crop (1)</td>
</tr>
<tr>
<td>No-till beans</td>
<td>0.2</td>
<td>Upper end of row crop range (2)</td>
</tr>
<tr>
<td>Conventional corn</td>
<td>0.08</td>
<td>(2)</td>
</tr>
<tr>
<td>Strip conventional corn</td>
<td>0.09</td>
<td>½ pasture, ½ corn</td>
</tr>
<tr>
<td>Strip no-till corn</td>
<td>0.2</td>
<td>Upper end of row crop range (2)</td>
</tr>
<tr>
<td>No-till corn</td>
<td>0.2</td>
<td>Upper end of row crop range, (2)</td>
</tr>
<tr>
<td>Minimum till corn</td>
<td>0.2</td>
<td>Upper end of row crop range, (2)</td>
</tr>
<tr>
<td>Sorghum</td>
<td>0.086</td>
<td>½ good across slope small grain (3)</td>
</tr>
<tr>
<td>Minimum till sorghum</td>
<td>0.2</td>
<td>Upper end of row crop range (2)</td>
</tr>
<tr>
<td>Small grain</td>
<td>0.032</td>
<td>(2)</td>
</tr>
<tr>
<td>Strip small grain</td>
<td>0.1</td>
<td></td>
</tr>
<tr>
<td>Min. till small grain</td>
<td>0.4</td>
<td>Upper end of small grain range (2)</td>
</tr>
<tr>
<td>Barley</td>
<td>0.032</td>
<td>Small grain (2)</td>
</tr>
<tr>
<td>Wheat</td>
<td>0.032</td>
<td>(2)</td>
</tr>
<tr>
<td>Oats</td>
<td>0.032</td>
<td>Good, across slope small grain (3)</td>
</tr>
<tr>
<td>Alfalfa</td>
<td>0.04</td>
<td>Normal, mature field crop, (1)</td>
</tr>
<tr>
<td>Clover</td>
<td>0.16</td>
<td>(2)</td>
</tr>
<tr>
<td>Grass</td>
<td>0.046</td>
<td>(3)</td>
</tr>
<tr>
<td>Summer annual</td>
<td>0.086</td>
<td>Same as sorghum</td>
</tr>
<tr>
<td>Pasture</td>
<td>0.1</td>
<td>Middle of grass/pasture range (3)</td>
</tr>
<tr>
<td>Hay</td>
<td>0.035</td>
<td></td>
</tr>
<tr>
<td>Idle</td>
<td>0.05</td>
<td>(3)</td>
</tr>
<tr>
<td>Plowed</td>
<td>0.055</td>
<td>(3)</td>
</tr>
<tr>
<td>Wetland</td>
<td>0.125</td>
<td>Sluggish river reach, very weedy, fair condition (4)</td>
</tr>
<tr>
<td>Waterway</td>
<td>0.08</td>
<td>(4)</td>
</tr>
<tr>
<td>Pond</td>
<td>0.08</td>
<td>Same as waterway</td>
</tr>
<tr>
<td>Loafing lot</td>
<td>0.040</td>
<td>Lower end of grass/pasture range (3)</td>
</tr>
<tr>
<td>Farmstead</td>
<td>0.025</td>
<td>½ short grass(2); ½ gravel (3)</td>
</tr>
<tr>
<td>Church</td>
<td>0.038</td>
<td>¼ good grass(3); ¼ concrete (2)</td>
</tr>
<tr>
<td>Residential</td>
<td>0.015</td>
<td></td>
</tr>
<tr>
<td>Light industry</td>
<td>0.013</td>
<td>Street pavement, (2)</td>
</tr>
<tr>
<td>Commercial</td>
<td>0.015</td>
<td></td>
</tr>
<tr>
<td>Road/rail road</td>
<td>0.02</td>
<td></td>
</tr>
</tbody>
</table>

Source: 1. Gray (Gray, 1973)
        2. Novotny and Olem (1994)
        3. Engman (1986)
        4. Brater and King (1976)

**Precipitation**

In DANSAT, the spatial distribution of precipitation is considered by assigning a different rain gauge station in the cell data block of the main input. Only four precipitation monitoring stations, including POB, POD, POF, and POH (Figure 5.19), were considered to generate the thieessen
polygons, because the other stations had missing data during the model simulation period of 1990 through 1993. Thiessen polygon shape file was generated using Arc/View extension and was converted to ASCII grid file based on the selected grid size of 100 m. Figure 5.26 shows the spatial distribution of thiessen polygons.

Figure 5.26. Spatial distribution of thiessen polygon in the Owl Run watershed.

Model Calibration

As mentioned previously, the internal validation approach was selected in this study. First, DANSAT was calibrated for QOA using sensitive parameters and then validated on two nested subwatersheds, QOC and QOD, over the same period without further calibration. Unlike the semi-distributed models such as HSPF and SWAT, there is no input parameter for calibrating a subwatershed because of the different concept and structure used in DANSAT. For example, changes in soil parameters of a specific soil type influence the characteristics of a local area where the soil type is located instead of the overall subwatershed. In particular, difficulties in the calibration of the watershed-scale, spatially-distributed, physically-based model arise because there are too many spatially-distributed parameters, which usually impact a small portion of the watershed. Therefore, watershed-scale parameters, which impact the overall watershed, were used for the calibration of QOA.
The sensitive watershed-scale parameters affecting the hydrology include effective soil depth for infiltration calculation, rainfall adjustment factor for effective hydraulic conductivity of the Green-Ampt equation, anisotropic factor for interflow calculation (a ratio of horizontal saturated hydraulic conductivity to vertical saturated hydraulic conductivity), and the considering depth for the interflow calculation (InterDep). Spatially distributed parameters, such as topographic and soil related parameters, were not used for the calibration while land use related initial parameters for forest, pasture, and hay areas were used to calibrate sediment loss. Selected land use related initial parameters include flat residue biomass, buried biomass, dead root biomass, and live root biomass, which are used for calculation of constant rill erodibility and critical shear stress of non-crop areas during the simulation period.

Rill space was used for the calibration of sediment load over QOA. The sediment loads’ results without further calibration showed underestimation in both QOC and QOD with total percent error of -13% -49%, respectively. Minimum calibration was first conducted to fit simulated total sediment load to the observed data. For the further calibration of sediment loads from QOC and QOD, different channel types were assigned to tributaries in QOA, QOC, and QOD. Detail information on properties of channel beds is not available in the soil database as they are not commonly measured. Thus, parameters of the fraction of unerodible channel soil and soil contents of streambed (percents of clay, sand and silt) were used for further adjustment of total sediment loads. Selected parameter values used for the model calibration are summarized in Table 5.13.
Table 5.13. Summary of sensitive watershed-scale parameters used for the calibration of hydrology and sediment in Owl Run watershed.

<table>
<thead>
<tr>
<th>Watershed-scale parameters</th>
<th>Parameter value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Effective soil depth for infiltration calculation (m)</td>
<td>0.7</td>
</tr>
<tr>
<td>Rainfall adjustment factor for effective hydraulic conductivity of Green-Ampt equation</td>
<td>0.0</td>
</tr>
<tr>
<td>Anisotropic factor for interflow calculation (a ratio of horizontal saturated hydraulic conductivity to vertical saturated hydraulic conductivity)</td>
<td>15.0</td>
</tr>
<tr>
<td>Considering depth for the interflow calculation (m)</td>
<td>1.0</td>
</tr>
<tr>
<td>Rill space (rills/meter)</td>
<td>0.4</td>
</tr>
<tr>
<td>Length for rill detachment calculation (m)</td>
<td>10.0</td>
</tr>
<tr>
<td>Length for channel detachment calculation(m)</td>
<td>10.0</td>
</tr>
</tbody>
</table>

Results and Discussion

Hydrology

A comparison of the observed and simulated annual total runoff for the subwatersheds, without further calibration, are provided in Table 5.14, along with a summary of model performance. The hydrology results for QOC and QOD were obtained from internal validation without any further calibration because there is no parameter in DANSAT for controlling hydrologic response in a specific subwatershed. Total runoff volume was well reproduced at the watershed outlet (QOA) with 0.03% error, while total runoff volume in QOC and QOD were overestimated by 39.76% and 7.84% errors, respectively. Total runoff in QOA and QOD are within the range of ±10%. For all three sites, monthly and daily Nash-Sutcliffe efficiency indexes (E) for total runoff were greater than 0.5, which is a suggested lower range value for acceptable model prediction by Ramanarayanan et al. (1997). Monthly E values, which were calculated based on observed and simulated monthly total runoff, were 0.78, 0.68, and 0.77 for QOA, QOC, and QOD, respectively. The daily E values, which were calculated based on daily total runoff, were smaller than monthly E values and ranged from 0.55 to 0.59. Similar to E values, the monthly NOFs for surface runoff were smaller than the daily NOFs. The differences in monthly NOF values for the three watersheds were small. The monthly NOF values ranged from the minimum of 0.49 in QOA to the maximum of 0.71 in QOD.
Table 5.14. Comparison of observed and simulated annual total runoff and summary of model performance criteria for Owl Run watershed.

<table>
<thead>
<tr>
<th>Year</th>
<th>QOA Obs.</th>
<th>QOC Obs.</th>
<th>QOD Obs.</th>
<th>QOA Sim.</th>
<th>QOC Sim.</th>
<th>QOD Sim.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1990</td>
<td>385</td>
<td>332</td>
<td>302</td>
<td>391</td>
<td>491</td>
<td>311</td>
</tr>
<tr>
<td>1991</td>
<td>328</td>
<td>227</td>
<td>254</td>
<td>390</td>
<td>427</td>
<td>361</td>
</tr>
<tr>
<td>1992</td>
<td>535</td>
<td>466</td>
<td>439</td>
<td>516</td>
<td>617</td>
<td>445</td>
</tr>
<tr>
<td>1993</td>
<td>626</td>
<td>562</td>
<td>485</td>
<td>578</td>
<td>682</td>
<td>479</td>
</tr>
<tr>
<td>Total</td>
<td>1874</td>
<td>1587</td>
<td>1480</td>
<td>1875</td>
<td>2217</td>
<td>1596</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Percent Error</th>
<th>Monthly NOF</th>
<th>Monthly $E$</th>
<th>Daily NOF</th>
<th>Daily $E$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Percent Error</td>
<td>0.03</td>
<td>39.76</td>
<td>7.84</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Monthly NOF</td>
<td>0.49</td>
<td>0.71</td>
<td>0.56</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Monthly $E$</td>
<td>0.78</td>
<td>0.68</td>
<td>0.77</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Daily NOF</td>
<td>2.14</td>
<td>2.47</td>
<td>2.36</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Daily $E$</td>
<td>0.55</td>
<td>0.59</td>
<td>0.56</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- NOF: normalized objective function (unit is mm/watershed)
- $E$: Nash-Sutcliffe model efficiency

Figure 5.27 shows scatter-plots and time-series of observed and simulated daily flow and monthly flow for QOA. Scatter-plot (Figure 5.27a) and time-series (Figure 5.27c) of observed and simulated daily flow show that DANSAT underpredicted the high flow during storm events and overpredicted low flow caused by interflow after rainfall ended. However, the daily total runoffs for the two major storm events (6/18/91 and 8/9/91) were grossly overpredicted. The thiesseen averaged rainfall amounts were 67.43 mm and 91.58 mm for 6/18/91 storm and 8/9/91 storm, respectively. The total runoff was very low for the two storm events, even though they were the 5th and 3rd largest storms during the simulation period from 1990 to 1993. The measured runoffs were 2.31 mm and 5.72 mm for the 6/18/91 and 8/9/91 storm events, respectively. In spite of large rainfall amounts, the small runoff amounts for these two storm events could be attributed to a very small amount of antecedent rainfall or errors in data collection and recording. During the growing season when the antecedent moisture content of the soil is low, most of the rainfall amount infiltrates into the soil and a large amount of soil water is extracted by crops. The storms with similar amounts of rainfall during winter and early spring season resulted in much higher runoff volumes in the Owl Run Watershed. For example, storms on 12/10/92 (102.01 mm) and 3/4/93 (67.57 mm) produced 100 mm and 57.27 mm of total runoff volume, respectively. The infiltration process in DANSAT can be controlled by two major factors, namely effective hydraulic conductivity ($K_{eff}$) and existing soil water amount at a specific depth. In this application, a dynamic approach for $K_{eff}$ was selected and daily $K_{eff}$ values were predicted by the model based on soil and surface cover characteristics. The rainfall adjustment factor for $K_{eff}$ was set as zero to decrease infiltration and increase runoff for big storm events such as those occurring on 12/10/92,
As a result, the $K_{\text{eff}}$ values during 6/18/91 and 8/9/91 storms were also decreased. Figure 5.28 shows the temporal changes in Thiessen averaged rainfall intensity for (a) 6/18/1991 and (b) 8/9/1991 storm events. The 6/18/1991 storm had higher rainfall intensity and smaller rainfall duration compared to the 8/9/1991 storm event. The actual rainfall intensity at each gauge station was higher than the averaged rainfall intensity. Figure 5.29 shows rainfall intensity at each raingauge station for 8/9/1991 storm event. Spatial variation in rainfall amount was high and the highest rainfall intensity occurred at QPF with 259.08 mm/hr intensity. Thus, it was difficult to increase or decrease infiltration amounts of specific storm events by changing $K_{\text{eff}}$ value.

Available soil moisture content is another factor considered in calibration. Effective soil depth for infiltration calculation (InfilDep) is used as the user input to calculate the amount of existing soil water within the depth. If the InfilDep is selected to be small and a large amount of rainfall occurs, the soil layer will be quickly filled with water and infiltration will decrease as the soil layer is saturated. An increase in InfilDep during the 6/18/1991 and 8/9/1991 storm events could increase the total infiltration amount and decrease the total runoff. However, the current version of DANSAT uses a constant InfilDep throughout the simulation period. It is recommended that a dynamic InfilDep approach be considered for DANSAT to enable temporal changes in infiltration depth.

Figure 5.27b and Figure 5.27d show the scatter-plot and time-series of observed and simulated monthly flow, respectively. The monthly total flow was well reproduced by DANSAT, except for the underpredictions on December 1992 and March 1993. Underpredictions for the two months are due to the underprediction of daily runoff for the two major storms of 12/10/92 and 3/4/93. The underprediction of high flow during storm events and overprediction of low flow after rainfall has ended improved the monthly performance criteria in Table 5.14. Model evaluation using daily and monthly runoff is recommended because sediment yield is more sensitive to the changes in daily than monthly flow rates. Sediment yield can be overestimated or underestimated when the daily flow is not correctly simulated even though the monthly flow is well reproduced by the model.

Scatter-plots and time-series of observed and simulated daily flow and monthly flow for QOC and QOD are shown in Figure 5.30 and Figure 5.31. Similar hydrologic responses to QOA were shown for QOC and QOD watersheds. Daily runoffs were overpredicted for the 6/18/1991 and 8/9/1991 storm events and underpredicted for the storms that occurred on 12/10/92, 3/4/93, and 11/28/93, as shown in Figure 5.27.
11/28/93. Overall, DANSAT predicted monthly runoff reasonably. However, the simulation of daily flows can be improved by considering temporally changing infiltration rates throughout the simulation period.
Figure 5.27. Comparison of observed and simulated runoff volumes for QOA: (a) scatter-plots for daily flow, (b) scatter-plots for monthly flow, (c) time-series for daily flow, and (d) time-series for monthly flow.
Figure 5.28. Temporal changes in thiessen averaged rainfall intensity for (a) 6/18/1991 and (b) 8/9/1991 storm events.
Figure 5.29. Actual rainfall intensity in (a) QPB, (b) QPD, (c) QPF, and (d) QPH raingauge stations.
Figure 5.30. Comparison of observed and simulated flow for QOC: (a) scatter-plots for daily flow, (b) scatter-plots for monthly flow, (c) time-series for daily flow, and (d) time-series for monthly flow.
Figure 5.31. Comparison of observed and simulated flow for QOD: (a) scatter-plots for daily flow, (b) scatter-plots for monthly flow, (c) time-series for daily flow, and (d) time-series for monthly flow.
Sediment

The overall comparison of observed and simulated annual total sediment load with minimum calibration is provided in Table 5.15, along with a summary of model performance. The total sediment load in QOA was slightly overestimated with 8.76% total error. However, total sediment loads in subwatersheds after minimum calibration showed overestimation in QOC and underestimation in QOD with 34.73% and -6.90% errors, respectively. The overall trend of total sediment load from each subwatershed was similar to the hydrology simulations. Simulated total runoffs and sediment loads in QOA and QOD were all within the range of ±10% error, while both total runoff and sediment load from QOC were greatly overpredicted with greater than 30% error. It should be noted that DANSAT overpredicted both total runoff and sediment loads from QOC.

The daily Nash-Sutcliffe efficiency indexes (E) for sediment load in QOA, QOC, and QOD were considerably low with the values of 0.31, 0.10, and 0.20, respectively. The low daily E values for sediment in these three watersheds can be attributed to the underprediction of runoff during high flow and overprediction of runoff during low flow periods. Figure 5.32 shows the comparison of daily runoff and sediment yields at watershed outlet (QOA) during a part of the simulation period (6/15/92 – 10/30/92). Underprediction of daily runoff during storm events resulted in the underprediction of daily sediment yields. Underestimation of surface runoff during the major storm events may be due to the underestimation of the effective hydraulic conductivity value for big storm events. Similarly, overprediction of daily runoff after rainfall has stopped resulted in the overprediction of sediment yields. Predicted soil loss was very sensitive to the changes in runoff.

Daily NOF values were relatively high in all watersheds compared to the monthly NOF. The higher daily NOF values may be attributed to the procedure used for calculating the daily sediment yields based on irregularly collected samples. Water quality samples do not exist for every single day during the simulation period. The daily sediment load for a day when samples were not collected was interpolated using the existing observed data around that day (estimated sediment loads). As a result, the estimated daily sediment loads contains a high degree of uncertainty between sampling dates. The daily NOF values shown in the parentheses in Table 5.15 were calculated based on the daily sediment loads, which were actually calculated using measured flow rates and sediment concentrations by excluding interpolated daily sediment loads (measured sediment loads). The daily NOF values based on measured sediment loads were less
than NOF values in parentheses, which were based on both measured and estimated daily sediment loads.

Similar to the hydrology, errors in daily sediment load during high flows and low flow periods canceled each other and increased the monthly Nash-Sutcliffe efficiency indexes (E) for sediment load in QOA, QOC, and QOD (0.63, 0.44, and 0.50, respectively). Only the monthly E value for QOC was less than 0.5. Similar to the hydrology, the monthly NOF values for sediment were smaller than the daily NOF values with a range of 0.69 to 1.40 at QOA and QOC, respectively.

Figure 5.33, 5.34 and 5.35 show scatter-plots and time-series of observed and simulated monthly sediment loads for QOA, QOC, and QOD, respectively. When observed monthly sediment loads from the three subwatersheds are compared with each other, the unusual trend in the monthly observed sediment loads should be noted. The monthly sediment loads were underestimated by DANSAT during November 1993 at QOA, April 1993 at QOC, and December 1992 at QOD. Sediment load was overestimated during December 1992 at QOD even though the monthly total runoff was underestimated during that month. The observed sediment load during this month is very low considering the high value of measured monthly total runoff for this month. The major difference between observed and simulated sediment load during this month can be attributed to the second largest storm event occurring during the simulation period (1990-1993) for which no water quality sample was collected due to malfunctioning equipment. The storm event produced 102mm of rain with a duration of 20 hours on December 10, 1992. Similarly, no water quality samples were collected for the major storms that occurred during November 1993 at QOA and April 1993 at QOC. The largest observed and predicted monthly sediment load occurred during March 1993; however, DANSAT underpredicted this monthly sediment load in all three subwatersheds. The underpredictions in sediment loads may be attributed to the underpredictions in hydrology during the month for the same reasons described in the previous section.
Table 5.15. Comparison of observed and simulated annual total sediment load and summary of model performance criteria.

<table>
<thead>
<tr>
<th>Year</th>
<th>QOA Obs.</th>
<th>QOA Sim.</th>
<th>QOC Obs.</th>
<th>QOC Sim.</th>
<th>QOD Obs.</th>
<th>QOD Sim.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1990</td>
<td>709</td>
<td>777</td>
<td>273</td>
<td>487</td>
<td>811</td>
<td>879</td>
</tr>
<tr>
<td>1991</td>
<td>605</td>
<td>734</td>
<td>150</td>
<td>383</td>
<td>568</td>
<td>981</td>
</tr>
<tr>
<td>1992</td>
<td>1147</td>
<td>962</td>
<td>417</td>
<td>580</td>
<td>966</td>
<td>1049</td>
</tr>
<tr>
<td>1993</td>
<td>1076</td>
<td>1374</td>
<td>816</td>
<td>781</td>
<td>2421</td>
<td>1529</td>
</tr>
<tr>
<td>Total</td>
<td>3537</td>
<td>3847</td>
<td>1656</td>
<td>2231</td>
<td>4767</td>
<td>4438</td>
</tr>
<tr>
<td>Percent Error</td>
<td>8.76</td>
<td>34.73</td>
<td>-6.90</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Monthly NOF</td>
<td>0.69</td>
<td>1.40</td>
<td>1.19</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Monthly $E$</td>
<td>0.63</td>
<td>0.44</td>
<td>0.50</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Daily NOF</td>
<td>3.58 (2.49)</td>
<td>6.27 (4.31)</td>
<td>5.13 (3.11)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Daily $E$</td>
<td>0.31</td>
<td>0.10</td>
<td>0.20</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(): criteria were calculated based on a set of daily sediment load which is estimated only if samples exist in a given day.

NOF: normalized objective function (unit is kg/ha)

$E$: Nash-Sutcliffe model efficiency

Figure 5.32. Comparison of daily runoff and sediment load from 6/15/92 to 10/30/92 for QOA.
Figure 5.33. (a) Scatter-plot and (b) time-series of observed and simulated monthly sediment load for QOA.
Figure 5.34. (a) Scatter-plot and (b) time-series of observed and simulated monthly sediment load for QOC.
y = 0.5535x
$R^2 = 0.3288$

Observed Monthly Sediment Load (kg/ha)
Simulated Monthly Sediment Load (kg/ha)

Figure 5.35. (a) Scatter-plot and (b) time-series of observed and simulated monthly sediment load for QOD.
Watershed-scale Evaluation with Integrated Ground Water Approach

Study Area

The Nomini Creek (NC) Watershed/Water Quality monitoring project was initiated in 1985 and completed in 1997 to quantify the impacts of agricultural best management practices (BMPs) on surface and ground water quality. Figure 5.36 shows the location and monitoring network of the Nomini Creek watershed. Nomini Creek watershed is located in Westmoreland County, Virginia. Meteorological, hydrologic, water quality, and land use information were measured at several locations within the watershed.

Seven precipitation monitoring stations (PN1 through PN7) were installed to characterize the spatial distribution of rainfall. Additional meteorological data were measured at station PN5. The meteorological data includes evaporation, wind direction and speed, air temperature, and relative humidity. Surface hydrology and water quality were monitored at two stations including QN1 and QN2. The runoff at the watershed outlet, QN1, is strongly influenced by the wetland that exists upstream from the station. Even though there is no wetland in the subwatershed, the influence of baseflow on total runoff at the subwatershed outlet (QN2) is significant because of high ground water tables. The average baseflow index, which is defined as the ratio of the total volume of the baseflow to the total volume of runoff for a given period, is greater than 0.85 at QN2 subwatershed. This indicates that a large portion of the rainfall falling on upland areas is lost to ground water by infiltration and percolation.

The NC watershed is agricultural with 49% cropland, 47% woodland, and 4% under residential and roads. Corn, soybeans, and small grains (wheat and barley) are the major crops in the watershed. The typical rotation in the watershed is conventionally-tilled corn, followed by small grains and no-till soybeans. Occasionally, some acreage is planted to conventionally-tilled full season soybean. Actual land use changes were recorded during the project period starting from 1985 through 1997 in a series of field boundary maps and attribute files. Spatial changes in land management practices were considered in the field boundary maps, which are in a digital format. Temporal land use changes were recorded to the attribute files three times a year. A pre- versus post-BMP monitoring design was implemented in the NC watershed using a combination of agronomic and structural BMPs. The pre-BMP implementation period ended in 1988. BMPs were
installed in 1989 and continued over approximately two years. The post-BMP period started in 1991 and continued until the end of the monitoring project.

![Figure 5.36. Location and monitoring network of Nomini Creek watershed.](image)

Both Suffolk and Rumford series, which cover about 90% of the watershed, are the major soils in Nomini Creek watershed. The Suffolk soil, which is characterized by a sandy loam texture, covers 58% of the watershed. The Rumford series, which is classified as sandy loam soil, covers approximately 33% of the watershed. Both soils are deep and well drained soils. Suffolk and Rumford soils show moderate (1.5 to 5.1 cm/hr) and moderately rapid (5.1 to 15 cm/hr) permeability characteristics, respectively.

The pesticide database contains the field number, applied pesticide amounts, and application dates. Additional information regarding the procedures for data collection and data analysis is given by Mostaghimi and others (Mostaghimi et al., 1989b).

**Development of Input Parameters**

The model was applied to the subwatershed, QN2. The subwatershed area was divided into a total of 265 uniform cells, 0.81 ha (90 × 90 meters) in size. The minimum time-step of DANSAT, 1 minute, was also used in this application. Most procedures used for developing physically-based input parameters as well as spatially distributed input parameters are similar to those described in
the previous sections. Topographic parameters were extracted from 90 m DEM, which was re-sampled from the original 30 m DEM. Similar procedures for developing topographic parameters for the Owl Run watershed simulation were employed for the integrated ground water approach. Figure 5.37.a and b show the re-sampled 90 m DEM and the derived channel segments, respectively. SSURGO soil database for the Westmoreland County was available at the NRCD webpage. DANSAT interface was developed and used to extract soil related parameters from the SSURGO database file. Spatial distribution of soil types on QN2 is depicted in Figure 5.37.c. Detailed equations and procedures for extracting general and layer-related soil parameters are included in Appendix D. Six years of land use data from 1987 to 1992 were manipulated using Arc/View GIS software to identify rotation number. Forty eight identical rotation polygons were derived through the Union geoprocessing (ESRI, 1992) according to the predefined grid size (Figure 5.37.d). The attribute file contains the unique field number and three land use activities for each year (LU1: from April through June, LU2: from July through September, and LU3: from October through March). Five non-crop rotation types such as forest, pasture, hay, low density developed, and high density developed were defined based on land use attribute data. For the remaining crop areas, each polygon was treated as identical rotation type to consider actual location where pesticide was applied. Typical dates for the crop area were decided based on the advice from professionals of Virginia Tech. Atrazine and metolachlor were selected for the validation of pesticide component because both atrazine and metolachlor were the most frequently detected or predominantly used pesticides in the watershed. Surveyed pesticide application information was combined in crop rotation sub-blocks by considering the actual location to which pesticides were applied based on the unique field number. Three precipitation monitoring stations were used to generate the thiessen polygons shown in Figure 5.37.e.
Figure 5.37. Major GIS layers used for creating spatially distributed parameters in Nomini Creek watershed: (a) DEM; (b) Channel network; (c) soil; (d) land use; and (e) Thiessen polygon.
Model Calibration and Validation

As mentioned previously, the split-sample validation approach was used to evaluate how the model simulates the temporal changes in land use. DANSAT was calibrated on pre-BMP and BMP implementation period and validated with data collected during the post-BMP period. Temporal land use changes between the calibration and validation periods were considered by using different tillage type and planting and harvesting dates and by increasing the percent of residue covers after harvesting crops. Table 5.16 shows the comparison of typical dates and types of the agricultural management operations during the calibration and validation periods.

Table 5.16. Comparison of typical dates and application types of agricultural management during the calibration and validation period.

<table>
<thead>
<tr>
<th>Date</th>
<th>Type</th>
<th>Description</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>04/09</td>
<td>Tillage</td>
<td>Planting</td>
<td></td>
</tr>
<tr>
<td>04/09</td>
<td>Planting</td>
<td>Corn</td>
<td></td>
</tr>
<tr>
<td>10/09</td>
<td>Harvesting</td>
<td>Corn</td>
<td>15% residue cover</td>
</tr>
<tr>
<td>10/10</td>
<td>Tillage</td>
<td>Chisel plow</td>
<td></td>
</tr>
<tr>
<td>10/14</td>
<td>Tillage</td>
<td>Disk</td>
<td></td>
</tr>
<tr>
<td>10/15</td>
<td>Planting</td>
<td>Winter wheat</td>
<td></td>
</tr>
<tr>
<td>06/24*</td>
<td>Harvesting</td>
<td>Winter wheat</td>
<td>70% residue cover</td>
</tr>
<tr>
<td>06/30*</td>
<td>Tillage</td>
<td>No-till drill</td>
<td></td>
</tr>
<tr>
<td>06/30*</td>
<td>Planting</td>
<td>Soybean</td>
<td></td>
</tr>
<tr>
<td>11/09*</td>
<td>Harvesting</td>
<td>Soybean</td>
<td>70% residue cover</td>
</tr>
</tbody>
</table>

*: Second year of rotation

General calibration parameters were used first. These parameters included effective soil depth for infiltration, rainfall adjustment factor for effective hydraulic conductivity, anisotropic factor for interflow calculation, and the depth for interflow calculation for calibration of hydrology. In addition, parameters in the ground water data block were used for calibrating hydrology because a great portion of total runoff at QN2 comes from baseflow. Rill space and length for rill detachment parameters are used for controlling sediment loss on overland area, while the length for channel detachment calculation, fraction of unerodible channel soil, and soil contents of the streambed (percents of clay, sand and silt) were used for controlling the sediment deposition and detachment in stream segments. Land use related initial parameters for non-crop areas, which include flat residue biomass, buried biomass, dead root biomass, and live root biomass, were used to calibrate sediment loss by controlling rill erodibility and critical shear stress. For pesticides, fraction of dissolved chemical available for runoff, partitioning coefficient, and half-life were used for calibration pesticide components. Selected parameter values for the model calibration and validation are summarized in Table 5.17.
Table 5.17. Summary of sensitive parameters calibrated for model application at QN2.

<table>
<thead>
<tr>
<th>Watershed-scale parameters</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Effective soil depth for infiltration calculation (m)</td>
<td>0.7</td>
</tr>
<tr>
<td>Rainfall adjustment factor for effective hydraulic conductivity of Green-Ampt equation</td>
<td>1.0</td>
</tr>
<tr>
<td>Anisotropic factor for interflow calculation (a ratio of horizontal saturated hydraulic conductivity to vertical saturated hydraulic conductivity)</td>
<td>1.0</td>
</tr>
<tr>
<td>Considering depth for the interflow calculation (m)</td>
<td>0.035</td>
</tr>
<tr>
<td>Rill space (rills/meter)</td>
<td>0.4</td>
</tr>
<tr>
<td>Length for rill detachment calculation (m)</td>
<td>10.0</td>
</tr>
<tr>
<td>Length for channel detachment calculation (m)</td>
<td>10.0</td>
</tr>
</tbody>
</table>

Results and Discussion

Hydrology

A comparison of observed and simulated annual total runoff along with a summary of model performance is provided in Table 5.18. Total runoff volume was well reproduced for both calibration and validation periods with 0.64% and -5.12% percent errors, respectively. Total runoff for both calibration and validation periods are within a range of ±10%. Total runoff at the watershed outlet consists of surface runoff, interflow, and baseflow from the ground water. The monthly normalized objective function (NOF) for the calibration period was about half the value of the daily NOF value. Both monthly and daily Nash-Sutcliffe efficiency indexes (E) for the calibration period were greater than 0.5, which is a suggested lower range value for acceptable model prediction by Ramanarayanan et al. (1997). The daily and monthly E values for the calibration period were 0.59 and 0.53, respectively. Figure 5.38 shows scatter-plots and time-series of observed and simulated daily and monthly flows for the calibration period. Time-series of observed and simulated daily and monthly flows showed that DANSAT simulates the overall fluctuation of baseflow well, even though monthly total runoff during 1989 was slightly overestimated and monthly total runoff during 1990 was underestimated. The discrepancies between the observed and simulated monthly total runoffs are due to the overprediction and underprediction of daily baseflow during 1989 and 1990, as shown in Figure 5.38.c, respectively.

Fluctuation of baseflow is simulated by the integrated ground water component of DANSAT using daily recharge values from intermediate zone to ground water zone as input. Figure 5.39 shows the simulated temporal changes in monthly total runoff and monthly average flux from intermediate to ground water zone. The higher recharge during the first month can be explained by the higher initial soil water content at every soil layer. Monthly total runoff positively responded to the changes in the monthly average recharge with decreased amplitude and
increased frequency. Model performance in the QN2 watershed is highly impacted by the subsurface components, which transform spatially assigned recharge input to baseflow at watershed outlet.

A utility program to convert flux output by DANSAT to Arc/View ASCII format was developed to examine the spatial distribution of flux from intermediate to ground water zone. The source code and sample input files are included in a compressed file in Appendix F. Spatial distribution of annual simulated total flux from intermediate to ground water zone is shown in Figure 5.40. The spatial distribution of cells with higher recharge values was related to the spatial distribution of cell numbers, which define the order of overland flow routing calculation. Higher cell number means that more water can be accumulated through overland during the routing procedure. The available water for infiltration in a given cell is considered by adding precipitation and inflow from adjacent cells during a given time-step. As a result, a cell with higher drainable soil characteristics and higher cell number has strong possibility to contribute more recharge to ground water.

Similar to the calibration period, total runoff for the validation period was underestimated by -5.12% compared to the observed data. Unlike the calibration period, daily Nash-Sutcliff efficiency indexes (E) for validation period were greater than 0.5, while the monthly E value was less than 0.5. The daily and monthly E values for validation period were 0.66 and 0.10, respectively. Figure 5.41 shows scatter-plots and time-series of observed and simulated daily and monthly flows for validation period. Time-series of observed and simulated daily and monthly flows showed that DANSAT underestimated the monthly total runoff from January 1991 to May 1991, failed to simulate the increase in baseflow from September 1991 to January 1992, and increase in baseflow during August 1992 was delayed by one month. These discrepancies in monthly total runoff resulted in a low value for the monthly Nash-Sutcliff efficiency index. Daily E values for both calibration and validation periods were higher than the monthly E values because the total runoffs by storm events were relatively well reproduced by overland flow and interflow components of DANSAT, while fluctuations in baseflow based on ground water recharge were difficult to simulate using the integrated ground water component.
Table 5.18. Comparison of observed and simulated annual total runoff and summary of model performance criteria for calibration and validation periods at QN2.

<table>
<thead>
<tr>
<th>Year</th>
<th>Runoff (mm)</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Obs.</td>
<td>Sim.</td>
<td>Obs.</td>
</tr>
<tr>
<td>1987</td>
<td>425</td>
<td>358</td>
<td></td>
</tr>
<tr>
<td>1988</td>
<td>356</td>
<td>323</td>
<td></td>
</tr>
<tr>
<td>1989</td>
<td>479</td>
<td>578</td>
<td></td>
</tr>
<tr>
<td>1990</td>
<td>586</td>
<td>574</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>1845</td>
<td>1833</td>
<td>897</td>
</tr>
</tbody>
</table>

Percent Error -0.64  -5.12
Monthly NOF 0.16  0.14
Monthly E 0.53  0.10
Daily NOF 0.33  0.22
Daily E 0.59  0.66

- NOF: normalized objective function (mm)
- E: Nash-Sutcliffe model efficiency
Figure 5.38. Comparison of observed and simulated flow for calibration period: (a) scatter-plots for daily flow, (b) scatter-plots for monthly flow, (c) time-series for daily flow, and (d) time-series for monthly flow.
Figure 5.39. Time-series of simulated monthly total runoff and monthly average flux from intermediate to ground water zone.

Figure 5.40. Spatial distribution of annual simulated total flux from intermediate to ground water zone (unit is mm/year-cell).
Figure 5.41. Comparison of observed and simulated flow for validation period: (a) scatter-plots for daily flow, (b) scatter-plots for monthly flow, (c) time-series for daily flow, and (d) time-series for monthly flow.
Sediment

A comparison of observed and simulated annual total sediment yield for both calibration and validation periods are provided in Table 5.19, along with a summary of model performance. The total sediment load for the calibration period was slightly overestimated with 5.64% in total error, while the total sediment load for the validation period was underestimated by -28.98%. The monthly Nash-Sutcliffe efficiency indexes \( (E) \) for calibration and validation periods were considerably low, with the values of -2.24 and -1.43, respectively. Figure 5.42 and Figure 5.43 show scatter-plot and time-series of observed and simulated monthly sediment load for calibration and validation periods, respectively. DANSAT failed to simulate the temporal fluctuations of monthly sediment loads for both calibration and validation periods. During the calibration period, monthly sediment loads during 1987 and 1988 (dry years) were underpredicted, while monthly sediment loads during 1989 and 1990 (wet years) were overpredicted by the model. During the validation period, monthly sediment loads were underpredicted for most months.

Table 5.19. Comparison of observed and simulated annual sediment yields and a summary of model performance criteria for calibration and validation periods at QN2.

<table>
<thead>
<tr>
<th>Year</th>
<th>Runoff</th>
<th>Obs.</th>
<th>Sim.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1987</td>
<td>1084</td>
<td>316</td>
<td></td>
</tr>
<tr>
<td>1988</td>
<td>706</td>
<td>334</td>
<td></td>
</tr>
<tr>
<td>1989</td>
<td>1115</td>
<td>2430</td>
<td></td>
</tr>
<tr>
<td>1990</td>
<td>1729</td>
<td>1816</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>4634</td>
<td>4896</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Year</th>
<th>Runoff</th>
<th>Obs.</th>
<th>Sim.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1991</td>
<td>1013</td>
<td>565</td>
<td></td>
</tr>
<tr>
<td>1992</td>
<td>1125</td>
<td>954</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>2138</td>
<td>1518</td>
<td></td>
</tr>
</tbody>
</table>

- NOF: normalized objective function (kg/ha)
- \( E \): Nash-Sutcliffe model efficiency

It should be noted that both monthly Nash-Sutcliffe efficiency indexes \( (E) \) for calibration and validation periods had negative values. The negative monthly \( E \) values for both calibration and validation periods can be attributed to the poor relationship between observed daily discharge and daily total sediment load. Figure 5.44 shows the relationship between observed daily runoff and daily sediment loads, which were calculated based on actual water quality samples taken during a simulation period (1987-1992). It should be noticed that ranges in daily sediment loads variations during low flow condition were very broad and within four orders of magnitude. Water quality samples were collected irregularly and do not exist for every single day. The daily sediment load for a day when samples were not collected was calculated based on the existing observed data around the day. Figure 5.45 shows an example of measured flow rate, measured sediment...
concentration, and representative interval for daily sediment load calculation during December 1987. Variations in measured sediment concentrations measured during similar flow rates during low flow conditions were very high. A sufficient number of samples was not taken during high flow condition by storms. For example, only one sample was used for representing storms on 12/10/87 and 12/27/87. In Figure 5.44, it also should be noticed that the observed daily sediment loads did not increase as the flow rates increased during the high flow condition. Figure 5.46.a through e show the temporal changes in observed flow rates and observed sediment concentrations for the five largest runoff events from the QN2 watershed (1987-1992). For all five storm events, observed sediment concentration had high values at the beginning of runoff and low values near the storm peak and recession limbs. Daily sediment load did not increase during storm events due to the low sediment concentration even though flow rates were high. Figure 5.46.f shows the temporal changes in observed flow rates and sediment concentrations for the storm event of 4/2/1990 at Owl Run watershed. As mentioned previously, sediment in Owl Run watershed showed a similar trend to the hydrology. Sediment concentration increased as the flow rate increased. This poor relationship between observed daily discharge and daily total sediment load may be attributed to bank erosion, agricultural management such as tillage, and cross sectional shape of streams. Only the response of DANSAT to the changes in the shapes of stream cross section was analyzed in this section because DANSAT is not able to consider bank erosion. Figure 5.47 shows the comparison of daily observed and simulated sediment loads for different stream cross sections such as rectangular and triangular. Sediment yields were not simulated during a low flow condition within the rectangular stream because transport capacity and soil detachment in rills and channels are simulated based on estimated flow depth by hydrology components. Soil detachment occurs only when effective shear stress (based on flow depth) is greater than the critical shear stress (based on soil characteristics). As a result, sediment loads in the rectangular stream were underpredicted during dry years and overpredicted during wet years. However, soil detachment occurs during low flow condition in triangular streams for same amount of water, because triangular cross section causes higher flow depth than the rectangular stream cross section in low flow conditions, while flow depth in triangular streams is smaller than rectangular streams for a high flow condition. For the triangular cross-section streams, small and consistent sediment loads were simulated for the low flow conditions and sediment loads during high flow condition were not sensitive to the changes in flow depth. Figure 5.48 shows a comparison of accumulated observed and simulated sediment loads for different
stream cross sections. Response of sediment components for different stream cross sections will be discussed in the sensitivity analysis part of the study.

![Graph](image)

**Figure 5.42.** (a) Scatter-plot and (b) time-series of observed and simulated monthly sediment load for the calibration period at QN2.
Figure 5.43. (a) Scatter-plot and (b) time-series of observed and simulated monthly sediment load for the validation period at QN2.
Figure 5.44. Relationship between observed daily discharge and daily total sediment load in QN2.

Figure 5.45. Example of flow rate, sediment concentration, and representative interval for daily sediment load calculation (December 1987).
Figure 5.46. Temporal changes in flow rates and sediment concentrations during five biggest runoff events: (a)-(e) from QN2 watershed and (f) from Owl Run watershed.
Pesticides

Rapid decrease in pesticide concentrations in runoff occurred between 1 minute and 10 minute time-steps. The 10 minute time-step was selected for the pesticide simulations after the preliminary time-step analysis. The detail time-step analysis will be discussed in the next chapter. The overall comparison of observed and simulated total pesticide loads for both calibration and validation periods are provided in Table 5.20, along with a summary of model performance criteria. Due to the lack of sufficient number of pesticide samples, the total pesticide loads were calculated based on the actual daily pesticide loads, which were estimated using measured flow rates and measured pesticide concentrations only if pesticide samples were available. A total of
74 and 44 daily pesticide loads were used for calculating total pesticide loads and performance criteria for calibration and validation periods, respectively.

Total atrazine loads were underestimated for both calibration and validation periods with -34.21% and -74.17% errors, respectively. The daily Nash-Sutcliffe efficiency indexes (E) for calibration and validation periods were considerably low with the values of 0.09 and 0.25, respectively. Figure 5.49 shows observed and simulated accumulated atrazine loads for calibration and validation periods. DANSAT failed to simulate the temporal trend in daily atrazine load for both calibration and validation periods.

Total metolachlor loads were overestimated for calibration period and underestimated for the validation period with 81.0% and -28.91% errors, respectively. The daily Nash-Sutcliffe efficiency indexes (E) for calibration and validation periods were considerably low with values of 0.42 and 0.20, respectively. Figure 5.50 shows observed and simulated accumulated metolachlor loads for calibration and validation periods. DANSAT failed to simulate the temporal trend in daily metolachlor load for both calibration and validation periods even though metolachlor predictions were better than for atrazine.

Table 5.20. Comparison of observed and simulated total pesticide loss and summary of model performance criteria for the calibration and validation periods at QN2.

<table>
<thead>
<tr>
<th>Criteria</th>
<th>Calibration</th>
<th>Validation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Atrazine</td>
<td>Metolachlor</td>
</tr>
<tr>
<td>Total</td>
<td>34.79 22.89</td>
<td>71.44 128.99</td>
</tr>
<tr>
<td>Percent Error</td>
<td>-34.21 81</td>
<td>-74.17 28.91</td>
</tr>
<tr>
<td>Daily NOF</td>
<td>5.48 4.44</td>
<td>0.09 0.25</td>
</tr>
<tr>
<td>Daily E</td>
<td>0.09 0.20</td>
<td></td>
</tr>
</tbody>
</table>

- NOF: normalized objective function (g/ha)
- E: Nash-Sutcliffe model efficiency
Figure 5.49. Observed and simulated daily atrazine loads for the (a) calibration and (b) validation periods at QN2.
Figure 5.50. Observed and simulated daily metolachlor loads for the (a) calibration and (b) validation periods at QN2.

Pesticide mass balance was computed to validate the pesticide component of the model. The amount of pesticide applied should be equal to the sum of pesticide amounts in all pesticide storages and pesticide losses to outside of the system. Pesticide storages inside of the modeling system include pesticides on foliage, in the soil profile, overland routing storage, channel routing storage and stream bed, and in lumped interflow storage. Pesticide losses include degradation on foliage, in soils, plant uptakes, pesticide flux from intermediate zone to ground water zone, and pesticide outflow at the watershed outlet. Figure 5.51 shows the temporal changes in pesticide mass in pesticide related modeling storages and simulated pesticide losses leaving the QN2 watershed. Most of applied pesticides disappeared through the degradation process or remained in the soil profile. The sum of pesticide amounts in all pesticide storages and pesticide loss were not
equal to the total amount of pesticide applied. A total of -0.06% total error at the end of simulation period was resulted.

Figure 5.51. Atrazine mass balance during the calibration period.
Watershed-scale Evaluation with Linked Ground Water Approach

Study Area and Methods
The Nomini Creek watershed was selected to validate the interface components for the surface and ground water interaction by linkage of DANSAT to existing ground water models such as MODFLOW and MT3D. Eight wells were installed to a depth ranging from 10 to 17 m in order to assess the underlying ground water quality. Figure 5.52 shows the location of eight ground water monitoring wells in the Nomini Creek watershed. The detail information on these wells is provided by Mostaghimi and others (Mostaghimi et al., 1999b).

Figure 5.52. Location of ground water monitoring wells in Nomini Creek watershed.

Only detail procedures for the ground water modeling will be described in this section because the procedures for the integrated ground water approach using DANSAT was described in previous sections in detail, and the accuracy of the linked ground water approach depends on the how reasonably the saturated area is simulated by the ground water models. The general procedure for validation of linked ground water approach consists of three steps: 1) calibrating surface water model using integrated approach, which is already explained in the previous section; 2) calibrating the ground water models in a steady-state condition; and 3) running the linked system with the transient mode of ground water models to simulate the impact of land use.
activities on the hydraulic head and stream flow. MODFLOW was run both in steady-state and in transient mode. In the steady-state simulation, the model runs until the system reaches equilibrium when the maximum residual between previous and current calculations is within the criterion specified in the Solver package (McDonald and Harbaugh, 1988). A steady-state simulation is usually performed during the calibration procedure to develop an optimal parameter set. The optimal parameter set is then used in a transient simulation to solve a time-dependent problem and to verify the available data for that time period (Cho et al., 2001).

MODFLOW was calibrated in a steady-state condition against the hydraulic head and stream flow rate. Calibration was performed by changing hydraulic conductivity of unconfined saturated layer and streambed conductance until the simulated solution matched the observed value. A trial-and-error method was employed to calibrate the model. Boundary and initial conditions, constructed based on the calibrated ground water model, were used for the application of the linked system in a transient mode.

**Development of Input Parameters**

The study area was divided into the 0.81 ha grid size (90m × 90m square cell), the same size as that of the integrated ground water application. The same input files developed for the integrated ground water application using DANSAT were used for the linked approach by turning off the integrated baseflow component and turning on the existing ground water models such as MODFLOW and MT3D. Only procedures for preparing input parameters for MODFLOW will be discussed in this section due to the lack of parameter information for the MT3D simulation. Procedures for preparing input parameters for DANSAT were already described in the previous section (watershed-scale evaluation with integrated ground water approach) of this chapter.

Available information and data were compiled for the study area to develop the conceptual model for the MODFLOW simulations. An appropriate time-step for the ground water models should be decided based on characteristics of stream and ground water flow. For example, if flow characteristics of stream and ground water vary significantly during a small period of time, a shorter time-step is necessary. In this study, a 10-day time-step for ground water simulations was selected.

*Average Ground Water Table Elevation*

Generation of reliable distribution of average ground water table elevation is critical for the calibration of ground water models. Spatial distribution of average ground water table cannot be
generated with only one pair of ground water monitoring stations (GN1-2) inside QN2. Sixteen points were sampled in streams to obtain approximate elevation of the ground water table. It is assumed that the ground water table is connected with the streambed considering that over 85 percent of total runoff came from ground water in QN2. Figure 5.53 shows the location of ground water monitoring stations (midpoints of paired monitoring wells), selected stream points for interpolating ground water table (red point in figure), and generated contours of average ground water table.

Multiple observation wells are required inside the watershed in order to calculate simulation error for calibration of the ground water model. Virtual observation wells were defined throughout the watershed as shown in Figure 5.53 because only one pair of ground water monitoring wells were available in QN2. Ground water table elevations from paired monitoring wells, GN1 and GN2, were averaged for comparison with the simulated value. Observed hydraulic head information for
virtual observation wells was generated based on interpolated average ground water table elevation.

**Model Layer**

Only one layer of saturated zone was considered in the ground water simulations with MODFLOW because the average ground water tables at eight monitoring stations (GN1-GN8) are about 10 meters below the ground surface, based on the 10 years of observed data. This layer represents the unconfined aquifer. The bedrock was not considered because QN2 is not big enough to consider deep ground water movement. The same surface elevation information, which was created in the integrated application, was used to represent the land surface of the conceptual model. The bottom boundary of the layer was assumed to be 5 m from the sea level. Hydraulic conductivity in a shallow unconfined aquifer can vary depending on the different soil types. Even though the NRCS hydrologic soil group is based on the soil's runoff potential, the hydrologic soil group was derived from soil survey to consider spatial distribution of hydraulic conductivity in the shallow unconfined saturated layer. However, one homogeneous hydraulic conductivity value was assigned for the unconfined layer because no significant spatial distribution of the hydrologic soil group was detected in QN2. Figure 5.54 shows the spatial distribution of the hydrologic soil group in the watershed. Soil group B covers 96 percent of the watershed and soil group D exists near the streams, covering 3.4 percent of the watershed. The spatial distribution near streams can be considered by changing the stream bed conductivity parameters.
**Stream Input**

In MODFLOW, streams can be simulated by using either *General Head Boundary* package, *River* package, or *Streamflow Routing* package (Cho et al., 2001). The *Streamflow Routing* package was selected to represent the stream in this study. Due to the difficulty in measuring stream bed conductance values, input parameters were determined through calibration. After calibrating the hydraulic conductivity of the unconfined layer, stream bed conductance was changed to match the observed and simulated stream flow rates. Observed average stream flow rate for the model calibration were calculated based on the observed daily runoff data at the QN2 watershed outlet. Total baseflow, estimated using baseflow separation filter (Arnold and Allen, 1999; Arnold et al., 1995), was used to calculate average stream flow rate, which needs to be compared with the simulated total flux between aquifer and streams.

**Boundary Conditions**

At the beginning, the closed boundary assumption was applied to the 265 ha of QN2 subwatershed to decrease the uncertainties in estimating average recharges. It was assumed that the boundary of the watershed is closed and all the recharged water that enters the saturated
regime returns to the stream as baseflow after a relatively long period of time. The assumption, which could be valid in a basin scale watershed, was changed later because the steady-state MODFLOW simulation did not converge. As a result, constant head boundary was added near the watershed outlet by considering the fact that contour lines of ground water table elevation are perpendicular to the watershed boundary near outlet areas. The water flux through the boundary is simulated by the ground water model. Thus, it increased the uncertainty in deciding average recharge values based on water balance.

**Average Recharge**

To consider spatial distribution of daily average recharges into the saturated zone, the approximate total recharge value throughout the watershed needs to be calculated. Because of specific head boundary near the watershed outlet, the assumption that all the water that enters the subsurface regime returns to the stream as baseflow after a relatively long period of time cannot be used. However, total annual recharge was estimated based on the closed bound assumption, and its uncertainty was considered by changing the daily average recharge values as a calibration parameter. Average annual recharge value was calculated based on the observed daily baseflow data during the four years of the simulation period (1987-1990). Daily baseflow was estimated based on daily total runoff using the filter, which is provided in the SWAT model (Arnold et al., 1995), and average annual recharge value was calculated based on estimated total baseflow. Then, the average annual recharge amount was distributed to the six land use types in order to consider spatial distribution based on the degree of perviousness for each land use type. The study area was divided into six recharge areas based on land use type. Figure 5.55 shows the spatial distribution of different land use types.
The selected land use categories include crop, forest, hay, pasture, low density, and high density developed areas. This distinction was made under the assumption that recharge values are related to the land use activities. For example, the recharge in urban areas would be smaller than recharge occurring in relatively pervious agricultural areas. Table 5.21 shows percent of land use, assumed degree of perviousness, and adjusted daily average recharge value for each land use type. The Recharge package of MODFLOW was used to simulate the hydrologic impact of different land use and agricultural managements on the ground water system (McDonald and Harbaugh, 1988).

### Table 5.21. Perviousness, and annual average recharge value for each land use type.

<table>
<thead>
<tr>
<th>Land use activity</th>
<th>Crop</th>
<th>Hay</th>
<th>Pasture</th>
<th>Forest</th>
<th>LDR</th>
<th>HDR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Degree of perviousness (%)</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>80</td>
<td>60</td>
</tr>
<tr>
<td>Land use percent (%)</td>
<td>33</td>
<td>2</td>
<td>4</td>
<td>59</td>
<td>0.4</td>
<td>2</td>
</tr>
<tr>
<td>Average annual recharge (mm/day)</td>
<td>1.052</td>
<td>1.066</td>
<td>1.052</td>
<td>1.052</td>
<td>0.841</td>
<td>0.631</td>
</tr>
</tbody>
</table>

**Results and Discussion**

*Steady-State Calibration of MODFLOW*

Table 5.22 shows a summary of the steady-state calibration results for both hydraulic head and stream-flow rate. Mean error for the hydraulic head was 3.07 m based on 33 observation points.
According to the spatial distribution of average ground water table elevation in Figure 5.53, maximum values occurred near the headwater of the watershed and minimum hydraulic head occurred near the watershed outlet. The simulated and observed minimum values are close to each other with 15.7 m and 15.2 m of hydraulic heads, respectively. Median value of simulation results was greater than that of observed values, while the maximum predicted value was greater. Figure 5.56 shows the scatter-plot of observed and simulated hydraulic head at monitoring wells described in Figure 5.53. According to the error statistics in Table 5.22 and Figure 5.56, the model closely reproduced the trend in ground water table elevations both near the watershed outlet and in the headwater of the watershed. However, most of overprediction occurred near the middle area of the watershed. As mentioned previously, the hydraulic head information at each calibration data points are not actually measured values. Only one point, GN1-2, has a measured value, which is an average ground water table elevation based on GN1 and GN2. The observed hydraulic head at GN1-2 was 28.47 m compared with the simulated hydraulic head of 31.78 m. Results indicate that the steady-state model reasonably reproduces the spatial distribution of the hydraulic head throughout the watershed. In the case of stream fluxes, the percent error was -7.1% with the flow rate of 2257 m³/day and 2097 m³/day values for the observed and simulated, respectively. These data also illustrate the performance of the model and show that the model does a relatively good job of matching the observed hydraulic head elevation and streamflow rates.

Table 5.22. Results of steady-state calibration of MODFLOW for the QN2 Subwatershed.

<table>
<thead>
<tr>
<th>Component</th>
<th>Criteria</th>
<th>Obs. (m)</th>
<th>Sim. (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydraulic head</td>
<td>Min. head</td>
<td>15.7</td>
<td>15.2</td>
</tr>
<tr>
<td></td>
<td>Max. head</td>
<td>42.5</td>
<td>40.7</td>
</tr>
<tr>
<td></td>
<td>Median head</td>
<td>27.9</td>
<td>31.8</td>
</tr>
<tr>
<td></td>
<td>Mean error</td>
<td></td>
<td>3.07</td>
</tr>
<tr>
<td></td>
<td>Mean abs. error</td>
<td>3.30</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Root mean sq. error</td>
<td>3.66</td>
<td></td>
</tr>
<tr>
<td>Stream flow</td>
<td>Flow rate (m3/day)</td>
<td>2257</td>
<td>2097</td>
</tr>
<tr>
<td></td>
<td>Percent error (%)</td>
<td></td>
<td>-7.1</td>
</tr>
</tbody>
</table>
Figure 5.56. Observed and simulated hydraulic head at monitoring wells of QN2.

**Transient Simulation of Linked Approach**

Comparison of observed and simulated annual total runoff and sediment yields, along with the summary of model performance criteria, by the linked and integrated GW approach for calibration period at QN2 are shown in Table 5.23. Integrated GW approach uses its own ground water components described in Equation 3.23 and Figure 3.10 for simulating baseflow based on spatially distributed recharge fluxes, while the linked GW approach uses existing ground water models such as MODFLOW and MT3D instead of the baseflow components in DANSAT. Results from both integrated and linked GW approaches were compared in this section since a major objective is to assess the effectiveness of BMPs on both hydrology and water quality by considering the interaction between surface and ground water. The purpose of comparison is not to decide which approach is better, but rather to provide model users with a better understanding of the response of baseflow based on different GW approaches. Cumulative total runoff volume was well predicted with -7.09% percent error. Total runoff by the linked approach during simulation period was decreased to 1714 mm compared to 1833 mm by the integrated approach.
Daily NOF values for the two different approaches were the same, while the daily Nash-Sutcliffe efficiency index (E) was slightly higher in the linked approach. However, monthly E value by the linked approach was much higher (0.60) compared to the value of 0.53 by the integrated approach. Monthly NOF also decreased with similar values for both approaches (0.16 for the linked approach and 0.15 for the integrated approach). Figure 5.57 shows temporal comparison of observed and simulated monthly runoff by the integrated and linked GW approaches. In the integrated GW approach, monthly runoffs were underestimated during 1987 and 1988, overestimated during 1989, and were close to the observed values during 1990. However, monthly runoff by the linked approach was closely reproduced from the beginning of simulation to October 1989 and was underestimated during the remaining period. The overall performance statistics can be improved (Monthly E value of up to 0.73) in the linked approach by increasing the infiltration and percolation values. However, model calibration was stopped at this point considering the reasonable ranges of parameters obtained. Hydrology components of DANSAT in both surface and subsurface are sensitive to soil related parameters such as total porosity and field capacity. Total porosity was increased and field capacity was decreased to increase baseflow. Similarly, performance statistics by the integrated approach can be improved when different input parameters set from the linked approach are used. However, same input parameters were used for both approaches except for the ground water component. As a result, a set of parameters was selected to satisfy both integrated and linked GW approaches.

The model underpredicted total sediment loss by the linked approach with -44.54% error when the same sediment related parameters obtained during the calibration in the integrated approach to fit the total sediment loss are used. The total sediment loss by the linked approach during the simulation period decreased from 4896 kg/ha to 2570 kg/ha for the integrated approach. Both monthly NOF and E values were improved in the linked approach compared with the integrated approach. Time-series comparisons of observed and simulated monthly sediment yields by integrated and linked GW approaches are shown in Figure 5.58. The monthly sediment losses were closely predicted by the two different ground water approaches during 1987 and 1988, while significant differences between the two approaches occurred during 1989 and 1990. This can be explained by the fact that sediment simulation by DANSAT is very sensitive to higher flow rates, and thus the integrated approach overestimated and the linked approach underestimated total runoff during 1989 and 1990 of high flow rates. Thus, better estimates of runoff during 1990 can be obtained by increasing baseflow, which could also improve the estimates of monthly trends in sediment loss by the linked approach. The prediction of monthly trends of sediment loss can also
be improved by using a different parameter set from the integrated approach and shifting up simulated total sediment loss close to the observed total sediment loss.

In summary, the linked approach was better for predicting the temporal trends of monthly runoff and sediment loss than the integrated approach. However, the differences were negligible. The linked GW approach has several advantages compared to the integrated approach in spite of the fact it requires a much longer calculation time and the difficulties in obtaining input parameters and observed data for the calibration of ground water models. The major advantage of the linked system is that the approach is able to provide the spatial distribution and temporal changes in ground water table elevation or pesticide concentration in ground water. Figure 5.59 shows the spatial distribution of ground water table elevation predicted by MODFLOW at the end of the simulation period.

Table 5.23. Comparison of observed and simulated annual total runoff and sediment yields by the linked GW approach for calibration period at QN2, along with the summary of model performance criteria.

<table>
<thead>
<tr>
<th>Year</th>
<th>Runoff</th>
<th>Sediment</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Obs.</td>
<td>Sim.</td>
<td>Obs.</td>
<td>Sim.</td>
<td></td>
</tr>
<tr>
<td>1987</td>
<td>425</td>
<td>403 (358)</td>
<td>1084</td>
<td>365 (316)</td>
<td></td>
</tr>
<tr>
<td>1988</td>
<td>356</td>
<td>350 (323)</td>
<td>706</td>
<td>329 (334)</td>
<td></td>
</tr>
<tr>
<td>1989</td>
<td>479</td>
<td>489 (578)</td>
<td>1115</td>
<td>1154 (2430)</td>
<td></td>
</tr>
<tr>
<td>1990</td>
<td>586</td>
<td>472 (574)</td>
<td>1729</td>
<td>721 (1816)</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>1845</td>
<td>1714 (1833)</td>
<td>4634</td>
<td>2570 (4896)</td>
<td></td>
</tr>
<tr>
<td>Percent Error</td>
<td>-7.09 (-0.64)</td>
<td>-44.54 (5.64)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Monthly NOF</td>
<td>0.15 (0.16)</td>
<td>0.97 (1.20)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Monthly E</td>
<td>0.60 (0.53)</td>
<td>-1.10 (-2.24)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Daily NOF</td>
<td>0.33 (0.33)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Daily E</td>
<td>0.60 (0.59)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

( ) : summary from linked GW approach
NOF: Normalized objective function (units are mm and kg/ha for hydrology and sediment, respectively)
E: Nash-Sutcliffe model efficiency
Figure 5.57. Time-series comparison of observed and simulated monthly runoff by integrated and linked GW approaches.

Figure 5.58. Time-series comparison of observed and simulated monthly sediment yields by integrated and linked GW approaches.
Summary and Conclusions

DANSAT was applied to one field plot and two agricultural watersheds in Virginia to validate the model components and evaluate the performance in predicting runoff, sediment loss, and pesticide loads. A newly developed user interface was used to generate intensive model inputs for both plot-scale and watershed-scale applications.

Cell components were validated on a corn plot with conventional tillage. The model performed well in predicting total surface runoff, sediment load, and pesticides loads during the simulation period in which only one cell was used without the use of routing components. Movements of percolated water and pesticides in the root zone of the plot were also well reproduced by the model. However, the model did not perform well when predicting the temporal changes in sediment load using the dynamic erodibility approach of the model in which rill and interrill erodibility parameters are predicted by soil components on a daily basis. The overall result showed that DANSAT needs to realistically simulate temporal changes in erodibility parameters by considering factors such as accumulated rainfall energy after tillage application, soil characteristics, and surface cover condition influenced by agricultural management practices.
The routing related components for hydrology and sediment were validated on the Owl Run watershed using the internal validation approach without considering the baseflow. The model, which was calibrated at the outlet of the watershed, predicts runoff and sediment load for internal subwatershed reasonably well with minimum calibration. Monthly and daily Nash-Sutcliffe efficiency indexes (E) for runoff were greater than 0.5 on all three watersheds, while the monthly E for sediment load were greater than 0.5 only in QOA and QOD watersheds. The overall trend in total sediment load in each subwatershed was similar to the hydrology. Simulated total runoff and sediment loads in QOA and QOD were within the range of ±10% error, while both total runoff and sediment load were highly overpredicted in QOC with the percent error of over 30%. The overprediction of runoff and sediment loads in QOC could be due to the fact that two reservoirs are located in QOC sub-watershed, and DANSAT does not have a reservoir component for considering evaporation and seepage losses and sediment deposition in reservoirs. Daily total runoff was underestimated for large storm events for which the effective hydraulic conductivity for Green-Ampt infiltration equation seems to be overestimated by the soil components. Underestimation of runoff during large storm events resulted in the underestimation of sediment yields. The overall results, including high Nash-Sutcliffe efficiency index (E) values, low total percent error, and negligible differences in normalized objective function (NOF) values among subwatersheds for both hydrology and sediment load, indicate that the model consistently predicts spatially distributed surface runoff and sediment load at watershed scale with minimum calibration.

The integrated baseflow components were validated for hydrology, sediment, and pesticide using the split-sample method on QN2 watershed, which is located in the Coastal Plain of Virginia. The model performed well in predicting the total runoff for both calibration and validation periods with 0.64% and -5.12% percent errors, respectively. The daily Nash-Sutcliffe efficiency index (E) was greater than the monthly E value for both calibration and validation periods. The daily E values were also greater than 0.5 for calibration and validation periods. DANSAT simulated the overall fluctuation of monthly total runoff reasonably well for the calibration period (with a 0.53 monthly E value), while DANSAT failed to simulate the fluctuations of baseflow for the validation period (monthly E value less than 0.5). Spatial distribution of simulated ground water recharge showed that higher recharge values were predicted in cells with higher drainable soil characteristics and higher accumulated flow during the overland routing procedure. DANSAT failed to simulate the temporal fluctuations of monthly sediment loads for the calibration and validation periods even though DANSAT predicted the total sediment yields for both periods.
relatively well. The poor relationship between observed daily discharge and daily total sediment load caused difficulties in simulating the temporal fluctuations of sediment loads. Predicted sediment yield by DANSAT was sensitive to the changes in the shapes of stream cross section. Rectangular and triangular stream cross sections resulted in different temporal changes in sediment yields, even though the same amount of water was available in each stream type. The rectangular stream cross section was more sensitive to the changes in flow rates, especially during high flows. The pesticide component was also validated using 10-minute time-step. DANSAT failed to simulate the temporal trend of daily atrazine load for both calibration and validation periods.

A linked ground water system using the dual simulation approach was evaluated on the QN2 watershed. Ground water model, MODFLOW, was calibrated against both hydraulic head and stream-flow rate using the steady-state simulation. Steady-state simulation results illustrated that MODFLOW reasonably reproduced the spatial distribution of the hydraulic head and stream flow rates throughout the watershed. Only runoff and sediment yields were simulated using the linked approach. Pesticide was not simulated because of a lack of input data for the saturated zone, even though the interface for linkage between DANSAT and MT3D is available. Results from the integrated and linked approaches were compared with the observed daily stream flow and sediment yields. The linked approach improved seasonal trend of baseflow prediction compared to the integrated approach, even though the ground water recharge during the wet years were not still enough to increase the baseflow in streams. The linked approach performed poorly in predicting total sediment loss with -44.54% percent error, while the linked approach was better in predicting the temporal trends of monthly sediment loss. Advantage of the linked approach was demonstrated by displaying the spatial distribution of ground water table elevation at the end of the simulation period.

References


Chapter 6: Sensitivity Analysis

Introduction

Parameters can be divided into two categories in the distributed model application: functional parameters and structural parameters. Functional parameters represent the general model input parameters, which usually can be used for model calibration and validation. Structural parameters, which should be decided before the preparation of functional parameters for the distributed modeling application, include grid size and time-step and could have a significant impact on the model results.

Grid size determination in NPS modeling is often based on manpower, database resolution and storage, and time constraint, even though it should be based on the spatial variability of the watershed and computational algorithm of the model (Vieux and Needham, 1993). Smaller grid size is recommended for distributed parameter models to satisfy the assumption that all properties, including soil and land use, are homogeneous within each grid (Dillaha, 1990). Considering the computational limitation of a physically-based and distributed parameter, selection of a coarser grid resolution is attractive because it would substantially reduce computational time and resources. However, selection of an appropriate grid resolution for particular hydrologic modeling is limited by lack of understanding of: 1) scale effects on land surface representation and 2) the concept and assumptions upon which the computational algorithms of a particular model are based.

The availability of spatial data and development of user interface, which is usually integrated with GIS, provides the basis for sensitivity analysis of distributed hydrological models to different grid size. Some previous researchers have only focused on the effects of different grid size, especially DEM, on the parameterization and representation of watershed characteristics (Armstrong and Martz, 2003; Moglen and Hartman, 2001). However, more attention has been given to the grid size sensitivity analysis of some models such as SWAT (Cho and Lee, 2001), TOPMODEL (Brasington and Richards, 1998; Bruneau et al., 1995; Saulnier et al., 1997; Valeo and Moin, 2000; WenLing et al., 1999; Zhang and Montgomery, 1994), CASC2D (Molnar and Julien, 2000), AGNPS (Panuska et al., 1991; Vieux and Needham, 1993), ANSWERS (Brown et al., 1993), MIKE SHE (Refsgaard, 1997; Styczen et al., 1999; Vzquez et al., 2002), and WEPP (Cochrane and Flanagan, 2005). Mankin et. al (2002) assessed AGNPS input data, which is generated using Arc/Info interface, by the cell-by-cell comparison with manually-created data.
Topographic data comparison showed the lowest degree of agreement due to inappropriate selection of grid size. Cho and Lee (2001) investigated the sensitivity of SWAT to the two different sources of DEM. In their study, the use of finer DEM resulted in higher runoff volume and the increased average slope was suggested as a major factor impacting the results. Molnar and Julien (2000) analyzed the effects of grid size on surface runoff using CASC2D model. Vieux and Needham (1993) investigated the grid size sensitivity of AGNPS. They reported that sediment yield increased with the coarser grid size where stream lengths were shortened. Bruneau et. al.(1995) studied the effect of grid and time resolutions on the hydrologic response of TOPMODEL. The results showed that appropriate ranges of grid and time resolutions can be defined for the input variables without significant degradation of modeling efficiency. The time-step needed to be decreased as grid size decreased in order to maintain stability of the numerical solutions. However, few studies have investigated the overall impact of grid size by separating it into the impact due to the mechanisms or algorithm of the distributed model and the impact due to the changes in model input parameter, which are usually defined based on grid size.

Borah and Bera (2003) summarized the temporal scale of existing distributed, continuous, watershed-scale hydrologic and NPS pollution models. AnnAGNPS uses daily time-step; the current version of ANSWERS-2000 uses dual time-steps: daily for dry days and 30 seconds for days with precipitation; MIKE SHE and CASC2D use variable steps depending on the numerical stability. Physically-based models usually have a short time-step. Short time-step increases the computational time. ANSWERS requires a small time-step of 60 seconds or less to minimize errors in the solution of the continuity equation even during no runoff producing precipitation (Bouraoui, 1994). It was also reported that CASC2D and MIKE SHE would be more appropriate for small watersheds in continuous simulation mode due to the computationally intensive numerical scheme (Borah and Bera, 2003). Bouraoui (1994) recommended determining the threshold time-step of ANSWERS for the time related efficiency.

Functional sensitivity analysis has been used for identifying critical model parameters and as guidelines for future sampling and experimental design (Ma et al., 1998). However, sensitivity analysis also can be used to find programming errors and gain insight into the nature of the model. Both deterministic and stochastic approaches have been used for the sensitivity analysis of NPS models. The stochastic approach usually varies multiple parameters simultaneously based on predefined parameter ranges and underlying probability distribution. This approach requires large number of simulation runs (Haan and Zhang, 1996). Deterministic sensitivity analysis is not
appropriate when dealing with the model’s uncertainties caused by errors in parameter estimation. This approach is commonly based on independent parameter changes in which one parameter is varied individually with the other parameter fixed at base values. Difficulties exist in performing deterministic sensitivity analysis because of complex interactions between parameters. Sensitivity of an individual parameter changes according to the values taken by other parameters and based on the state of the system (Anderton et al., 2002). Ferreira et al. (1995) discussed the site- and condition-specific nature of sensitivity analysis and demonstrated that user-side sensitivity analysis is an essential step in model application even though general sensitivity analyses are provided by model developers. In the deterministic sensitivity analysis, parameter values can be changed based on the specific percentage of base value or reasonable range determined by measurement.

Generally, difficulties in the sensitivity analysis of watershed-scale, distributed, physically-based model rise because there are too many parameters, which usually impact a local area of watershed. Changes in spatially distributed parameter value influence the characteristics of one cell or a local area where the parameter value is assigned. Only watershed-scale parameters influence changes in the characteristics of the overall watershed. As models become more complex, data and parameter requirements and uncertainty in model prediction may increase (Anderton et al., 2002). Models having unnecessary complexity will require more efforts to achieve expected results. From this point of view, the deterministic sensitivity analysis approach is more appropriate for the distributed, physically-based model, which requires long computational time. Few efforts have been made to evaluate the sensitivity of the three-dimensional watershed models by considering the horizontal- and vertical-distribution of parameter values. Byrne (2000) reduced the number of soil, crop, and channel types to one in order to simplify the sensitivity analysis of ANSWERS-2000.

The overall goal of this chapter is to analyze the sensitivities of newly developed watershed-scale, distributed, physically-based model, DANSAT, to different grid size, time-step, and functional model input parameters. Specific objectives are to 1) find programming errors as an extended validation procedure by checking the expected model response to a specific model input parameter; 2) provide 3-dimensional sensitivity analysis approach by considering the model response to model parameters, which are horizontally distributed on overall watershed and vertically distributed in multi-soil layers; 3) provide an approach for deciding the appropriate range of grid size in which spatial distribution of soil, land use, and topographic parameters can
be appropriately represented and reasonable accuracy of model simulation can be achieved; and 4) provide appropriate ranges of time-step without significant reduction of model accuracy in order to decrease the computational time.

**Parameter Sensitivity Analysis**

**Methods**

**Statistics**

Relative sensitivity, which describes how model output varies over changes of input parameters, was selected as an evaluation parameter and is estimated using the equation:

\[
S_r = \frac{\Delta O}{O} \times \frac{\Delta P}{P} \quad (6.1)
\]

Where, \( S_r \) = relative sensitivity, \( \Delta O \) = change in the output, \( O \) = base output, \( \Delta P \) = the change in the parameter value, and \( P \) = the base parameter value.

If the reasonable range of a parameter value is available, the relative sensitivity \( (S_r) \) can be expressed by:

\[
S_r = \frac{(O_2 - O_1)}{O_{12}} \times \frac{(P_2 - P_1)}{P_{12}} \quad (6.2)
\]

Where, \( P_1 \) and \( P_2 \) = the least and greatest values of the parameter used, respectively, \( P_{12} \) = average of \( P_1 \) and \( P_2 \), \( O_1 \) and \( O_2 \) = output for the two parameter values, and \( O_{12} \) = average of the two outputs.

The parameter \( S_r \) is a function of selected input parameter range because of the nonlinear response of model to input parameters. The approach of using specific percentage of the base value is common and was selected in this study for parameters for which reasonable ranges are not available. The sensitivity \( (S_r) \) is expressed by:

\[
S_r = \frac{(O - O_b)}{O_b} \times \frac{(P - P_b)}{P_b} \quad (6.3)
\]

Where, \( b \) represents a base value.
Limitations of linear methods used for sensitivity analysis (Equation 6.1 through 6.3), as mentioned by previous researchers (Anderton et al., 2002; Beven, 1989), include 1) the linear form of sensitivity parameter does not consider the entire range of the parameter because of the nonlinear response of the model, 2) it is difficult to consider interaction between variables, and 3) this approach gives a deterministic single value of the sensitivity parameter. Even though the stochastic approach can resolve some of these limitations, the deterministic approach was selected because of the intensive computation time required by the distributed and physically-based model, DANSAT. The sensitivity parameter was calculated at six different levels (+50%, +25%, +10%, -10%, -25%, and -50% changes from base value) to consider the non-linear response of the model to input parameters. Relatively wide ranges of the input parameters were selected in order to test the model response to the extreme parameter values.

A sensitivity index providing a method to compare overall relative sensitivities of output variables was then calculated using the equation:

\[ SI = \frac{1}{N} \sum_{i=1}^{N} |S_r(i)| \]  

(6.4)

Where, SI = sensitivity index for each output variable and N = total number of theoretically possible occurrences for S_r.

**Procedures**

Sensitivity analysis for three-dimensional distributed parameter models such as DANSAT is very complex. For example, horizontal distribution of soil parameters is considered in DANSAT by assigning different soil types to grid cells, and the soil parameter also varies vertically in the soil layers. In this study, sensitivity analysis was done in two different scales including field-scale and watershed-scale. First, field-scale sensitivity analysis involved two steps: 1) preliminary sensitivity analysis to assort sensitive field-scale parameters without considering multiple soil layers and 2) soil layer sensitivity analysis to determine the model response to the changes in soil parameters for different soil layers. Watershed-scale sensitivity analysis was also performed in two steps: 1) to compare relative sensitivity between selected field-scale parameters and watershed-scale parameters and 2) to understand how the model responds to changes of soil parameters in different locations in the watershed. A sensitive parameter at the field-scale may not be sensitive at the watershed-scale because the impacts of the field-scale parameter can be
alleviated during the cell routing related processes. Parameters used in both field-scale and watershed-scale sensitivity analyses are listed in Table 6.1.

Table 6.1. List of field-scale, watershed-scale, and channel related parameters used in sensitivity analysis

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Parameter description analysis.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Spatial parameters (Field-scale parameters)</strong></td>
<td></td>
</tr>
<tr>
<td>TPor</td>
<td>Total porosity</td>
</tr>
<tr>
<td>FCap</td>
<td>Field capacity</td>
</tr>
<tr>
<td>PClay</td>
<td>Percent clay</td>
</tr>
<tr>
<td>PSand</td>
<td>Percent sand</td>
</tr>
<tr>
<td>PSilt</td>
<td>Percent silt</td>
</tr>
<tr>
<td>POM</td>
<td>Percent of organic matter</td>
</tr>
<tr>
<td>Ksat</td>
<td>Saturated hydraulic conductivity for soil layers</td>
</tr>
<tr>
<td>K_eff</td>
<td>Effective hydraulic conductivity for Green-Ampt infiltration equation</td>
</tr>
<tr>
<td>Kinter</td>
<td>Constant interrill erodibility</td>
</tr>
<tr>
<td>MRtDep</td>
<td>Maximum root depth (m)</td>
</tr>
<tr>
<td>D2GWT</td>
<td>Depth to the ground water table from surface (m)</td>
</tr>
<tr>
<td>RR2nd</td>
<td>Random roughness of secondary tillage immediately after tillage (m)</td>
</tr>
<tr>
<td>HLsoil</td>
<td>Half-Life on soil</td>
</tr>
<tr>
<td>Koc</td>
<td>Partitioning coefficient</td>
</tr>
<tr>
<td>AppDep</td>
<td>Pesticide application depth</td>
</tr>
<tr>
<td><strong>General parameters (Watershed-scale parameters)</strong></td>
<td></td>
</tr>
<tr>
<td>InfilDep</td>
<td>Effective soil depth for infiltration calculation</td>
</tr>
<tr>
<td>RainFac</td>
<td>Rainfall adjustment factor for K_eff</td>
</tr>
<tr>
<td>RSpace</td>
<td>Rill space</td>
</tr>
<tr>
<td>ManRill</td>
<td>Manning's n in the rill</td>
</tr>
<tr>
<td>FDroff</td>
<td>Fraction of dissolved chemical avail for runoff</td>
</tr>
<tr>
<td>InterDep</td>
<td>Interflow depth</td>
</tr>
<tr>
<td>AnioFac</td>
<td>Anisotropic factor for interflow (Khor/Kver)</td>
</tr>
<tr>
<td>LenRill</td>
<td>Length for rill detachment calculation (m)</td>
</tr>
<tr>
<td>LenChan</td>
<td>Length for channel detachment calculation (m)</td>
</tr>
<tr>
<td>GwCoeff</td>
<td>Baseflow coefficient</td>
</tr>
<tr>
<td>GwPow</td>
<td>Power coefficient for baseflow equation</td>
</tr>
<tr>
<td>GwSlope</td>
<td>Slope coefficient for baseflow equation</td>
</tr>
<tr>
<td>GwInter</td>
<td>Intercept for the baseflow equation</td>
</tr>
<tr>
<td>GwThr</td>
<td>Threshold value for the baseflow equation</td>
</tr>
<tr>
<td>GwBD</td>
<td>Average bulk-density in ground water zone</td>
</tr>
<tr>
<td>GwTPor</td>
<td>Average total porosity in ground water zone</td>
</tr>
<tr>
<td>Disp</td>
<td>Dispersivity</td>
</tr>
<tr>
<td>AHGrad</td>
<td>Average hydraulic gradient</td>
</tr>
<tr>
<td><strong>Channel related parameters</strong></td>
<td></td>
</tr>
<tr>
<td>ChaWid</td>
<td>Channel width</td>
</tr>
<tr>
<td>FUES</td>
<td>Fraction of Unerodible channel Soil, or erosion resistant</td>
</tr>
<tr>
<td>CClay</td>
<td>Percent clay in channel</td>
</tr>
<tr>
<td>CSand</td>
<td>Percent sand in channel</td>
</tr>
<tr>
<td>CSilt</td>
<td>Percent silt in channel</td>
</tr>
<tr>
<td>COM</td>
<td>Percent organic matter in channel</td>
</tr>
</tbody>
</table>

* Only for constant hydraulic conductivity approach

Preliminary sensitivity analysis was applied to the QNB plot using the same data set used in the validation chapter, except for the assumption of homogeneous soil layers. Total runoff, sediment
load, and pesticide loads in the surface runoff, as well as water and pesticides fluxes to ground water table, were used as output variables. A homogeneous soil profile was assumed to exclude the impact of soil layers on a selected output variable. Effective hydraulic conductivity parameter for infiltration calculation is an important parameter to distribute excess rainfall into surface and subsurface related processes. The parameter can be predicted daily by DANSAT based on several one-cell parameters selected in Table 6.1 (dynamic method) or a user-defined constant value can be used throughout the simulation period (constant method). Preliminary sensitivity of field-scale parameters was conducted based on both dynamic and constant methods for the effective hydraulic conductivity parameter. To adequately reflect the physical meaning, simultaneous changes in two or more parameters was occasionally necessary. The sum of clay, sand, and silt percent should be 100% and increase in clay percent should cause decrease in silt or sand percent. In this study, increase or decrease of percent of a soil particle class such as clay, silt, or sand was considered by equally distributing the changes to the remaining soil particle classes.

Among selected field-scale parameters based on the preliminary sensitivity analysis, only the soil layer related parameters were changed to determine the sensitivity of the location of soil layer to water quantity and quality in both surface and ground water. Soil layer sensitivity was analyzed based on the dynamic approach for the effective hydraulic conductivity. Soil related parameters were changed in three different locations of soil layer: top (0-1.52m), middle (1.52-5.26m), and bottom (5.26-9.0m). Top, middle, and bottom locations of the soil layer represent root zone soil layers, upper half of intermediate zone soil layers, and the remaining half of intermediate zone soil layers, respectively. Weighted changes in input parameters for each layer location were used to consider different depth of soil layers. The weighted change in soil parameters for different layer location was calculated based on the total depth of the soil profile by:

$$\frac{\Delta P}{P} = \frac{D_1 \cdot \Delta P_1 / P_1 + D_2 \cdot \Delta P_2 / P_2 + \cdots + D_n \cdot \Delta P_n / P_n}{D_1 + D_2 + \cdots + D_n}$$

(6.5)

Where, $D_n$ = thickness of the soil layer using parameter value $P_n$ and $n$ = total number of soil layers.

Watershed-scale sensitivity analysis was applied to the QN2 subwatershed. Changes in the watershed-scale parameters, listed in Table 6.1, have impact on overall watershed response. In order to compare relative sensitivity between selected field-scale parameters and watershed-scale parameters, one homogeneous soil and crop rotation was assumed throughout the watershed area.
The calculated sensitivity index based on field-scale parameters was compared with the result based on watershed-scale parameters. Total runoff, sediment load, and pesticide loads at the watershed outlet, as well as water and pesticide fluxes through the interface between intermediate and ground water zones, were used as output variables in watershed-scale sensitivity analysis.

The user can change the spatially distributed field-scale parameters in a specific location or throughout the watershed. Parameter changes in a specific soil type impacts the specific location where the soil type is located in a watershed. Sensitivity of selected output variables based on the changes in soil related parameters at different locations was analyzed based on weighted changes in soil parameters using the equation:

$$\frac{\Delta P}{P} = \frac{NC_1 \cdot \Delta P_1 / P_1 + NC_2 \cdot \Delta P_2 / P_2 + \cdots + NC_n \cdot \Delta P_n / P_n}{NC_1 + NC_2 + \cdots + NC_n}$$

(6.6)

Where, $NC_n$ = the number of cells using parameter value $P_n$, which is distributed horizontally in a watershed, and $n$ = total number of parameter types (soil types) in a watershed.

For the sensitivity analysis, the entire soil depth was assumed homogeneous. Two different soil groups were assigned for considering the changes in soil related parameters at different locations. The two soil groups included 1) soils existing near the watershed boundary and 2) soils existing near streams. Figure 6.1.a shows the spatial distribution of soil groups for location sensitivity analysis. Instead of using the actual spatial distribution of soil types, which is shown in Figure 6.1.b, one of the two soil groups was assigned to each cell based on the cell number. Among 265 total number of cells, near watershed boundary soil group was assigned to the cells where cell numbers 1 to 132 were assigned, while near stream soil group was assigned to the remaining cells. The simulated outflow in a cell is added to the downstream cell according to the order of routing calculation, which is defined by the cell number. Flow path from a boundary cell to a stream cell is an important factor to be considered in a distributed parameter model. As a result, soil type was assigned to each cell by considering the flow routing pass rather than the straight distance from a cell to a nearest stream segment.
Figure 6.1. Spatial distribution of soil groups for the soil location sensitivity analysis according to (a) cell number and (b) actual soil types.

Results and Discussion

Field-scale Sensitivity Analysis

Table 6.2 shows the selected field-scale parameters from preliminary sensitivity analysis and calculated sensitivity index for each output variable. RSpace and FDruff parameters, which were used for model calibration in the previous chapter, were treated as field-scale parameters in the analysis even though they are watershed-scale parameters. Surface related output variables included total runoff amount, total sediment load, and total pesticide load during simulation period. Subsurface related output variables included recharge flux and pesticide flux through the interface between intermediate zone and saturated zone. Atrazine was selected for the pesticide output variables for both surface and subsurface. Figure 6.2 through Figure 6.18 show the sensitivity index for five different output variables based on changes in each selected parameter value.
Table 6.2. Summary of preliminary field-scale sensitivity analysis of DANSAT for surface and subsurface output variables.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Baseline</th>
<th>Approach</th>
<th>Surface runoff</th>
<th>Surface sediment load</th>
<th>Surface pesticide load</th>
<th>Recharge to GW</th>
<th>Pesticide flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>TPor</td>
<td>0.387</td>
<td>D</td>
<td>0.04</td>
<td>0.02</td>
<td>-0.08</td>
<td>-2.82</td>
<td>-1.40</td>
</tr>
<tr>
<td></td>
<td></td>
<td>C</td>
<td>0.01</td>
<td>0.01</td>
<td>0.10</td>
<td>-1.73</td>
<td>-2.22</td>
</tr>
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<td>FCap</td>
<td>0.192</td>
<td>D</td>
<td>0.49</td>
<td>0.48</td>
<td>0.95</td>
<td>-1.02</td>
<td>-0.65</td>
</tr>
<tr>
<td></td>
<td></td>
<td>C</td>
<td>0.38</td>
<td>0.34</td>
<td>0.74</td>
<td>-0.91</td>
<td>-1.07</td>
</tr>
<tr>
<td>PClay</td>
<td>11.7</td>
<td>D</td>
<td>0.70</td>
<td>0.95</td>
<td>0.53</td>
<td>-0.41</td>
<td>-0.14</td>
</tr>
<tr>
<td></td>
<td></td>
<td>C</td>
<td>-0.09</td>
<td>-0.08</td>
<td>-0.12</td>
<td>0.05</td>
<td>0.03</td>
</tr>
<tr>
<td>PSand</td>
<td>61.5</td>
<td>D</td>
<td>-0.46</td>
<td>-1.32</td>
<td>-0.15</td>
<td>0.31</td>
<td>0.11</td>
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<tr>
<td></td>
<td></td>
<td>C</td>
<td>1.46</td>
<td>1.52</td>
<td>1.74</td>
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<td>-0.30</td>
</tr>
<tr>
<td>PSilt</td>
<td>26.4</td>
<td>D</td>
<td>-0.89</td>
<td>-0.80</td>
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<td>0.18</td>
</tr>
<tr>
<td></td>
<td></td>
<td>C</td>
<td>-0.38</td>
<td>-0.34</td>
<td>-0.41</td>
<td>0.09</td>
<td>0.05</td>
</tr>
<tr>
<td>POM</td>
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<td>D</td>
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<td>0.05</td>
<td>1.37</td>
<td>-0.03</td>
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</tr>
<tr>
<td></td>
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<td>1.50</td>
<td>0.00</td>
<td>-0.93</td>
</tr>
<tr>
<td>Ksat</td>
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<td>D</td>
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<td>-0.02</td>
<td>-0.57</td>
<td>1.77</td>
<td>1.41</td>
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<tr>
<td></td>
<td></td>
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<td>-0.02</td>
<td>-0.33</td>
<td>1.03</td>
<td>1.33</td>
</tr>
<tr>
<td>K_{eff}</td>
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<td></td>
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<td>0.00</td>
<td>0.00</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>C</td>
<td>0.00</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>MRtDep</td>
<td>1.52</td>
<td>D</td>
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<td>-0.02</td>
<td>-0.20</td>
<td>0.59</td>
<td>0.30</td>
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<td></td>
<td></td>
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<td>-0.18</td>
<td>0.57</td>
<td>0.59</td>
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<td>0.00</td>
<td>0.00</td>
<td>-2.73</td>
<td>-1.67</td>
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<tr>
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<td></td>
<td>C</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>-1.45</td>
<td>-1.96</td>
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<td>RR2nd</td>
<td>0.30</td>
<td>D</td>
<td>-0.26</td>
<td>-0.49</td>
<td>-0.75</td>
<td>0.14</td>
<td>0.05</td>
</tr>
<tr>
<td></td>
<td></td>
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<td>-0.02</td>
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<td>0.09</td>
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<td></td>
<td></td>
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<td>1.00</td>
</tr>
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<td>Koc</td>
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<td>0.00</td>
<td>-0.94</td>
</tr>
<tr>
<td></td>
<td></td>
<td>C</td>
<td>0.00</td>
<td>0.00</td>
<td>1.41</td>
<td>0.00</td>
<td>-0.94</td>
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<td>D</td>
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<td>0.00</td>
<td>2.58</td>
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</tr>
<tr>
<td>RSpace*</td>
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<td>D</td>
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<td>0.82</td>
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<td>D</td>
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<td>0.79</td>
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<tr>
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<td>C</td>
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<td>0.00</td>
<td>0.78</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

D: dynamic approach for the effective hydraulic conductivity
C: constant approach for the effective hydraulic conductivity
* : treated as field-scale parameters

Sensitivities of output variables to changes in total porosity (TPor) of soil are shown in Figure 6.2. Subsurface outputs such as recharges and pesticide flux to ground water were sensitive to changes in total porosity while surface outputs were not. An increase in the total porosity decreased subsurface outputs by -2.82 and -1.40 of sensitivity index in the dynamic approach, respectively. An increase in the total porosity of the soil resulted in an increase of soil space in which more...
infiltrated water can be stored and extracted through evapotranspiration process. If the same amount of water is infiltrated and more water is extracted through evapotranspiration, less water will be percolated through soil profile. Atrazine has moderate solubility in water and a similar trend to the hydrology was expected in pesticide flux to ground water.

Results of the sensitivity of output variables to changes in field capacity (FCap) of the soil are shown in Figure 6.3. The model was very sensitive to variations in the field capacity of the soil (FCap). Surface runoff increased and ground water recharge decreased as the field capacity increased. Since the field capacity is not related to the calculation of effective hydraulic conductivity, both dynamic and constant approaches showed similar trends. As expected, increased field capacity within a capacity-based percolation approach reduces the volume of available water for percolation resulting in the decrease in recharge. More water can be stored in soil layers with an increased field capacity, and effective matrix potential for Green-Ampt infiltration can be decreased resulting in a decrease in infiltration and an increase in surface runoff. Increases in sediment and pesticide loads were expected with the increased total runoff. Subsurface pesticide flux to ground water showed a similar trend to the recharge to ground water, and as expected, increased field capacity resulted in decreased pesticide flux to ground water.

Sensitivities of output variables to changes in clay content (PClay) of the soil are shown in Figure 6.4. Only the dynamic approach results showed sensitivity to changes in clay content of the soil because clay content is directly used in estimation of effective hydraulic conductivity ($K_{eff}$) for Green-Ampt infiltration. Since the $K_{eff}$ value is fixed as user-input, neither surface and subsurface outputs were impacted by changes in clay content with the constant approach. An increase in the clay content of the soil resulted in a decrease in $K_{eff}$ value, which decreases infiltration rate and finally increases runoff volume. Increased runoff volume also resulted in a decrease in the ground water recharge.

Sensitivities of output variables to changes in sand content of the soil are shown in Figure 6.5. Both the dynamic and constant approaches sensitively responded to changes in sand content of the soil. However, the two approaches showed the opposite responses. As sand content of the soil increased, surface output variables decreased in the dynamic approach and increased in the constant approach. Sand content of the soil is connected with infiltration rates in two different ways. Sand content is related to the estimation of the effective hydraulic conductivity ($K_{eff}$), and it is also used in predicting the wetting front capillary potential ($S_f$) for Green-Ampt infiltration method. The $K_{eff}$ increases and $S_f$ decreases as sand content of the soil increases. In the constant
approach, infiltration decreased and resulted in an increase in runoff volume as sand percent increased because the $K_{eff}$ value is fixed as user-input and only $S_f$ is affected by changes in sand content. However, the impact of increases in sand content on $K_{eff}$ and $S_f$ values can cancel each other within the dynamic variable approach. In this analysis, the impact of sand content on $K_{eff}$ was greater than its impact on $S_f$ and resulted in a different response compared to the constant approach. In addition, sand content of the soil is related to soil erodibility parameters. As a result, an increase in sand content makes the soil more sensitive to the erosion process, which is driven by flow rate changes.

Sensitivity results of output variables to changes in silt content of the soil are shown in Figure 6.6. An increase in the silt content of the soil resulted in a decrease in the total runoff volume and an increase in the groundwater recharge. However, silt content of the soil is not directly connected with any parameter, which is related to surface and subsurface hydrologic model response. Silt content is only involved in estimating the sealing and crusting adjustment factor for rill erodibility. Sensitivity results in this analysis may be attributed to the changes in both clay and sand contents. Therefore, changes in silt content of the soil do not significantly impact hydrologic calibration.

Sensitivity results of output variables to changes in organic matter content (POM) of the soil are shown in Figure 6.7. Only the pesticide related model components were sensitive to variations in organic matter content (POM) of the soil, even though surface runoff slightly increased as organic matter content increased. An increase in the organic matter content value increased total pesticide loads from the surface and decreased the pesticide flux from intermediate to groundwater zone. The partitioning coefficient is a function of the organic matter content. Higher organic matter content resulted in higher sediment-bound pesticides and lower dissolved pesticides in runoff. Higher organic matter content increases the persistence of pesticides in a soil profile. As a result, pesticide load in surface runoff increased with sediment load and pesticide movement in soil water to groundwater decreased as organic matter content increased.

Sensitivity results of output variables to changes in Effective hydraulic conductivity ($K_{eff}$) for Green-Ampt infiltration are shown in Figure 6.8. Effective hydraulic conductivity ($K_{eff}$) for Green-Ampt infiltration is one of the very sensitive parameters to hydrologic response of the model. If the user decides to use the dynamic approach for $K_{eff}$ analysis, the model will determine daily $K_{eff}$ values based on soil and land use characteristics and disregards the user-defined $K_{eff}$ values. In a constant approach, the user-defined constant $K_{eff}$ values are used throughout the simulation period. An increase in $K_{eff}$ value with the constant approach increased the infiltration
rates, which resulted in reduction of surface runoff volume. Increases in recharges and pesticide flux to ground water were also expected with increased $K_{eff}$ values.

Sensitivities of output variables to changes in the saturated hydraulic conductivity of soil layers ($K_{sat}$) are shown in Figure 6.9. Subsurface related components were more sensitive to changes in the saturated hydraulic conductivity of soil layer ($K_{sat}$) compared to surface related components. The $K_{sat}$ value is used in the percolation process for controlling the leaching velocity of soil water. An increase in $K_{sat}$ value increased the percolation, resulting in an increase of ground water recharge. Decreased soil water content in root zone soil layers increases the effective matrix potential in Green-Ampt equation, which enhances infiltration and decreases of surface runoff. However, the sensitivity of surface output variables to changes in $K_{sat}$ value were negligible except for the pesticide loads in runoff.

Sensitivities of output variables to changes in interrill erodibility ($K_{inter}$) are shown in Figure 6.10. In the constant approach, user-defined interrill erodibility ($K_{inter}$) values are used throughout the model simulation without considering temporal changes for various agricultural management practices. As a result, the user-defined $K_{inter}$ values are ignored in the dynamic approach. The $K_{inter}$ value is only used in the soil detachment process for estimating interrill erosion. An increase in interrill erodibility increased the sediment yields at the outlet because only one overland cell was considered without considering a channel. $K_{inter}$ did not impact the subsurface output variables and surface runoff and pesticide loads.

Sensitivities of output variables to changes in the maximum root depth are shown in Figure 6.11. An increase in maximum root depth increased the recharges and pesticide flux to the ground water. However, responses to the surface output variables were negligible. Increased values of MRTDep may increase soil water extraction from soil layers through the crop transpiration.

Sensitivities of output variables to changes in the depth to ground water table (D2GWT) are shown in Figure 6.12. Subsurface related components were very sensitive to changes in the depth to ground water table (D2GWT). D2GWT defines the travel time required for infiltrated water to reach the ground water table. The other factor to be considered is the initial condition of soil water content in each soil layer. If the soil water contents in soil layers are greater than the field capacity, excess water in the soil profile will increase the total recharges to ground water. If the initial soil water content is less than the field capacity, more water will be stored in the soil, resulting in decreased recharges. Changes in D2GWT did not impact surface output variables. An increase in the depth to ground water table increases the travel time, which can be a sensitive
factor in an application with a short simulation period. In this application, decreased depth to ground water table increased the recharges and pesticide flux to ground water.

Sensitivities of output variables to changes in roughness of secondary tillage (RR2nd) are shown in Figure 6.13. An increase in random roughness of secondary tillage (RR2nd) increased infiltration rates and decreased the surface runoff because RR2nd is used for adjusting effective hydraulic conductivity (K_{eff}) of fallow soil. The dynamic approach was more sensitive to variations in the random roughness of secondary tillage compared to the constant approach.

Sensitivities of output variables to changes in pesticide half-life in soil (HL_{soil}) are shown in Figure 6.14. An increase in the pesticide half-life in soil (HL_{soil}) increased the pesticides’ persistence in the soil profiles. More pesticide movements in both surface and soil water were expected in both the constant and dynamic approaches because of the increased possibility of interaction among water, soil, and pesticide with the increased residence time. The changes in HL_{soil} values did not impact the hydrology and sediment related output variables.

Sensitivities of output variables to changes in the pesticide partitioning coefficient (K_{oc}) are shown in Figure 6.15. Similar to the organic matter content of the soil, only pesticide related model components were sensitive to variations in the pesticide partitioning coefficient (K_{oc}). An increase in the K_{oc} values increased total pesticide loads in surface and decreased the pesticide flux to ground water. Higher K_{oc} value increases pesticides’ persistence in a soil profile and enhances the possibility that more pesticides attach to soil particles. As a result, pesticide load in surface runoff increased with an increase in sediment-bound pesticide in runoff, and pesticide movement through soil profile to ground water decreased when dissolved pesticides in soil water decreased.

Sensitivities of output variables to changes in pesticide application depth (AppDep) are shown in Figure 6.16. Only surface pesticide output was sensitive to variations in pesticide application depth (AppDep). An increases in the application depth increased surface pesticide loads in both the dynamic and constant approaches.

Sensitivities of output variables to changes in rill space (RSpace) are shown in Figure 6.17. Only sediment loads in runoff was sensitive to changes in rill space (RSpace). A decrease in rill space decreased the sediment detachment of rill because contributing flow rate per rill decreased as rill space decreased. Sediment routing was not considered in this field-scale application. Deposition
of detached soil in channel or downstream cells was ignored because the field was considered to be one cell.

Sensitivities of output variables to changes in fraction of dissolved chemical available for runoff (FDRoff) are shown in Figure 6.18. Similar to the pesticide application depth, only pesticide in runoff was sensitive to changes in fraction of dissolved chemical available for runoff (FDRoff). An increase in the FDRoff value increased surface pesticide loads simulated by both approaches.
Figure 6.2. Sensitivity of parameters to changes in total porosity.

Figure 6.3. Sensitivity of parameters to changes in field capacity.
Figure 6.4. Sensitivity of parameters to changes in clay percent.

Figure 6.5. Sensitivity of parameters to changes in sand percent.
Figure 6.6. Sensitivity of parameters to changes in silt percent.

Figure 6.7. Sensitivity of parameters to changes in organic matter content.
Figure 6.8. Sensitivity of parameters to changes in Green-Ampt effective hydraulic conductivity.

Figure 6.9. Sensitivity of parameters to changes in saturated hydraulic conductivity in soil layer.
Figure 6.10. Sensitivity of parameters to changes in interrill erodibility.

Figure 6.11. Sensitivity of parameters to changes in maximum root depth.
Figure 6.12. Sensitivity of parameters to changes in depth to ground water table.

Figure 6.13. Sensitivity of parameters to changes in random roughness of secondary tillage.
Figure 6.14. Sensitivity of parameters to changes in pesticide half-life in soil.

Figure 6.15. Sensitivity of parameters to changes in pesticide partitioning coefficient.
Figure 6.16. Sensitivity of parameters to changes in pesticide application depth.

Figure 6.17. Sensitivity of parameters to changes in rill space.
Figure 6.18. Sensitivity of parameters to changes in fraction of dissolved chemical available for runoff.
Soil Layer Sensitivity Analysis

Table 6.3 and Figure 6.19 through Figure 6.25 show the calculated sensitivity index of DANSAT for surface and subsurface output variables based on the changes in different soil layers. Soil parameters in Table 6.3 can be classified into three groups: 1) surface related parameters related to infiltration and soil detachment processes; 2) subsurface parameters related to percolation process; and 3) combined parameters involved in both surface and subsurface processes.

Surface related parameters are used in estimating infiltration and soil detachment rates, which are based on the characteristics of top soil layers. Clay content (PClay), sand content (PSand), and very fine sand content (PVFSand) can be categorized into surface related parameters. Changes in the surface related parameters within the middle or bottom layers of the soil profile did not impact the output variables including surface and subsurface parameters. Sensitivities of output variables to changes in PClay, PSand, and PVFSand values in different soil layers are shown in Figure 6.19, Figure 6.20, and Figure 6.21, respectively. Similar to the results from the field-scale sensitivity analysis, an increase in the clay content of the top soil layers resulted in a decrease in the infiltration rate and an increase in runoff volume. Increased runoff volume also resulted in a decrease in the ground water recharge. Sand content sensitivity analysis in the top soil layers also showed a similar trend to the results from the dynamic approach used in the field-scale sensitivity analysis. Surface output variables decreased and subsurface output variables increased as sand content in the top soil layers increased. However, only sediment yield was sensitive to the changes in the sand content of the top soil layers because impacts of increased sand content on the hydrologic parameters, such as effective hydraulic conductivity ($K_{\text{eff}}$) and the wetting front capillary potential ($S_f$) values, can cancel each other out while impacts on the soil erodibility parameters make the soil more sensitive to the erosion process. The very fine sand content, VFSand, was not used in any hydrologic process; however, it is used in the soil detachment process for estimating soil erodibility and critical shear stress. As a result, only sediment yield in surface runoff was sensitive to the changes in VFSand value in the top soil layer.

Subsurface related parameters are used to control the percolation rates and pesticide leaching rates within each soil layer. Therefore, changes in the subsurface related parameters in any soil layer could significantly impact the subsurface output variables such as recharge and pesticide flux to the ground water. In addition, the infiltration process can be indirectly affected by percolation process. Higher soil water content in the top soil layers may decrease effective matrix potential in Green-Ampt equation and it could impact the surface output variables. However, the
influence of subsurface related parameters to the infiltration process are generally negligible below a certain soil depth.

Total porosity (TPor), field capacity (FCap), and saturated hydraulic conductivity (Ksat) can be classified under subsurface related parameters. Sensitivities of output variables to changes in TPor, FCap, and Ksat values in different soil layers are shown in Figure 6.22, Figure 6.23, and Figure 6.24, respectively. In all three cases, changes in each parameter of bottom soil layers did not impact the surface output variables. Both surface and subsurface output variables were sensitive to the changes in the FCap values. Similar to the results from the previous field-scale analysis, surface runoff increased and ground water recharge decreased as the field capacity increased. However, changes in TPor and Ksat values of only bottom soil layers impacted subsurface output variables, including recharges and pesticide flux to ground water. An increase of TPor in bottom soil layers decreased the recharge and pesticide flux to the ground water, while an increase in Ksat in bottom soil layers increased subsurface output variables.

Organic matter content (POM) can be classified under a surface related parameter from the hydrologic point of view and can be classified under a subsurface related parameter from the water quality point of view. Organic matter content is also involved in estimating infiltration related parameters. As a result, changes in POM value within middle or bottom layers of the soil profile did not impact surface runoff and subsurface recharge to ground water. Changes in POM in top soil layers had an impact on hydrology and sediment yield but the impact was negligible. However, surface pesticide loss was sensitive to the changes in top soil layers, while subsurface pesticide flux was more sensitive to the changes in bottom soil layers.
Table 6.3. Sensitivity index of DANSAT for surface and subsurface output variables for different soil layer depths.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Layer location</th>
<th>Baseline</th>
<th>Surface runoff</th>
<th>Surface sediment load</th>
<th>Surface pesticide load</th>
<th>Recharge to GW</th>
<th>Pesticide flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>PClay</td>
<td>Top</td>
<td>11.7</td>
<td>0.53</td>
<td>0.52</td>
<td>0.53</td>
<td>-0.27</td>
<td>-0.17</td>
</tr>
<tr>
<td></td>
<td>Middle</td>
<td>16.7</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>Bottom</td>
<td>5.5</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>PSand</td>
<td>Top</td>
<td>61.5</td>
<td>-0.27</td>
<td>-1.19</td>
<td>-0.02</td>
<td>0.13</td>
<td>0.08</td>
</tr>
<tr>
<td></td>
<td>Middle</td>
<td>63.9</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>Bottom</td>
<td>90.8</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>PVFSand</td>
<td>Top</td>
<td>10.3</td>
<td>0.00</td>
<td>0.28</td>
<td>0.00</td>
<td>0.00</td>
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<td>Middle</td>
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<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>Bottom</td>
<td>15.2</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>TPor</td>
<td>Top</td>
<td>0.387</td>
<td>0.06</td>
<td>0.02</td>
<td>0.13</td>
<td>0.06</td>
<td>0.02</td>
</tr>
<tr>
<td></td>
<td>Middle</td>
<td>0.369</td>
<td>-0.03</td>
<td>-0.01</td>
<td>-0.13</td>
<td>-0.05</td>
<td>-0.07</td>
</tr>
<tr>
<td></td>
<td>Bottom</td>
<td>0.410</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>-0.65</td>
<td>-0.64</td>
</tr>
<tr>
<td>FCap</td>
<td>Top</td>
<td>0.192</td>
<td>0.54</td>
<td>0.45</td>
<td>0.96</td>
<td>-0.51</td>
<td>-0.43</td>
</tr>
<tr>
<td></td>
<td>Middle</td>
<td>0.241</td>
<td>0.02</td>
<td>0.01</td>
<td>0.20</td>
<td>-0.41</td>
<td>-0.34</td>
</tr>
<tr>
<td></td>
<td>Bottom</td>
<td>0.127</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>-0.88</td>
<td>-1.23</td>
</tr>
<tr>
<td>Ksat</td>
<td>Top</td>
<td>0.00313</td>
<td>-0.04</td>
<td>-0.01</td>
<td>-0.44</td>
<td>0.08</td>
<td>0.05</td>
</tr>
<tr>
<td></td>
<td>Middle</td>
<td>0.00359</td>
<td>0.00</td>
<td>0.00</td>
<td>-0.01</td>
<td>0.05</td>
<td>0.04</td>
</tr>
<tr>
<td></td>
<td>Bottom</td>
<td>0.00613</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.05</td>
<td>1.27</td>
</tr>
<tr>
<td>POM</td>
<td>Top</td>
<td>0.94</td>
<td>0.06</td>
<td>0.05</td>
<td>1.41</td>
<td>-0.03</td>
<td>-0.03</td>
</tr>
<tr>
<td></td>
<td>Middle</td>
<td>0.42</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>Bottom</td>
<td>0.23</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>-0.83</td>
</tr>
</tbody>
</table>

Figure 6.19. Comparison of sensitivity index based on changes in clay percent at various soil depths.
Figure 6.20. Comparison of sensitivity index based on changes in sand percent at various soil depths.

Figure 6.21. Comparison of sensitivity index based on changes in very fine sand percent at various soil depths.
Figure 6.22. Comparison of sensitivity index based on changes in total porosity at various soil depths.

Figure 6.23. Comparison of sensitivity index based on changes in field capacity at various soil depths.
Figure 6.24. Comparison of sensitivity index based on changes in saturated hydraulic conductivity at various soil depths.

Figure 6.25. Comparison of sensitivity index based on changes in organic matter percent at various soil depths.
Watershed-scale Sensitivity Analysis

Table 6.4 shows the calculated sensitivity index for changes in spatial, general, and channel related parameters for five selected output variables. The output variables selected for sensitivity analysis include surface runoff, sediment in runoff, pesticide in runoff, recharge to ground water, and pesticide flux to ground water. Systematic calibration should be performed beginning with hydrology, followed by sediment, and finally followed by pesticide. Thus, the sediment or pesticide components need to have separate sensitive parameter sets from the hydrology component to calibrate the sediment or pesticide components without changing hydrologic results. Grouping the parameters in Table 6.4 according to the sensitivity to five output variables will be useful as a guideline for calibrating DANSAT for each specific situation. For example, common parameters for calibrating hydrology, sediment, and pesticide include TPor, FCap, AnioFac, and Ksat. If a user wants to calibrate the pesticide component only, POM and FDroff parameters can be selected. Even though Table 6.4 can be used as a guideline for a calibration of the model, it should be noted that the sensitivity index for each output variable can be changed in other watersheds with different hydrologic characteristics. Subsurface output variables were more sensitive to changes in parameters than surface output variables, as shown by the maximum and minimum values in Table 6.4.
Table 6.4. Summary of sensitivity index for changes in field-scale and watershed-scale parameters.

<table>
<thead>
<tr>
<th>Category</th>
<th>Parameters</th>
<th>Sensitivity index (SI)</th>
<th>Sensitivity index (SI)</th>
<th>Sensitivity index (SI)</th>
<th>Sensitivity index (SI)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Surface runoff</td>
<td>Surface sediment load</td>
<td>Surface pesticide load</td>
<td>Recharge to GW</td>
</tr>
<tr>
<td>Spatial (field-scale)</td>
<td>TPor</td>
<td>-0.19</td>
<td>-0.47</td>
<td>-0.63</td>
<td>4.16</td>
</tr>
<tr>
<td>parameters</td>
<td>FCap</td>
<td>-0.03</td>
<td>0.14</td>
<td>0.70</td>
<td>-7.12</td>
</tr>
<tr>
<td></td>
<td>PClay</td>
<td>0.03</td>
<td>0.07</td>
<td>0.00</td>
<td>0.04</td>
</tr>
<tr>
<td></td>
<td>PSand</td>
<td>-0.01</td>
<td>-0.04</td>
<td>-0.35</td>
<td>-0.03</td>
</tr>
<tr>
<td></td>
<td>POM</td>
<td>0.00</td>
<td>0.00</td>
<td>-0.28</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>Ksat</td>
<td>0.08</td>
<td>0.50</td>
<td>0.26</td>
<td>-0.06</td>
</tr>
<tr>
<td></td>
<td>D2GWT</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>-0.03</td>
</tr>
<tr>
<td>General (watershed-scale)</td>
<td>InfilDep</td>
<td>0.00</td>
<td>0.00</td>
<td>-0.03</td>
<td>0.00</td>
</tr>
<tr>
<td>parameters</td>
<td>RainFac</td>
<td>0.00</td>
<td>-0.02</td>
<td>-0.10</td>
<td>0.02</td>
</tr>
<tr>
<td></td>
<td>RSpace</td>
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<td>0.00</td>
<td>0.01</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>FDroff</td>
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<td>0.00</td>
<td>0.17</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>InterDep</td>
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<td>0.00</td>
<td>-0.03</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>AnioFac</td>
<td>0.13</td>
<td>0.61</td>
<td>0.21</td>
<td>-0.78</td>
</tr>
<tr>
<td></td>
<td>LenChan</td>
<td>0.00</td>
<td>0.90</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>GwSlope</td>
<td>0.02</td>
<td>0.02</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
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<td>GwInter</td>
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<td>-0.01</td>
<td>0.00</td>
<td>0.00</td>
</tr>
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<td></td>
<td>GwThr</td>
<td>0.42</td>
<td>0.46</td>
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<td>0.00</td>
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<td>Channel related parameters</td>
<td>ChaWid</td>
<td>0.00</td>
<td>-1.03</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>FUES</td>
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<td>-0.89</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>CClay</td>
<td>0.00</td>
<td>-0.53</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>CSand</td>
<td>0.00</td>
<td>0.50</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>Summary</td>
<td>Min.</td>
<td>-0.19</td>
<td>-1.03</td>
<td>-0.63</td>
</tr>
<tr>
<td></td>
<td>Max.</td>
<td>0.42</td>
<td>0.90</td>
<td>0.70</td>
<td>4.16</td>
</tr>
</tbody>
</table>

Figure 6.26 shows a comparison of sensitivity index for surface runoff based on changes in selected parameters. Runoff was sensitive to changes in threshold value for the baseflow equation (GwThr), anisotropic factor for interflow (AnioFac), and total porosity (TPor). GwThr parameter, which is included in the general parameter group, is included in the integrated baseflow component to consider ground water inflow from outside of the watershed boundary. Constant amount of baseflow is added to the stream flow during the stream routing process, resulting in an increased amount of total runoff at the watershed outlet. The other watershed-scale parameter, AnioFac, is used in the interflow calculation. An increase in AnioFac value increases the horizontal velocity through soil layers considered in interflow calculation, which, in turn, results in an increase in interflow and decrease in recharges to ground water.

Figure 6.27 shows a comparison of sensitivity index for sediment in runoff for changes in selected parameters. Sediment yield is directly related to the runoff volume, and a similar trend to runoff is expected in the response of sediment components to the changes in selected sensitive
parameters. Sediment yield was also sensitive to changes in TPor, AnioFac, and GwThr, which are selected sensitive parameters for runoff. Sediment yield was sensitive to the changes in the length for channel detachment calculation (LenChan) and channel related parameters including percent sand in channel (CSand), percent clay in channel (CClay), fraction of unerodible channel soil (FUES), and channel width (ChaWid). Nonerodible streambed due to armoring by rocks or exposed shale can be considered by FUES parameters. An increase in FUES values decreases the soil detachment from the streambed. Soil texture information in the streambed, including CClay and CSand, is used for estimating erodibility and critical shear stress values in a stream. An increase in CSand or decrease in CClay increased the sediment yields at the watershed outlet. Change in ChaWid value indirectly impacts the transport capacity in a stream segment. Transport capacity is calculated based on Yalin’s equation as a function of flow depth. In a stream with a rectangular-shaped cross section, an increase in channel width decreased flow depth, resulting in a decrease in transport capacity.

Figure 6.28 shows a comparison of sensitivity index for pesticide in runoff for changes in selected parameters. Atrazine is moderately soluble in water, and a similar trend to runoff is expected in the response to the changes in sensitive parameters such as AnioFac, TPor, and GwThr. However, pesticide in runoff was only sensitive to the changes in AnioFac and TPor parameters with negligible sensitivity to GwThr. The amount of pesticide lost through runoff was sensitive to the changes in soil depth for considering interflow calculation (InterDep), saturated hydraulic conductivity (Ksat), sand content of the soil (PSand), and field capacity (FCap). The total amount of available water for interflow calculation increases as the InterDep increases. As a result, a portion of interflow in total flow increases as the InterDep increases. An increase in Ksat value also may increase interflow amount by increasing the horizontal velocity in the soil profile. An increase in FCap also may increase available water for interflow by reducing percolation and may increase surface runoff by decreasing the effective matrix potential for the Green-Ampt equation. Possible paths of pesticide transport from field to stream segment include overland flow, interflow, and baseflow. It can be inferred based on the sensitivity results that most pesticide movement in a stream is simulated by the model through overland flow and interflow components. In addition, pesticide in runoff was sensitive to changes in a fraction of the dissolved chemical available for runoff (FDroff) and organic content (POM). FDroff and POM did not impact the hydrology and sediment results.
A comparison of sensitivity index of selected parameters for ground water recharge is shown in Figure 6.29. Recharge to ground water was sensitive to changes in soil depth used for estimating interflow calculation (InterDep), anisotropic factor for interflow (AnioFac), field capacity (FCap), and total porosity (TPor). Recharge was negatively sensitive to InterDep, AnioFac, and FCap, while it was positively sensitive to TPor. As mentioned previously, increases in AnioFac, InterDep, and FCap may increase interflow or overland flow, which results in a decrease in recharges to ground water.

Figure 6.30 shows a comparison of sensitivity index for pesticide flux to ground water for selected parameters listed in Table 6.4. Downward movement of pesticide in a soil profile is expected to vary in a similar manner as the water movement. However, pesticide flux to ground water was not sensitive to the changes in AnioFac, while it responded in a similar manner to the changes in InterDep, FCap, and TPor. As expected, subsurface pesticide movement was sensitive to the changes in organic matter content (POM). As OPM increases, more pesticide is attached to soil particles, which results in a decrease in pesticide movement in soil water. Pesticide flux to ground water was also sensitive to the changes in depth to the ground water table (D2GWT). The method by which this parameter impacts pesticide movement in a soil profile was explained in the previous field-scale sensitivity analysis section.
Figure 6.26. Comparison of sensitivity index values for total runoff for changes in field-scale and watershed-scale parameters.
Figure 6.27. Comparison of sensitivity index values for sediment load for changes in field-scale and watershed-scale parameters.
Figure 6.28. Comparison of sensitivity index valued for pesticide load for changes in field-scale and watershed-scale parameters.
Figure 6.29. Comparison of sensitivity index values for recharge to ground water for changes in field-scale and watershed-scale parameters.
Figure 6.30. Comparison of sensitivity index values for pesticide flux to ground water zone for changes in field-scale and watershed-scale parameters.
Soil Location Sensitivity Analysis

Table 6.5 and Figure 6.31 through Figure 6.34 show the estimated sensitivity index values for selected surface and subsurface output variables for changes in soil parameters at different locations in the watershed. In some cases, changes in the same parameter at different locations showed different responses in the same output variable. For example, an increase in total porosity (TPor) of a soil located near the watershed boundary decreased spatially averaged pesticide flux, while an increase in TPor near streams increased the value of same output variable. The opposite response to the same output variable for changes in the same parameter at different locations can be explained by considering the possible paths of water and pollutants from overland area to a stream segment. Compared to the response of model to parameter changes near the watershed boundary, response of the model to changes in parameters near streams showed more similar trends to the results in Table 6.4 where one homogeneous soil type was assumed throughout the watershed. Parameter changes near the watershed boundary may also influence the downward routing process in the path from the overland cells where changes occurred to the stream cells. For example, increase in infiltration near the watershed boundary may increase the ground water recharges near the watershed boundary area. However, decreased runoff rate to the down stream cells may decrease the ground water recharges near stream areas, thus the overall spatially averaged recharges is reduced. If the same situation is considered using one cell without considering the routing processes, increases in infiltration rates would decrease the surface runoff and increase the recharge to the ground water. Parameter changes in cells located near the stream decreases the possibility of interactions among output variables during the routing process because of the reduced travel distance. Both pesticides in runoff and pesticide flux to ground water were sensitive to the change in total porosity (TPor), field capacity (FCap), and organic matter content (POM). Pesticide in runoff was more sensitive to the changes in TPor, FCap, and POM near stream cells than to the parameter changes near watershed boundary cells. Pesticide flux was more sensitive to the changes in FCap and POM values for near stream cells and the changes in TPor value in near watershed boundary cells. Ground water recharge was sensitive to the changes in TPor and FCap. Parameter changes of TPor and FCap in near stream cells had greater impacts on the ground water recharges than changes in watershed boundary cells. Sediment yield was also sensitive to the changes in TPor and FCap. However, changes in TPor and FCap in watershed boundary cells had greater impacts on the sediment yield than changes in near stream cells. With regard to runoff, no significant differences in the calculated sensitivity index values were detected for various parameter values at different locations. Overall, the
selected output variables were more sensitive to the parameter changes in cells located near the stream. However, it should be noted that the soil location sensitivity results can change in other watersheds with different characteristics and hydrologic response.

Table 6.5. Summary of sensitivity index values based on spatial location of soils in a field.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Layer location</th>
<th>Surface runoff</th>
<th>Surface sediment load</th>
<th>Surface pesticide load</th>
<th>Recharge to GW</th>
<th>Pesticide flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>TPor</td>
<td>Boundary</td>
<td>0.06</td>
<td>0.55</td>
<td>-5.43</td>
<td>-0.03</td>
<td>-5.04</td>
</tr>
<tr>
<td></td>
<td>Stream</td>
<td>-0.01</td>
<td>-0.23</td>
<td>-17.14</td>
<td>1.16</td>
<td>1.76</td>
</tr>
<tr>
<td>FCap</td>
<td>Boundary</td>
<td>-0.73</td>
<td>-1.41</td>
<td>3.22</td>
<td>-1.29</td>
<td>3.81</td>
</tr>
<tr>
<td></td>
<td>Stream</td>
<td>-0.48</td>
<td>-0.07</td>
<td>12.83</td>
<td>-2.13</td>
<td>-4.35</td>
</tr>
<tr>
<td>PClay</td>
<td>Boundary</td>
<td>0.10</td>
<td>0.10</td>
<td>-0.12</td>
<td>0.14</td>
<td>-0.09</td>
</tr>
<tr>
<td></td>
<td>Stream</td>
<td>0.05</td>
<td>0.01</td>
<td>0.11</td>
<td>0.15</td>
<td>-0.02</td>
</tr>
<tr>
<td>PSand</td>
<td>Boundary</td>
<td>-0.09</td>
<td>-0.10</td>
<td>0.84</td>
<td>-0.28</td>
<td>0.53</td>
</tr>
<tr>
<td></td>
<td>Stream</td>
<td>-0.02</td>
<td>0.19</td>
<td>0.10</td>
<td>-0.34</td>
<td>0.46</td>
</tr>
<tr>
<td>POM</td>
<td>Boundary</td>
<td>0.00</td>
<td>0.01</td>
<td>0.55</td>
<td>0.00</td>
<td>0.21</td>
</tr>
<tr>
<td></td>
<td>Stream</td>
<td>0.00</td>
<td>0.01</td>
<td>0.66</td>
<td>0.00</td>
<td>-3.65</td>
</tr>
<tr>
<td>Ksat</td>
<td>Boundary</td>
<td>0.07</td>
<td>0.31</td>
<td>-0.08</td>
<td>0.07</td>
<td>0.18</td>
</tr>
<tr>
<td></td>
<td>Stream</td>
<td>0.10</td>
<td>0.41</td>
<td>0.47</td>
<td>-0.03</td>
<td>-0.14</td>
</tr>
</tbody>
</table>

Figure 6.31. Comparison of sensitivity index values for changes in total porosity soil parameter at different locations in the watershed.
Figure 6.32. Comparison of sensitivity index values for changes in field capacity soil parameter at different locations in the watershed.

Figure 6.33. Comparison of sensitivity index values for changes in clay percent soil parameter at different soil locations in the watershed.
Figure 6.34. Comparison of sensitivity index values for changes in sand percent soil parameter at different soil locations in the watershed.

Figure 6.35. Comparison of sensitivity index values for changes in OM content soil parameter at different soil locations in the watershed.
Figure 6.36. Comparison of sensitivity index values for changes in saturated hydraulic conductivity soil parameter at different soil locations in the watershed.
Grid Size Sensitivity Analysis

Methods

The overall model response to different grid sizes can be separated into two categories: 1) changes in input parameter values due to the changes in grid size (parameter impacts) and 2) systematic response of the model due to the selected algorithm and equations (model impacts). To separate these two different sources of impacts, a grid size analysis was conducted based on three steps shown in Table 6.6. These three steps in grid size sensitivity analysis are limited to the integrated ground water approach. Table 6.6 shows the overall procedure used for grid size sensitivity analysis.

Table 6.6. Procedures used for conducting grid size sensitivity analysis.

<table>
<thead>
<tr>
<th>Step</th>
<th>Procedure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Step 1</td>
<td>- Analyze GIS manipulation errors</td>
</tr>
<tr>
<td></td>
<td>- Assess the watershed delineation error and rasterization error</td>
</tr>
<tr>
<td>Step 2</td>
<td>- Analyze the model response</td>
</tr>
<tr>
<td></td>
<td>- Evaluate the response of model to the different grid size using rectangular watershed of imagination.</td>
</tr>
<tr>
<td>Step 3</td>
<td>- Analyze Overall response</td>
</tr>
<tr>
<td></td>
<td>- Analyze the overall response to the grid size considering both GIS manipulation error and model response</td>
</tr>
</tbody>
</table>

Collection and manipulation of spatial data is the first step in the watershed-scale application of the distributed model. Common general categories of spatial data include topographic, soil, and land use information. DEM is commonly used to derive topographic data such as watershed boundary, slope, aspect, and stream networks. Delineation of the watershed boundary is significantly influenced by the selected resolution of DEM. Minimum grid size was selected based on finest cell resolution among available DEM. To calculate watershed delineation error, the original 30 m DEM was resampled (aggregated) successively to coarser grids of 60, 90, 120, 150, 180, 210, 240, and 270 m resolutions using a bilinear interpolation method. The Arc/View hydrology extension was used to delineate watershed boundaries based on the original and aggregated DEMs. The effects of DEM resolution on watershed delineation were examined by visual comparison of spatial distribution of boundary and calculated statistical error. Delineated watershed boundary for each selected resolution was resampled back to 30m resolution to calculate the error using cell-by-cell comparison. Figure 6.37 shows the procedure used for the analysis of watershed boundary delineation error. It is assumed that the watershed boundary derived from the base DEM resolution (30 m) is the most accurate. Watershed boundary delineated using finer DEM resolution has a higher possibility of being closer to the actual
watershed boundary. The discrepancy between the DEM based watershed boundary and actual watershed boundaries can be resolved based on the type of model being used. Input parameters of semi-lumped watershed models, such as SWAT and HSPF, are not less sensitive to the watershed boundary. Thus, the user can manually derive input parameters such as average slope and land use percent using any GIS tool based on a predefined watershed boundary. However, DANSAT is sensitive to routing related parameters, especially flow direction. The model will crash if flow directions throughout the watershed are not correct after adjusting watershed boundary. Thus, the watershed boundary, which is automatically delineated based on DEM using a GIS tool, needs to be close to the actual watershed boundary. Watershed boundaries derived from aggregated DEMs were compared to the reference boundary based on 30m grid size by calculating errors using the following equation:

\[
E_{\text{boundary}} = \frac{1}{2} \left( \frac{NC_{\text{in}}}{NC_{\text{ref}}} + \frac{NC_{\text{out}}}{NC_{\text{ref}}} \right)
\]  

(6.7)

Where, \( E_{\text{boundary}} \) = watershed boundary delineation error for each resampled resolution, \( NC_{\text{ref}} \) = total number of cells inside reference, \( NC_{\text{in}} = NC_{\text{ref}} - \) number of cells overlapped by reference and resampled boundary, and \( NC_{\text{out}} = \) total number of cells inside the resampled - number of cells overlapped by reference and resampled boundary.

Figure 6.37. Procedures used for analysis of watershed delineation error.

The temporal maximum grid size was selected based on boundary delineation error. Soil and rotation data usually exist in vector format. Vector format data were transformed into grid format using Arc/View GIS within the range of minimum and maximum grid sizes, which were selected in the delineation procedure. Error matrix, which is commonly used in image processing for the calculation of land use classification accuracy, was selected to calculate the error occurring
during the rasterization procedure. The procedure used to calculate the rasterization error of soil and rotation data is shown in Figure 6.38. A new maximum grid size was selected by considering the rasterization error from both soil and rotation data.

Two user-created virtual watersheds were defined to evaluate the response of the model to different grid sizes. At first, response of overland routing and channel routing components to different grid sizes were evaluated using one large cell and linearly connected watershed (Figure 6.39). Both watersheds consist of impervious overland area to simplify the system by excluding the subsurface components such as infiltration and percolation. A set of data was simulated without considering a channel component (Figure 6.39a) for evaluating the overland routing component based on the continuity equation and Manning’s equation. For the evaluation of the channel component, one channel segment was considered in each cell with the same channel width and channel slope (Figure 6.39b). If a cell contains a stream segment, all the waters from the adjacent overland cell and remaining water on the overland area after infiltration takes place goes into the stream segment for channel routing. In this case, there is no water from the adjacent cell and all the rainfall on the overland area and stream surface are added to stream segment for considering channel flow routing, which is based on the variable storage routing method.

Figure 6.38. Procedures used for rasterization error analysis.

Figure 6.39. User-created watersheds used for evaluating overland component and channel routing components for different grid sizes.
Secondly, a user-created rectangular watershed (600 m × 600 m) with constant overland slope (3.27%) and channel slope (0.83%) was generated to analyze the response of the model itself to the grid size by considering subsurface components and connections between overland cells. Figure 6.40 shows the concept of a created rectangular watershed for the analysis of model impacts.

![Figure 6.40. A user-created rectangular watershed with constant overland and channel slopes and homogeneous soil and rotation type.](image)

The previously mentioned GIS manipulation error including watershed delineation error and rasterization error can be eliminated by the user-created V-shaped rectangular watershed. The rectangular shape prevents the watershed boundary from changing due to different grid sizes. Both overland and channel slopes remain constant in different grid sizes by considering a V-shaped watershed, which is shown in Figure 6.40. One soil and one rotation type are also assigned to the overall watershed to remove the rasterization error. Four different grid sizes of 120, 85.71, 66.67, and 31.58 m were selected. As a result, only systematic response of the model to the different grid sizes (model impacts) can be analyzed and the results will be used to understand the overall response of the model in an actual watershed application.

Finally, QN2 in Nomini Creek watershed was used to analyze the overall response to the different grid sizes by considering both GIS manipulation error (parameter impacts) and model-itself response (model impacts). Several different grid sizes were considered within the range of minimum grid resolution (30 m) and maximum grid resolution, which was decided based on the spatial accuracy during the GIS data manipulation processes such as watershed delineation and rasterization. Watershed average values for sensitive parameters, which were selected in parameter sensitivity analysis, were calculated for each grid size. The Arc/View hydrology extension was used to derive overland and channel related parameters for each grid size.
Calculated watershed average values were used as basic information to understand the model response to the different grid sizes. Table 6.7 shows the data categories and selected sensitive parameters.

Table 6.7. Selected sensitive parameters used for calculation of watershed average values.

<table>
<thead>
<tr>
<th>Category</th>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Topographic</td>
<td>Overland: slope, elevation</td>
<td>Watershed average</td>
</tr>
<tr>
<td></td>
<td>Channel: length, slope</td>
<td>Channel average</td>
</tr>
<tr>
<td>Soil</td>
<td>Total porosity, field capacity, sand percent</td>
<td>Watershed average</td>
</tr>
<tr>
<td>Land use</td>
<td></td>
<td>Watershed average</td>
</tr>
</tbody>
</table>

Delineation of the stream networks gives different results depending on the arbitrary threshold value (number of cells) of the contributing drainage area above which a cell is considered as a channel. To derive similar stream networks independent of grid size, the threshold value should be selected for each grid size using a trial-and-error method, because the threshold values decrease as the grid size increases. In this study, the longest first-order stream networks were delineated to keep the consistency among stream network distributions generated based on different grid sizes.

Results and Discussion

Parameter Impact

The watershed boundary and channel networks generated at each DEM resolution are shown in Figure 6.41. First, 30m DEM-based boundary was compared with the boundary that was delineated on the base of contours of USGS quad maps. Discrepancies occur at the southeastern and western parts of the watershed. The difference in watershed areas between the two different sources is less than 0.64 percent. Stream networks derived from the 30m DEM compares well with the digitized networks. The 30m DEM-based boundary was used as a reference for the comparison of boundaries from different grid sizes.

Variations in watershed boundary for the 60 to 240 m resolution seems to be relatively small compared with the boundary at 30 m resolution. Maximum grid resolution of 240m for rasterization analysis of soil and rotation maps was decided due to dramatic change in watershed boundary at grid sizes larger than 240 m.
Figure 6.41. Watershed boundary and channel network maps for various grid resolutions.

Figure 6.42 and Figure 6.43 show variations in the spatial distribution of the soil type and rotation at each resolution for the QN2 subwatershed, respectively. With increased grid resolution, there is a difficulty in representing spatial distribution of soil types and rotation types. Small polygons of soil and rotation types disappeared or were exaggerated as resolution increased, mainly because Arc/View uses centroid algorithm for the rasterization processes. The algorithm chooses any polygon that exists at the center of each grid even though the polygon is not the dominant type within the grid (ESRI, 1998).
Figure 6.42. Variations in spatial distribution of the soil type for QN2 watershed.

Figure 6.43. Variations in spatial distribution of crop rotation type for QN2 watershed.
Table 6.8 shows the watershed delineation and rasterization errors for the soil and rotation maps for each grid resolution. With 80% accuracy considered to be the minimum acceptable criterion, maximum resolution of 240m was decided based on watershed delineation analysis and 90m was decided based on rasterization analysis. Thus, a maximum grid resolution of 90m was selected for modeling applications based on visual comparison of spatial distribution of soil and rotation types and error statistics. The spatial distributions of watershed boundary, soil types, and rotation types are represented with sufficient accuracy for any grid size smaller than 90 m for QN2 watershed.

<table>
<thead>
<tr>
<th>Grid size (m)</th>
<th>Boundary Accuracy (%)</th>
<th>Area (ha)</th>
<th>Rotation Accuracy (%)</th>
<th>Types</th>
<th>Soil Accuracy (%)</th>
<th>Types</th>
</tr>
</thead>
<tbody>
<tr>
<td>30m</td>
<td>100.0</td>
<td>210</td>
<td>100.0</td>
<td>53</td>
<td>100.0</td>
<td>7</td>
</tr>
<tr>
<td>60m</td>
<td>96.6</td>
<td>210</td>
<td>89.1</td>
<td>44</td>
<td>87.2</td>
<td>7</td>
</tr>
<tr>
<td>90m</td>
<td>94.5</td>
<td>215</td>
<td>83.0</td>
<td>43</td>
<td>80.2</td>
<td>7</td>
</tr>
<tr>
<td>120m</td>
<td>92.8</td>
<td>223</td>
<td>78.3</td>
<td>37</td>
<td>73.6</td>
<td>6</td>
</tr>
<tr>
<td>150m</td>
<td>90.9</td>
<td>207</td>
<td>73.7</td>
<td>31</td>
<td>67.6</td>
<td>6</td>
</tr>
<tr>
<td>180m</td>
<td>90.8</td>
<td>214</td>
<td>69.8</td>
<td>28</td>
<td>63.7</td>
<td>7</td>
</tr>
<tr>
<td>210m</td>
<td>88.8</td>
<td>212</td>
<td>70.3</td>
<td>20</td>
<td>62.8</td>
<td>5</td>
</tr>
<tr>
<td>240m</td>
<td>87.6</td>
<td>225</td>
<td>68.1</td>
<td>18</td>
<td>63.6</td>
<td>5</td>
</tr>
<tr>
<td>270m</td>
<td>70.2</td>
<td>299</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The accuracy of rasterized data depends on the characteristics of vector data as well as selected encoding methods such as centroid, predominant type, most important type, and percentage breakdown. For example, soil polygons in SURRGO with rapid changes in curve will show dramatic decrease in accuracy within smaller grid sizes compared to soil polygons in STATGO data that have fluent curves. As a result, an acceptable maximum grid size can be changed based on available data in a specific watershed and required spatial accuracy of data to fit the purpose of the research.

**Model Impact**

One storm event with constant rainfall intensity (0.3mm/min) and 3 hour duration was applied for evaluating overland routing and channel routing components. Figure 6.44 a and b show the hydrologic response of the overland flow routing component and the channel routing component to the storm event for different grid sizes, respectively. As expected, the peak of hydrograph reached the constant rainfall intensity at some point and flow rate started to decrease right after the rainfall stopped. The watershed without a channel reached the peak earlier than the watershed with a channel. Comparison of the results for different grid size indicates that flow rate from the one large cell increases faster during rising limb and decreases faster during recession limb of the hydrograph, compared to the result from the watershed consisting of ten 30 m cells in both
overland and channel routing simulation. The discrepancies could be due to differences in watershed sizes. The area of one 300 m cell is ten times greater than the watershed with ten 30m cells. Both the overland routing component in combination with continuity and Manning’s equations and the channel routing component by variable storage routing methods seem to accurately predict runoff.

Figure 6.44. Hydrologic response of (a) overland routing and (b) channel routing components to a storm event with constant intensity (0.3 mm/min) for different grid sizes.
The model response to different grid sizes and different stream cross sections (rectangular and triangular) was evaluated. Response of the hydrology components to different grid sizes on an idealized rectangular watershed are summarized in Table 6.9 and Figure 6.45. Results based on a 30 m grid size were assumed to be the baseline. Total runoff linearly decreased as the grid size increased in both rectangular and triangular stream shapes. Runoff slightly decreased (by 8 percent) at a 120 m grid size compared to the results from a 30 m grid size. Runoff in a rectangular stream was greater than that in a triangular stream for all different grid sizes. Total runoffs during the simulation period were 1191 mm and 1177 mm in rectangular and triangular stream shapes, respectively. Overall, total runoff was not sensitive to the changes in grid sizes and stream cross sections.

Table 6.9. Summary of the response of hydrology component of DANSAT to different grid size on user-created rectangular watershed.

<table>
<thead>
<tr>
<th>Grid size (meters)</th>
<th>Rectangular cross section</th>
<th>Triangular cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Runoff (mm/ha)</td>
<td>Ratio to 30m</td>
</tr>
<tr>
<td>30</td>
<td>1191</td>
<td>1.00</td>
</tr>
<tr>
<td>60</td>
<td>1146</td>
<td>0.96</td>
</tr>
<tr>
<td>90</td>
<td>1126</td>
<td>0.95</td>
</tr>
<tr>
<td>120</td>
<td>1096</td>
<td>0.92</td>
</tr>
</tbody>
</table>

Figure 6.45. Summary of response of hydrology component to different grid size on user-created rectangular watershed

The response of sediment components to different grid sizes on user-created rectangular watersheds are summarized in Table 6.10 and Figure 6.46. Even though sediment yields fluctuated as the grid size increased, the overall trend shows a decrease in sediment yield as grid
size increased. Maximum sediment yields occurred at 30 m grid size in both rectangular and triangular stream shapes. However, total sediment yield in a rectangular stream was greater than that of a triangular stream in all different grid sizes. Total sediment yields at 30 m grid-sizes were 698 kg/ha and 403 kg/ha in rectangular and triangular streams, respectively. The reason for the difference in sediment yield for different shapes of stream cross sections are discussed in the time-step analysis section.

Table 6.10. Summary of response of sediment component of DANSAT to different grid sizes on a user-created rectangular watershed.

<table>
<thead>
<tr>
<th>Grid size (meters)</th>
<th>Rectangular cross section</th>
<th>Triangular cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Sediment (kg/ha)</td>
<td>Ratio to 30m</td>
</tr>
<tr>
<td>30</td>
<td>698</td>
<td>1.00</td>
</tr>
<tr>
<td>60</td>
<td>678</td>
<td>0.97</td>
</tr>
<tr>
<td>90</td>
<td>684</td>
<td>0.98</td>
</tr>
<tr>
<td>120</td>
<td>674</td>
<td>0.97</td>
</tr>
</tbody>
</table>

Figure 6.46. Summary of response of sediment component to different grid sizes on a user-created rectangular watershed.

Overall, sediment yield was not sensitive to the changes in grid size. However, sediment yield was sensitive to the changes in flow depth, which is also influenced by the dimension of stream cross sections. Figure 6.47 shows a comparison of simulated daily total runoffs and daily sediment yields for different shapes of stream cross sections. Daily runoff volumes by two different stream cross sections were similar except for the two largest storms on 9/16/1989 and 9/11/1989. Daily runoff volumes by the triangular cross section were smaller than those simulated for the rectangular cross section during big storm events. The overall trend in sediment yields
showed that daily sediment yield in the rectangular stream was always greater than that for the triangular stream. Sediment yields were sensitive to the changes in flow rate during the storm events on 9/16/1989 and 9/11/1989.

Response of pesticide components to different grid sizes on user-created rectangular watersheds are summarized in Table 6.11 and Figure 6.48. Similar to the hydrology component, pesticide in runoff was not sensitive to the changes in shape of stream cross sections. However, pesticide was sensitive to the changes in grid size. Total pesticide load decreased as the grid size increased with the maximum and minimum values of 370.83 g/ha at 30 m and 230.15 g/ha at 120 m grid size for rectangular stream, respectively. An increase in grid size from 30 m to 120 m decreased total pesticide load by 38 percent.

Table 6.11. Summary of response of the pesticide component of DANSAT to different grid size on a user-created rectangular watershed.

<table>
<thead>
<tr>
<th>Grid size (meters)</th>
<th>Rectangular cross section</th>
<th>Triangular cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Pesticide (mg/ha)</td>
<td>Ratio to 30m</td>
</tr>
<tr>
<td>30</td>
<td>37083</td>
<td>1.00</td>
</tr>
<tr>
<td>60</td>
<td>28594</td>
<td>0.77</td>
</tr>
<tr>
<td>90</td>
<td>26116</td>
<td>0.70</td>
</tr>
<tr>
<td>120</td>
<td>23015</td>
<td>0.62</td>
</tr>
</tbody>
</table>
Overall Impact
Sensitivity analysis of hydrology, sediment, and pesticide components to different grid sizes by considering both GIS manipulation error (parameter impacts) and model response (model impacts) was conducted on the QN2 watershed. The time-step was fixed at 1 minute as minimum storm event time-step (SET). Results based on the smallest grid size (30 m) were considered to be the baseline.

Response of the hydrology component to different grid sizes was summarized in Table 6.12 and Figure 6.49. Total runoff at the watershed outlet increased as the grid size increased in both rectangular and triangular stream shapes. An increase in grid size from 30 m to 120 m increased total runoff by 6% in both rectangular and triangular streams. Runoff was not sensitive to the changes in the shape of the stream cross section even though runoff in the rectangular stream was insignificantly greater than that in the triangular stream for all different grid sizes. The hydrologic response in QN2 showed an opposite trend to the results from the user-defined rectangular watershed. The major difference between QN2 and the user-defined rectangular watershed is that only one homogeneous rotation, soil, and overland slope combination was applied to the overall user-defined watershed while the multiple rotation, soil, and overland slope combinations were present in QN2 watershed.
The increase in total runoff with an increase in grid size can be explained by the baseflow related components. Figure 6.50 shows the response of ground water recharge during the simulation period to the different grid sizes. Recharge decreased between 30 m and 60 m grid sizes and increased again after 60 m grid sizes. The minimum recharge was 644 mm/cell at 60 m grid size. The reason for the smallest recharge value at 60 m grid size could be explained by considering spatial distribution of rotation and soil types and changes in topographic parameters due to the changes in grid size. To examine the effects of various grid sizes on ground water recharge, variations in elevation, overland slope, and depth to the ground water table, various grid sizes were examined (Table 6.13). The table shows that the mean and maximum values of overland slopes decreased as the grid size increased. Reductions in surface slope may increase infiltration, which results in an increase in ground water recharge. The changes in elevation and depth to the ground water table were negligible. As a result, none of the topographic parameters were able to explain the decrease in ground water recharge at 60 m grid size. Thus, we examined the spatial distribution of the combination of rotation and soil type by considering the flow path. If a cell with the most permeable soil type and the most intensive tillage application exists near a stream with a higher accumulated flow depth, the recharge will be higher. The combination of soil, rotation, and flow path can be changed during the resampling procedures for each grid size. Figure 6.51 shows the comparison of temporal changes in daily total runoff for different grid sizes. The fluctuation in baseflow components is simulated by integrated ground water components using the ground water recharge as an input. The baseflow component was most sensitive at 120 m grid size, and the sensitivity decreased as the grid size increased. Since the relationship between spatial distribution of ground water recharge and baseflow in streams is defined as a function of saturated hydraulic conductivity and the distance from current cell where recharge occurs to the nearest stream cell, spatial distribution of ground water recharge and streams for different grid sizes were analyzed (Figure 6.52). It should be noted that cells with higher ground water recharge exist at a point with higher accumulated flow depth in an overall flow path while conversion from recharge to baseflow is based on the straight distance between cells. Even though maximum recharge in a cell decreased as the grid size increased, the straight distance from a cell with higher recharge value to a stream cell decreased at 60 m grid size. As a result, the sensitivity of the baseflow component to the ground water recharges decreased at 30 m grid size.

Computational times for 4 years of simulation (1987-1990), according to different grid sizes based on a fixed 1 minute time-step, are shown in Table 6.12. A machine with 3.4 ghz dual Zeon
processor and 2 gigabytes of ram was used to compare simulation time. Simulation time dramatically decreased from 612 minutes to 48 minutes as grid size increased from 30 m to 120 m.

Table 6.12. Summary of overall response of hydrology component of DANSAT to different grid sizes on QN2.

<table>
<thead>
<tr>
<th>Grid size (meters)</th>
<th>Rectangular cross section</th>
<th>Triangular cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Runoff (mm/ha)</td>
<td>Ratio to 30m</td>
</tr>
<tr>
<td>30</td>
<td>1738 (612)</td>
<td>1.00</td>
</tr>
<tr>
<td>60</td>
<td>1795 (168)</td>
<td>1.03</td>
</tr>
<tr>
<td>90</td>
<td>1812 (84)</td>
<td>1.04</td>
</tr>
<tr>
<td>120</td>
<td>1849 (48)</td>
<td>1.06</td>
</tr>
</tbody>
</table>

( ) : Computational time in minutes for a 4 year simulation period (1987-1990) based on fixed 1 minute time-step, using 3.4 ghz dual Zeon processor workstation with 2 gigabytes of ram.

Figure 6.49. Summary of overall response of hydrology component to different grid sizes on QN2.
Table 6.13. Variation in elevation and slope for various grid sizes.

<table>
<thead>
<tr>
<th>Grid size (m)</th>
<th>Elevation (m)</th>
<th>Overland slope (%)</th>
<th>Depth to GW table (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean</td>
<td>Max</td>
<td>Mean</td>
</tr>
<tr>
<td>30m</td>
<td>39.1</td>
<td>52.4</td>
<td>23.8</td>
</tr>
<tr>
<td>60m</td>
<td>38.8</td>
<td>52.4</td>
<td>19.4</td>
</tr>
<tr>
<td>90m</td>
<td>38.6</td>
<td>51.6</td>
<td>16.6</td>
</tr>
<tr>
<td>120m</td>
<td>38.8</td>
<td>52.1</td>
<td>13.8</td>
</tr>
</tbody>
</table>

Figure 6.50. Response of ground water recharge to different grid sizes.

Figure 6.51. Comparison of temporal changes in daily total runoff for different grid sizes.
Figure 6.52. Spatial distribution of ground water recharge and streams for different grid sizes in QN2.

The response of sediment components to different grid sizes are summarized in Table 6.14 and Figure 6.53. The general trend in sediment yield was similar to that of the hydrology component. However, the sediment yield was sensitive to the changes in grid size. Sediment yield increased as the grid size increased except for the 120 m grid size with a rectangular shape stream. Response of total runoff during storm events to the different grid sizes should be considered in explaining the impacts of grid size on sediment yields. Figure 6.54 shows a comparison of daily runoff and sediment yield for different grid sizes in the rectangular stream in QN2 watershed. During high flow rates, (Figure 6.54a), daily total runoff at 90 m grid size was greatest, followed by 60 and 120 m grid sizes. Sediment yields presented in Figure 6.54.b show a similar trend to the runoff even though the sediment component was more sensitive to grid size than the hydrology component. Higher sediment yield was predicted as the flow rate increased for various grid sizes. Examination of the spatial distribution of crop rotation and soil type by considering the flow paths could be helpful in explaining the reason for the higher runoff volume at 90 m grid
size. The sediment yield was sensitive to the changes in the shape of stream cross section as well. Sediment yields in a rectangular stream were greater than those in a triangular stream with 30 m through 90 m of grid sizes. The rapid increase in sediment yield occurred in a triangular stream at the 120 m grid size. An increase in grid size from 30 m to 120 m increased sediment yields by 128% in a stream of rectangular cross section and by 1223% in a stream of triangular cross section. A possible reason for the difference in sediment yield for different shape of the stream cross section is discussed later in this chapter (time-step sensitivity analysis using QN2).

Table 6.14. Summary of overall response of sediment component of DANSAT to different grid sizes in QN2.

<table>
<thead>
<tr>
<th>Grid size (meters)</th>
<th>Rectangular cross section</th>
<th>Triangular cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sediment (kg/ha)</td>
<td>Ratio to 30m</td>
<td>Sediment (kg/ha)</td>
</tr>
<tr>
<td>30</td>
<td>1177</td>
<td>1.00</td>
</tr>
<tr>
<td>60</td>
<td>2430</td>
<td>2.07</td>
</tr>
<tr>
<td>90</td>
<td>3223</td>
<td>2.74</td>
</tr>
<tr>
<td>120</td>
<td>2677</td>
<td>2.28</td>
</tr>
</tbody>
</table>

Figure 6.53. Summary of overall response of sediment component to different grid sizes in QN2.
Response of pesticide components to different grid sizes are summarized in Table 6.15 and Figure 6.55. Pesticide in runoff slightly increased within the range of 30 m and 60 m grid sizes and decreased as the grid size increased. This trend is related to the pesticide flux from the intermediate to ground water zone. Figure 6.56 shows a comparison of pesticide flux for different grid sizes based on average and maximum values. A trend in pesticide amounts in runoff followed the trend of pesticide flux based on maximum values instead of average values. The pesticide in runoff was less sensitive to the straight distance between the overland cell where pesticide flux occurred and the stream cell compared to the hydrology component. The unstable response of pesticide components to different time-steps could be an indication that the lumped interflow pool approach for pesticide movement via interflow has problems.
Table 6.15. Summary of response of pesticide component of DANSAT to different grid sizes on QN2.

<table>
<thead>
<tr>
<th>Grid size (meters)</th>
<th>Rectangular cross section</th>
<th>Triangular cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Pesticide (mg/ha)</td>
<td>Ratio to 30m</td>
</tr>
<tr>
<td>30</td>
<td>282</td>
<td>1.00</td>
</tr>
<tr>
<td>60</td>
<td>294</td>
<td>1.04</td>
</tr>
<tr>
<td>90</td>
<td>242</td>
<td>0.86</td>
</tr>
<tr>
<td>120</td>
<td>128</td>
<td>0.46</td>
</tr>
</tbody>
</table>

Figure 6.55. Summary of response of pesticide component of DANSAT to different grid sizes in QN2.

Figure 6.56. Ratio of pesticide flux to 30 m grid size based on average and maximum values.
Time-step Sensitivity Analysis

Methods

Time-step analysis for both integrated and linked ground water approaches are necessary for understanding the responses of each modeling system to different time-steps and for presenting a guideline for selecting appropriate time-steps. Time-steps of interest for both approaches are the Storm Event Time-step (SET) and Ground water Time-step (GWT) as shown in Figure 4.2.

Time-step analysis by changing storm event time-step (SET) was conducted for the integrated ground water approach in this study. In the integrated approach, the default Surface Water Time-step (SWT) is defined as one day and is used for the simulation of evapotranspiration, percolation, and pesticide degradation components in a non-rainfall day. If there is rain, SWT is divided into three different time-steps including Before Rainfall Time-step (BRT), Storm Event Time-step (SET), and After Runoff Time-step (ART). The percolation and pesticide leaching components are considered in both BRT and ART. During the SET, storm related components such as interception, infiltration, sediment detachment, and overland and channel routing components are simulated by DANSAT. The user can choose different SET, which should be equal to or greater than the minimum time-step (one minute), based on available rainfall data, required simulation time, and the purpose of model simulation. SET is an important structural parameter because the required computational time is determined according to SET. If the model is stable on large SET and provides similar results to those by smaller SET, one major limitation of physically-based and distributed models can be resolved.

The same watersheds used in model validation were selected for the time-step analysis. The Owl Run watershed was selected to evaluate the model response to different time-step without considering the baseflow component. Only overland and interflow components were turned on in this analysis, and the recharge into ground water was considered as a deep percolation loss to the outside of the system being modeled. QN2 in Nomini Creek watershed was selected to evaluate the response of the integrated systems including overland, interflow, and baseflow components to different time-steps. Sensitivity of stream cross-section shape to different time-steps was also tested using Owl Run and QN2 watersheds. The two different stream cross-section types include rectangular and triangular stream cross-sections. Different Storm event time-steps of 1, 5, 10, 15, 45, and 60 minutes were selected for the time-step sensitivity analysis. For each time-step, only the rainfall input file was replaced for the selected time-step without changing any other input
Parameters. The rainfall breakpoint input file was generated using the newly developed model interface.

Results and Discussion

Results Based on Owl Run Watershed

Sensitivity analysis of hydrology and sediment components to different time-steps without considering the baseflow component was conducted using the Owl Run watershed. Response of hydrology components to different time-steps is summarized in Table 6.16 and Figure 6.57. The result from the smallest time-step in DANSAT (1 minute time-step) was considered as baseline and results from bigger time-steps were compared to the baseline. Total runoff at the watershed outlet decreased as the time-step increased in both rectangular and triangular stream shapes. An increase in time-step from 1 minute to 60 minutes decreased total runoff by 24% in the rectangular stream and 25% in the triangular stream. Runoff was not sensitive to the changes in the dimension of the stream cross section even though runoff in the rectangular stream was greater than that in the triangular stream in all different time-steps. The rapid decrease occurred between 1 minute and 15 minute time-steps. This decrease was expected, because the greater the storm event time-step (SET), the smaller the rainfall intensity. In Owl Run watershed, most runoff volume is directly related to infiltration and is also indirectly related to evapotranspiration, which controls the soil water balance. Decreases in rainfall intensity could decrease the overland runoff and increase water in soil profile estimated by the Green-Ampt infiltration method. Increased soil water would increase the total runoff by being routed to the stream segments through the interflow. However, interflow process is relatively slower compared to the direct overland runoff. Figure 6.58 shows the calculated maximum and average rainfall intensities based on rainfall input files for different time-steps. Average rainfall intensity linearly decreased as time-step increased, and maximum rainfall intensity decreased rapidly between 1 minute and 5 minute time-steps. Even though vertical movement of soil water through the impermeable soil layer was not allowed, flux from the intermediate to ground water zone through the permeable soil types in Figure 5.20 was treated as deep percolation loss. The deep percolation loss was not considered in total runoff calculation. Increases in infiltrated water may increase the deep percolation. Summaries of the response of sediment component to different time-steps are shown in Table 6.17 and Figure 6.59. General response of sediment yield is directly related to the runoff volume and is expected to vary in a similar manner as the runoff. Total sediment yields for the simulation period decreased as the time-step increased in both rectangular and triangular stream...
shapes. An increase in time-step from 1 minute to 60 minutes decreased total runoff by 33% in a rectangular stream and 36% in a triangular stream. However, sediment yield in a rectangular stream was almost twice greater than that of a triangular stream. Sediment yields were 4458 kg/ha and 2611 kg/ha for rectangular and triangular streams at 1 minute time-step, respectively. It will be explained in a later section of this chapter (time-step sensitivity analysis using QN2).

Table 6.16. Summary of the model response of hydrology component to different time-steps without considering baseflow component.

<table>
<thead>
<tr>
<th>Time-step (minutes)</th>
<th>Rectangular cross section</th>
<th>Triangular cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Runoff (mm/ha)</td>
<td>Ratio to 1-min</td>
</tr>
<tr>
<td>1</td>
<td>1912</td>
<td>1.00</td>
</tr>
<tr>
<td>5</td>
<td>1737</td>
<td>0.91</td>
</tr>
<tr>
<td>10</td>
<td>1611</td>
<td>0.84</td>
</tr>
<tr>
<td>15</td>
<td>1545</td>
<td>0.81</td>
</tr>
<tr>
<td>30</td>
<td>1465</td>
<td>0.77</td>
</tr>
<tr>
<td>45</td>
<td>1452</td>
<td>0.76</td>
</tr>
<tr>
<td>60</td>
<td>1447</td>
<td>0.76</td>
</tr>
</tbody>
</table>

Figure 6.57. Summary of the model response of hydrology component to different time-steps without considering baseflow component.
Figure 6.58. Maximum and average rainfall intensity for different time-steps.

Table 6.17. Summary of the model response of sediment component to different time-steps without considering baseflow component.

<table>
<thead>
<tr>
<th>Time-step (minutes)</th>
<th>Rectangular cross section</th>
<th>Triangular cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Sediment (kg/ha)</td>
<td>Ratio to 1-min</td>
</tr>
<tr>
<td>1</td>
<td>4458</td>
<td>1.00</td>
</tr>
<tr>
<td>5</td>
<td>3883</td>
<td>0.87</td>
</tr>
<tr>
<td>10</td>
<td>3483</td>
<td>0.78</td>
</tr>
<tr>
<td>15</td>
<td>3278</td>
<td>0.74</td>
</tr>
<tr>
<td>30</td>
<td>3040</td>
<td>0.68</td>
</tr>
<tr>
<td>45</td>
<td>3011</td>
<td>0.68</td>
</tr>
<tr>
<td>60</td>
<td>2983</td>
<td>0.67</td>
</tr>
</tbody>
</table>

Figure 6.59. Summary of the model response of sediment component for different time-steps without considering baseflow component.
Results Based on QN2 Watershed

Sensitivity analysis of hydrology, sediment, and pesticide components to different time-steps by considering the baseflow component was conducted on QN2 watershed. Grid size was fixed as 0.81 ha (90 m by 90 m) of rectangular shape. Results based on the smallest time-step (1 minute) were considered as baseline. Responses of the hydrology component to different time-steps are summarized in Table 6.18 and Figure 6.60. Total runoff at the watershed outlet increased as the time-step increased in both rectangular and triangular stream cross sections. An increase in time-step from 1 minute to 60 minutes increased total runoff by 8% in both rectangular and triangular streams. Runoff was not sensitive to the changes in the shape of a stream cross section even though runoff in a rectangular stream was slightly greater than that in a triangular stream for all different time-steps. Hydrologic response in QN2 showed an opposite trend to the results from Owl Run watershed where total runoff decreased as the time-step increased. The difference between QN2 and Owl Run watersheds is that recharge from intermediate to ground water zones was considered in the stream routing process as baseflow in QN2 watershed while recharge to ground water was not considered for total runoff calculation in Owl Run watershed. Compared to the Owl Run watershed, constant or slower decrease in total runoff was expected in QN2 watershed as the time-step increased because the recharge to the ground water does not disappear and reaches the stream segment as baseflow. However, total runoff was increased as the time-step increased in QN2 watershed. The increase in total runoff with an increase in time-step can be explained with baseflow related components of DANSAT. Amount of baseflow increase due to increased recharge seems to be greater than the reduction in direct runoff due to decreased rainfall intensity as time-step increased. Figure 6.61 shows the response of ground water recharge during the simulation period (1989-1990) to different time-steps. The results show that the ground water recharge increased as time-step increased, as expected. Figure 6.62 also shows the time-series of daily total runoff for different time-steps. An increase in baseflow and decrease in total runoff for storm events occurred as time-step increased. The most significant changes in both baseflow and total runoff for storm events occurred between 1 minute and 5 minute time-steps. Computational times for the 4 years of simulation (1987-1990) for different time-steps based on 265 cells of 90 m × 90 m grid size, are shown in Table 6.18. A machine with 3.4 ghz dual Zeon processor and 2 gigabytes of ram was used to compare simulation time. Simulation time dramatically decreased from 84 minutes to 2 minutes as the time-step increased from 1 minute to 60 minutes.
Table 6.18. Summary of the model response of hydrology component to different time-step by considering baseflow components.

<table>
<thead>
<tr>
<th>Time-step (minutes)</th>
<th>Rectangular cross section</th>
<th>Triangular cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Runoff (mm/ha)</td>
<td>Ratio to 1-min</td>
</tr>
<tr>
<td>1</td>
<td>1812 (84)</td>
<td>1.00</td>
</tr>
<tr>
<td>5</td>
<td>1880 (16)</td>
<td>1.04</td>
</tr>
<tr>
<td>10</td>
<td>1910 (8)</td>
<td>1.05</td>
</tr>
<tr>
<td>15</td>
<td>1923 (6)</td>
<td>1.06</td>
</tr>
<tr>
<td>30</td>
<td>1937 (4)</td>
<td>1.07</td>
</tr>
<tr>
<td>45</td>
<td>1945 (3)</td>
<td>1.07</td>
</tr>
<tr>
<td>60</td>
<td>1949 (2)</td>
<td>1.08</td>
</tr>
</tbody>
</table>

( ) : Computational time in minutes for a 4 year simulation period (1987-1990) based on 265 cell of 90 m × 90 m grid size, using 3.4 ghz dual Zeon processor workstation with 2 gigabytes of ram.

Figure 6.60. Summary of the model response of hydrology component to different time-steps by considering baseflow component.
Figure 6.61. Response of ground water recharge to different time-steps in the rectangular stream.

Figure 6.62. Time-series of daily total runoff for different time-steps.

Summaries of the response of the sediment component to different time-steps are shown in Table 6.19 and Figure 6.63. Response of sediment yields to different time-steps varied for the two stream cross sections. Sediment yields increased in a triangular stream as time-step increased. In a rectangular stream, sediment yield decreased as the time-step increased. Increases in time-step
from 1 minute to 60 minutes decreased sediment yield by 51% in a rectangular stream and increased sediment yield by 21% in a triangular stream. Sediment yield in a triangular stream was almost twice greater than that of a rectangular stream.

Different response of sediment yields to different time-steps in QN2 and Owl Run watershed can be explained by looking into the sediment detachments with respect to flow rates. Sediment detachment in a stream occurs only when effective shear stress by flow is greater than the adjusted critical shear stress, which is estimated based on soil characteristics. Details in selected equations are described in Chapter 3. Figure 6.64 shows the possible cases of sediment detachment in a stream with respect to the shape of the stream cross section and flow depth. In Owl Run watershed, sediment yields for the two stream shapes showed similar trends to the total runoff but sediment yield in the rectangular stream was higher than that of the triangular stream. Considering that most runoff water originates from direct runoff and baseflow is negligible in the watershed, majority of the flow rates may occur in zones IV in Figure 6.64. Sediment yields in rectangular streams are higher when most of the flow rates occur in zone IV. In QN2 watershed, over 80% of total runoff is due to baseflow. If most of the flow rates belong to zone II and flow rates occasionally occur in zone III or IV during storm events, sediment yields in the triangular stream would occur in every stream flow rate, while sediment yield in the rectangular stream will occur only when flow rate exceeds critical point between zone II and III during storm events. As a result, sediment yields in both the triangular and rectangular streams were sensitive to the total runoff volume and flow rate of storm events, respectively. As mentioned previously, daily runoff during a storm event decreased and ground water recharge increased as the time-step increased. However, sediment yield in the rectangular stream decreases with a decrease in storm runoff as time-step increases. Sediment yield in the triangular stream decreases because flow rates during storm events decrease with increases in time-step (Figure 6.62).

Table 6.19. Summary of the model response of sediment component for different timesteps by considering baseflow component.

<table>
<thead>
<tr>
<th>Time-step (minutes)</th>
<th>Rectangular cross section</th>
<th>Triangular cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Sediment (kg/ha)</td>
<td>Ratio to 1-min</td>
</tr>
<tr>
<td>1</td>
<td>1229</td>
<td>1.00</td>
</tr>
<tr>
<td>5</td>
<td>998</td>
<td>0.81</td>
</tr>
<tr>
<td>10</td>
<td>986</td>
<td>0.80</td>
</tr>
<tr>
<td>15</td>
<td>976</td>
<td>0.79</td>
</tr>
<tr>
<td>30</td>
<td>793</td>
<td>0.64</td>
</tr>
<tr>
<td>45</td>
<td>747</td>
<td>0.61</td>
</tr>
<tr>
<td>60</td>
<td>606</td>
<td>0.49</td>
</tr>
</tbody>
</table>
Figure 6.63. Summary of the model response of sediment component for different time-steps by considering baseflow component.

Figure 6.64. Possible cases for sediment detachment in streams for various stream shape and flow rates.

Response of the pesticide component to different time-steps is summarized in Table 6.20 and Figure 6.65. The amount of pesticide in runoff was not sensitive to the shape of the stream cross
section even though the triangular stream had a slightly higher pesticide load for all time-steps than the rectangular stream. Total pesticide in runoff decreased rapidly between 1 minute and 5 minute time-steps in both stream shapes. The pesticide mass in runoff were 2385 mg/ha and 496 mg/ha at 1 and 5 minute time-steps for the rectangular stream shape, respectively. Pesticide in runoff in rectangular stream shape fluctuated between 496 mg/ha at 5 minute time-step and 338 mg/ha at 30 minute time-step. Possible paths of pesticide movement from crop area where pesticide is applied to a stream segment include overland flow, interflow, and baseflow. Figure 6.66 shows the response of pesticide flux from intermediate to ground water zone for different storm event time-steps on QN2 watershed. Response of pesticide flux to ground water for different time-steps showed a similar trend to the response of pesticides in runoff. Simulated pesticides in runoff seem to have close correlation with pesticide flux to ground water. Pesticide flux from an aquifer to a stream is not directly predicted by DANSAT. However, a similar trend between total pesticide load at the watershed outlet (Figure 6.65) and spatially averaged pesticide flux from the intermediate zone to ground water zone (Figure 6.66) shows that a large portion of pesticide load in a stream comes through the pesticide movement through baseflow.

Response of pesticide leaching components to different time-steps was examined on QNB plot by treating it as one cell. Table 6.21 and Figure 6.67 show the model response of the pesticide leaching component to different time-steps in QNB plot. The pesticide flux to the ground water was not sensitive to the different time-steps. The difference between ONB and QN2 applications is that the interflow and baseflow components were turned off in QNB while they were considered in QN2. The reason for the large reduction in pesticide losses in runoff between 1 and 5 minute time-step is not known. One possible component that caused this problem to occur could be the interflow related components. As mentioned previously, soil water exceeding field capacity of each soil layer are lumped into the interflow pool and then interflow to the adjacent cell is calculated based on the depth of water in the pool. When excessive amounts of soil water moves to the lumped pool, dissolved pesticide also moves and is lumped into a lumped pesticide pool. Then, water and pesticide in the lumped interflow pool are used for the calculation of infiltration and pesticide leaching. Error can occur during the complicated circulation of water and pesticide between actual soil layers and the lumped interflow pool. Error seems to be caused by some bug within the pesticide-related components rather than an intrinsic problem of the selected approach or algorithm. As a result, it is recommended to start checking errors from the interflow-related pesticide components in future model applications.
Table 6.20. Summary of the model response of pesticide component for different time-steps by considering baseflow components.

<table>
<thead>
<tr>
<th>Time-step (minutes)</th>
<th>Rectangular cross section</th>
<th>Triangular cross section</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Pesticide (mg/ha)</td>
<td>Ratio to 1-min</td>
</tr>
<tr>
<td>1</td>
<td>2385</td>
<td>1.00</td>
</tr>
<tr>
<td>5</td>
<td>496</td>
<td>0.21</td>
</tr>
<tr>
<td>10</td>
<td>360</td>
<td>0.15</td>
</tr>
<tr>
<td>15</td>
<td>409</td>
<td>0.17</td>
</tr>
<tr>
<td>30</td>
<td>338</td>
<td>0.14</td>
</tr>
<tr>
<td>45</td>
<td>367</td>
<td>0.15</td>
</tr>
<tr>
<td>60</td>
<td>410</td>
<td>0.17</td>
</tr>
</tbody>
</table>

Figure 6.65. Summary of the model response of pesticide component for different time-steps by considering baseflow component.

Figure 6.66. Response of pesticide flux from intermediate to ground water zone for different storm event time-steps.
Table 6.21. Response of pesticide leaching components to different time-step in QNB plot.

<table>
<thead>
<tr>
<th>Time-step (minute)</th>
<th>1</th>
<th>5</th>
<th>10</th>
<th>15</th>
<th>30</th>
<th>45</th>
<th>60</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pesticid flux to GW (mg)</td>
<td>1548</td>
<td>1521</td>
<td>1514</td>
<td>1498</td>
<td>1509</td>
<td>1506</td>
<td>1517</td>
</tr>
</tbody>
</table>

Figure 6.67. Comparison of daily pesticide flux to ground water for different time-steps in QNB plot.

Summary and Conclusions

Sensitivity of DANSAT to functional and structural parameters (grid size and time-step) was analyzed in this chapter. Responses of five output variables to the changes in the selected functional parameters were examined on field-scale and watershed-scale. Three surface output variables (runoff, sediment yield, and pesticides in runoff) and two subsurface output variables (ground water recharge and pesticide flux to the ground water) were selected for considering surface and subsurface responses of DANSAT, respectively. Model sensitivity to the changes in soil parameters for different soil layers was examined in the field-scale sensitivity analysis, while sensitivity to the changes in soil parameters at different locations within a watershed was examined in watershed-scale sensitivity analysis. Model response to different grid sizes was analyzed by separately considering 1) changes in input parameter values due to GIS manipulation (parameter impacts) and 2) systematic response of the model due to the selected algorithm and
equations (model impacts). Model response to different time-steps was also analyzed using varied storm event time-steps (SET) from 1 minute to 60 minutes.

Soil related parameters such as field capacity and soil particle sizes (clay, sand, and silt) were sensitive parameters for five output variables. Interrill erodibility and rill space were the sensitive parameters for sediment yields, while pesticide half-life in soil, pesticide partitioning coefficient, pesticide application depth, and fraction of dissolved chemical available for runoff were the sensitive parameters for the pesticide components. Depth to ground water table was sensitive to the subsurface components including both ground water recharge and pesticide flux to the ground water. Surface parameters related to infiltration and soil detachment processes include clay content, sand content, and very fine sand content. Subsurface parameters related to percolation rates and pesticide leaching rates within each soil layer include total porosity, field capacity, and saturated hydraulic conductivity. Surface output variables (runoff, sediment yield, and pesticide in runoff) were exclusively sensitive to the changes in soil parameters of the top soil layer, while subsurface output variables (recharge and pesticide flux to ground water) were sensitive to the changes in soil parameters in all soil layers.

Sensitivity index values for the spatial (plot-scale parameters), general (watershed-scale parameters), and channel related parameters were compared to select sensitive parameters for each output variable at the watershed-scale. Runoff was sensitive to changes in both general parameters, such as threshold value for the baseflow equation, and the anisotropic factor for interflow and spatial parameters, such as total porosity. In addition to the mentioned parameters, sediment yield was sensitive to channel parameters including percent sand in channel, percent clay in channel, fraction of unerodible channel soil, and channel width. Pesticide in runoff was sensitive to the changes in the anisotropic factor for interflow, total porosity, soil depth for considering interflow calculation, saturated hydraulic conductivity, sand content, and field capacity. Recharge to ground water was sensitive to changes in soil depth for considering interflow calculation, anisotropic factor for interflow, field capacity, and total porosity. Pesticide flux to ground water was sensitive to the changes in soil depth for considering interflow calculation, field capacity, total porosity, organic matter content, and depth to the ground water table. Total porosity and field capacity were sensitive to most output variables. Impacts of changes in soil parameter at different spatial locations on output variables were analyzed. Both surface and subsurface output variables were more sensitive to the parameter changes in near stream cells compared to the parameter changes in near watershed boundary cells. Changes in soil
parameters in near stream cells directly impacts surface and subsurface output variables because of less chance of interaction during the routing from cell of changes to stream cells.

The maximum acceptable grid size of 90 m was decided for QN2 watershed based on accuracy during GIS data manipulation such as watershed boundary delineation and rasterization. Response of DANSAT to different grid sizes at a user-created watershed was analyzed by excluding changes in input parameters according to the changes in grid size. First, one storm event of constant rainfall intensity and 3 hour duration was applied to the impervious land of one 9 ha (300 m by 300 m) cell and ten 0.09 ha (30 m by 30 m) cells for evaluating overland routing and channel routing components. Flow rates from the one large cell responded faster during both the rising and recession limbs of the hydrograph compared to the flow rates from the ten 0.09 ha cells. Second, the model response to the different grid sizes was analyzed in a user-created rectangular watershed (600m × 600m) with constant overland slope and channel slope. Total runoff linearly decreased as the grid size increased. Overall trend showed a decrease in sediment yield as the grid size increased. Neither runoff nor sediment yields were sensitive to the changes in grid size. However, pesticide loads were sensitive to the changes in grid size. An increase in grid size from 30 m to 120 m decreased the total pesticide load by 38%. Sensitivity of DANSAT to different grid sizes was analyzed on QN2 watershed with a fixed 1 minute time-step by considering both parameter impacts and model impacts. An increase in grid sizes from 30 m to 120 m increased total runoff by 6%. The general trend in sediment yield was similar to that of the hydrology component. However, the sediment yield was sensitive to the changes in grid size. Increase in grid size from 30m to 120m dramatically decreased simulation time from 612 minutes to 48 minutes.

Sensitivity analysis of hydrology and sediment components to different time-steps without considering the baseflow component was conducted using the Owl Run watershed. Both total runoff and sediment yields at the watershed outlet decreased as the time-step increased. Sensitivity analysis of hydrology, sediment, and pesticide components to different time-steps by considering the baseflow component was also conducted on QN2 watershed. Total runoff at the watershed outlet increased as the time-step increased. Sediment yields were sensitive to the changes in the shape of stream cross sections. Sediment yields in a triangular stream increased following a similar trend to the total runoff as time-step increased. In a rectangular stream, sediment yield decreased as the time-step increased. Total pesticide load in runoff decreased
rapidly between 1 minute and 5 minute time-steps. Increase in time-step from 1 minute to 60 minutes dramatically decreased simulation time from 84 minutes to 2 minutes.

Intensive simulation time can be a restricting factor in the application of DANSAT, using a small grid size and time-step at a watershed-scale. Use of a larger grid size with an acceptably larger time-step exponentially reduced computational time, compared to an application using a smaller grid size and time-step. Selection of appropriate grid size and time-step is important at the early stage of the modeling process from a practical point of view. In general, it is recommended that the grid size be decided first, then, an appropriate time-step based on the fixed grid size can be decided by considering the characteristics of the watershed and the purpose of the research. First, the largest grid size can be selected within the limits of acceptable representations in spatial distributions of topographic, soil, and land use. Then, appropriate time-step should be selected by considering the major goal of the research. If the main focus of the research is to determine long-term hydrologic impacts, a larger time step is recommended. However, if the research focuses on short-term impacts on hydrology and water quality such as storm peak and sediment yields, smaller time-steps are recommended. It also should be noted that different responses of DANSAT to the changes in grid size and time-sep are possible for watersheds with different characteristics and hydrologic response.

References


Chapter 7: Model Application

Introduction

The BMP impacts on hydrology and water quality at watershed vary considerably based on their location and implementation time. Watershed-scale non-point source models such as HSPF, SWAT, ANSWERS-2000, and AnnAGNPS have been used to evaluate the impacts of temporally and spatially variable BMPs on hydrology and water quality. Most current applications of existing watershed-scale and continuous simulation models use rough land use classification and typical management information as input data. Agricultural management data include a sequence of crop rotations, planting and harvesting dates, and tillage and pesticide application dates. Semi-distributed models such as HSPF and SWAT have difficulties in simulating the impacts of different locations of BMPs because the size of subwatershed or HRU is too big to consider the spatial distribution of BMPs in a field. Application of distributed and watershed-scale models such as ANSWERS-2000, AnnAGNPS, and MIKE-SHE also has been simplified due to a lack of detail information on temporal changes of management practices. As a result, rough land use classification with typical crop rotations is used in the simulations even though these models have the capability to consider spatial distribution and temporal changes in management practices. Few watershed-scale models consider actual changes in management practices in both temporal and spatial scales because of the limitation by model structure or lack of data. In DANSAT, temporal changes in management practices are included in the rotation data block and spatial distribution is considered in the cell data block by assigning the pre-defined rotation number to each cell.

The goal of this chapter is to analyze the response of DANSAT to different levels of information on management practices. There are three specific objectives for this chapter:

1. To introduce the methodology for considering actual dynamic rotation changes in DANSAT.
2. To understand impacts of different levels of information on crop rotation input data on hydrology and water quality.
3. To provide guidelines to future model users for preparing rotation input data.
Methods

In order to consider different levels of information on crop rotation information, the Nomini Creek (NC) watershed was selected because over ten years of land use data are available in a geographic information system (GIS) format. The GIS database consists of spatial maps and attribute data containing the unique field number and land use activities for each year. Each year of land use activity data was divided into three land use periods: 1st (LU1): April-June, 2nd (LU2): July-September, 3rd (LU3): October-March.

Figure 7.1 shows the procedure used for manipulating original land use GIS data for identifying a possible rotation number and considering spatial distribution and temporal changes. Arc/View GIS (ESRI, 1998) software, which has several geoprocessing capabilities such as union, clipping, and merging, was used to generate final rotation shape file based on yearly land use data. First, yearly land use GIS data were overlaid sequentially throughout the model simulation period using a geoprocessing technique, Union. The resulting shape file was clipped using the watershed boundary shape file to exclude the areas outside of the watershed. Yearly land use spatial data could have different field boundaries each year, because one specific field can be divided into two or more subfields and two or more subfields can be merged into one field, depending on the farmer’s crop rotation strategies. These changes in field boundaries were recorded and later digitized based on the visual examination of each field. This procedure could result in digitizing error, and it causes differences in the boundaries of a specific field, even though no boundary changes occurred in the actual field. Thus, mismatches, known as slivers, are resulted during Union geoprocessing. The clipped shape file was rasterized based on the user-defined grid size because the final format of rotation input is not in vector format (shape file) but rather in the raster format (grid file). Slivers disappear during this procedure, because slivers are small enough, compared with the grid cell size, to be removed. The unique rotation number based on the attribute file also needs to be defined before the rasterization of the clipped rotation files. All records of significant fields, which are big enough to remain during rasterization, were sorted by LU1, LU2, and LU3 fields. The same rotation number was assigned if the sequence of the land use code (CO, SB, and SG) in the LU-fields is exactly the same as the other. Finally, a unique rotation number was assigned to every record of significant field size.
Figure 7.1. Procedures used for manipulating land use data for the crop rotation input.

After defining spatial distribution of unique rotation types, each polygon was classified as having one broad land use category such as crop, pasture, hay, low-density developed, high-density developed, and forest based on the predominant crop types. Detailed land use changes in the fields, which were classified as crop rotation, were handled by two different approaches: the dynamic rotation approach and typical rotation approach. However, the same rotation information was used for non-crop areas in both dynamic and typical rotation approaches. In the dynamic rotation approach, different tillage applications such as no-till and conventional-till were considered, but similar crops such as wheat, oat and barley were all designated as small grains. The actual crop rotations were considered in the dynamic approach. For the typical rotation approach, typical crop rotation was assumed for crop areas. Table 7.1 shows the dates and types of agricultural managements used for the typical rotation approach. Typical crop management dates were decided based on the advice from professionals at Virginia Tech. Two different types of crop rotations are available within the typical crop rotation approach based on the starting crop
in the rotation. The starting crop for the first year can be either corn or winter wheat. Crop rotation type was decided based on the actual land use during the first year of the crop rotation.

Table 7.1. Dates and types of agricultural management information for the typical rotation approach in QN2.

<table>
<thead>
<tr>
<th>Land-use type</th>
<th>Date</th>
<th>Application type</th>
<th>Comment</th>
<th>Land use (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non-crop</td>
<td>01/01/01</td>
<td>Pasture</td>
<td>Grazing considered</td>
<td>4.5</td>
</tr>
<tr>
<td></td>
<td>12/31/01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Non-crop</td>
<td>01/01/01</td>
<td>Hay</td>
<td>Hay-cut considered</td>
<td>1.5</td>
</tr>
<tr>
<td></td>
<td>12/31/01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Non-crop</td>
<td>01/01/01</td>
<td>Forest</td>
<td></td>
<td>56.2</td>
</tr>
<tr>
<td></td>
<td>12/31/01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Non-crop</td>
<td>01/01/01</td>
<td>Low-density developed</td>
<td>20% impervious area and grass-cut considered</td>
<td>0.8</td>
</tr>
<tr>
<td></td>
<td>12/31/01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Non-crop</td>
<td>01/01/01</td>
<td>High-density developed</td>
<td>80% impervious area and grass-cut considered</td>
<td>1.1</td>
</tr>
<tr>
<td></td>
<td>12/31/01</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Typical Crop

+----------------+-----------------+---------------------+-----------------------------------------------+--------------+
<table>
<thead>
<tr>
<th>Date</th>
<th>Application type</th>
<th>Comment</th>
<th>Land use (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>04/09/01</td>
<td>Tillage (Planter)</td>
<td></td>
<td>35.8</td>
</tr>
<tr>
<td>04/09/01</td>
<td>Planting (Corn)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10/09/01</td>
<td>Harvesting (Corn)</td>
<td>15% cover after harvesting</td>
<td></td>
</tr>
<tr>
<td>10/10/01</td>
<td>Tillage (Chisel plow)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10/14/01</td>
<td>Tillage (Disk)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10/15/01</td>
<td>Planting (Wheat)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>06/24/02</td>
<td>Harvesting (Wheat)</td>
<td>70% cover after harvesting</td>
<td></td>
</tr>
<tr>
<td>06/30/02</td>
<td>Tillage (No-till drill)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>06/30/02</td>
<td>Planting (Soybean)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11/09/02</td>
<td>Harvesting (Soybean)</td>
<td>70% cover after harvesting</td>
<td></td>
</tr>
</tbody>
</table>

A rotation data block can be generated using either the Interface method or the Rotation Builder method. If the actual tillage application date and planting/harvesting dates are available for each field, the Interface method is recommended. The advantage of this method is that actual application dates can be considered, while its disadvantage is that it is time consuming because only one line of rotation information can be inserted at a time. The Rotation Builder method can be used in cases where actual agricultural management data for each field are not collected. In this method, typical application dates are assumed for frequently repeated land use changes such as corn-winter wheat-soybean 2 year rotation. A block of predefined rotation information can be inserted in the method. The Rotation Builder method was used in this study because actual application dates were not surveyed in the Nomini Creek watershed for individual fields even though the actual crop rotations were collected for each field.

The impact of different levels of information on crop rotation on pesticide losses was not considered in this study because the amount of applied pesticide in the typical rotation approach can be different from the pesticide amount in the actual rotation approach. The influence of
applied pesticide amount on pesticide losses in runoff is greater than the indirect influence of different crop rotations on pesticide losses. Temporal changes in dynamic parameters at user defined cells were compared for analyzing the impacts of two different rotation information levels on hydrology and sediment components. Effective hydraulic conductivity for the Green-Ampt equation was selected as one of the most sensitive dynamic variables for hydrology results, while rill and interrill erodibilities were selected as sensitive soil erosion related variables. This comparison will be useful for understanding the final response of hydrology and sediment results by considering how DANSAT responds to the changes in agricultural management practices. Both surface and subsurface hydrologic impacts were considered by comparing simulated total runoff and recharge from two different rotation approaches.

**Results and Discussion**

**Hydrology**

A total of 48 identical rotation types were derived based on actual land use changes and user defined grid size. Surface and subsurface hydrologic responses of DANSAT to the typical and dynamic approaches are provided in Table 7.2. Total runoff and total average recharges by the typical rotation approach were greater than those resulting from the dynamic approach during the simulation period (1987-1992). Changes in rotation information from dynamic to typical rotation approaches on crop areas (35.8% of the watershed) increased total runoff and ground water recharge by 1.3% and 1.8%, respectively. Figure 7.2 shows a comparison of daily total runoff at the watershed outlet and monthly total recharge in each cell for the two rotation approaches. Variations in total runoff during both low and high flow conditions were negligible, while variations in monthly total recharge were high for the cells with small recharge and low for the cells with large recharge. Total runoff from QN2 watershed was not sensitive to the different rotations on crop areas because the majority of total runoff in the watershed is due to baseflow. Impacts of high variations in the monthly recharge on total runoff for different rotation information can be attenuated through the subsurface components of DANSAT, which convert ground water recharge to baseflow by reducing the intensity and increasing lag time. Figure 7.3 shows a temporal comparison of differences in monthly total runoff at the watershed outlet and differences in spatially averaged monthly recharge between the two different rotation approaches. Spatially averaged monthly recharge values were calculated based on the flux output file (Flux_Inter2Ground.OUT) of DANSAT by averaging the recharge fluxes from the intermediate to ground water zone in all cells. The overall trend of difference in the monthly total runoff
followed the trend of difference in spatially average monthly recharge with smoothed and attenuated amplitude.

Table 7.2. Comparison of surface and subsurface hydrology results using the two rotation approaches.

<table>
<thead>
<tr>
<th>Year</th>
<th>Total runoff (mm/year)</th>
<th>Yearly average recharge (mm/year·cell)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Typical</td>
<td>Dynamic</td>
</tr>
<tr>
<td>1987</td>
<td>358.2</td>
<td>353.5</td>
</tr>
<tr>
<td>1988</td>
<td>323.9</td>
<td>320.4</td>
</tr>
<tr>
<td>1989</td>
<td>577.4</td>
<td>568.5</td>
</tr>
<tr>
<td>1990</td>
<td>574.1</td>
<td>565.3</td>
</tr>
<tr>
<td>1991</td>
<td>461.3</td>
<td>455.0</td>
</tr>
<tr>
<td>1992</td>
<td>500.3</td>
<td>496.4</td>
</tr>
<tr>
<td>Total</td>
<td>2795.1</td>
<td>2759.1</td>
</tr>
</tbody>
</table>

Changes in agricultural management practices due to different crop rotations may impact the infiltration process. Figure 7.4 shows an example of temporal variation in effective hydraulic conductivity \((K_{\text{eff}})\), used in the Green-Ampt Equation, at a specific cell (cell number 86) for different levels of information on crop rotation. Difference in \(K_{\text{eff}}\) values resulted in differences in infiltration and overland flow. Different levels of information on crop rotation also affect transpiration values. The longer the land is covered by crop, the larger the transpiration losses. In the typical crop rotation approach, no crop exists during the winter (between soybean and corn). However, winter wheat can be present during the entire winter seasons within the dynamic rotation approach. As a result, more transpiration could occur in the dynamic rotation approach, which may result in the decrease in recharge despite increased infiltration. The direct distance from a cell where ground water recharges occur to the nearest stream segment is also another important factor to consider. Predicted monthly fluxes from the intermediate zone to ground water zone in each cell were averaged for both typical and dynamic rotation approaches, and the spatial distribution of the differences between the two approaches (typical – dynamic) are shown in Figure 7.5. Most of the difference in recharge values occurred in the crop areas because rotation information was not changed in the non-crop areas. Areas with greater recharge are displayed with red and dark green for the typical rotation approach and the dynamic rotation approach, respectively. The shorter the distance between the overland cell and stream cell, the faster the conversion from the ground water recharge to the baseflow. More ground water recharge in the typical rotation approach may be converted to baseflow and added to the total runoff than those in the dynamic rotation approach because areas with greater recharge in the typical approach were closer to the stream compared to the areas with greater recharges in the dynamic approach.
Figure 7.2. Comparison of (a) daily total runoff and (b) monthly total recharge in each cell for the two levels of information on crop rotation.
Figure 7.3. Temporal comparison of difference in monthly total runoff (monthly total runoff by typical approach – monthly total runoff by dynamic approach) and difference in spatially averaged monthly recharge (spatially averaged monthly recharges by typical approach – spatially averaged monthly recharges by dynamic approach) for the two levels of information on crop rotation.

Figure 7.4. Comparison of effective hydraulic conductivity values for Green-Ampt for the two rotation approaches at cell number 86.
Figure 7.5. Spatial distribution of difference in average monthly recharge for the two crop rotation approaches.

Sediment

Table 7.3 shows variations in yearly total sediment loads for the two crop rotation approaches used in this study. As expected, total sediment loads in the typical rotation approach were higher during the entire simulation period compared to the total sediment load in the dynamic approach. Changes in crop rotation information from the dynamic to the typical rotation approach on crop areas increased total sediment yield by 6.5%. Figure 7.6 shows a comparison of the simulated daily total sediment loads by the two crop rotation approaches. It is difficult to identify the specific dates with big differences in daily sediment loads between the two crop rotation approaches. Time-series of differences in monthly total sediment loads during the simulation period are shown in Figure 7.7. Most of the differences occurred during the wet years such as 1989 and 1990. Even though direct runoff by the typical crop rotation approach was greater than that from the dynamic approach, most of the differences in total runoff were due to the baseflow component. As a result, changes in sensitive soil parameters such as rill and interrill erodibility factors on overland areas may not significantly impact the total sediment yields in streams, even
though the rill and interrill erodibility factors are sensitive parameters to overland soil erosion. Soil erodibility factors are estimated by DANSAT based on temporal and spatial changes in agricultural management practices. Figure 7.8 shows the temporal variation in rill and interrill erodibilities and critical shear stress in a rill at a specific cell (cell number 86) for the two crop rotation approaches. Erodibility factors such as rill and interrill erodibilities showed similar trends. Rill and interrill erodibilities increased right after a tillage application and decreased with time. Critical shear stress in a rill showed the opposite response to the erodibility factors and increased when erodibility factors decreased.

Table 7.3. Comparison of surface and subsurface hydrology results for the two crop rotation information levels used in this study.

<table>
<thead>
<tr>
<th>Year</th>
<th>Total sediment load (mm/yr)</th>
<th>Difference (Typical-Dynamic)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Typical</td>
<td>Dynamic</td>
</tr>
<tr>
<td>1987</td>
<td>315.2</td>
<td>305.5</td>
</tr>
<tr>
<td>1988</td>
<td>333.5</td>
<td>324.0</td>
</tr>
<tr>
<td>1989</td>
<td>2431.9</td>
<td>2255.9</td>
</tr>
<tr>
<td>1990</td>
<td>1814.1</td>
<td>1647.0</td>
</tr>
<tr>
<td>1991</td>
<td>738.6</td>
<td>712.9</td>
</tr>
<tr>
<td>1992</td>
<td>1108.1</td>
<td>1081.8</td>
</tr>
<tr>
<td>Total</td>
<td>6741.4</td>
<td>6327.0</td>
</tr>
</tbody>
</table>

Figure 7.6. Comparison of the simulated daily total sediment loads for the two crop rotation approaches used in this study.
Figure 7.7. Time-series of differences in monthly total sediment loads (monthly total sediment load by typical approach – monthly total sediment load by dynamic approach) during the simulation period.
Figure 7.8. Comparison of (a) interrill erodibility, (b) rill erodibility, and (c) critical shear stress in a rill for the two crop rotation approaches at cell number 86.
Summary and Conclusions

The overall goal of this chapter was to analyze the response of DANSAT to different levels of information available on management practices. Changes in crop rotation information on the crop area influenced both surface and subsurface regimes. The use of different levels of information on crop rotation caused changes in effective hydraulic conductivity and soil erodibility parameters on the ground surface. In the subsurface area, both temporal distribution of soil water extraction by evapotranspiration and spatial distribution of ground water recharge were influenced by the changes in crop rotations. Changes in surface characteristics on the overland area influenced the recharge to the ground water, and the changes in the ground water recharge influenced the total runoff in a stream, which also impacted the total sediment yield.

Even though the differences in total runoff and recharge were not significant, the typical rotation approach showed greater total runoff and ground water recharge than the dynamic crop rotation approach. Sediment yield was more sensitive to the level of crop rotation information on crop areas compared to the hydrology component, especially during the wet years. Changes from the dynamic rotation approach to typical approach on crop areas (35.8% of watershed) increased total runoff and ground water recharge by 1.3% and 1.8%, respectively. Whereas, the total sediment yield increased by 6.5% as the crop rotation approach changed from dynamic to typical.

The objective of this application was not to select a better approach for simulating hydrology and sediment in QN2 watershed. Rather, the application demonstrated that DANSAT is able to consider the impacts of temporal and spatial changes in crop rotation information on surface and subsurface hydrology and water quality. Rotation information considered on the crop area included 1) different date of planting, harvesting, and tillage applications, 2) different types of crop and tillage application, and 3) different residue management during harvesting. In addition, DANSAT also proved to be useful for simulating the impacts of land use changes from crop areas to non-crop areas on surface and subsurface areas.

Reference
Chapter 8: Summary and Conclusions

Summary

Goal and Intended Model Use
The overall goal of this study was to develop a comprehensive tool for assessing the effectiveness of selected BMPs on both hydrology and water quality and to demonstrate the applicability of the system by considering 1) temporally and spatially changing land use management practice in an agricultural watershed and 2) interaction between surface and ground water over the entire system.

DANSAT is a management model developed for planning purposes within a small agricultural watershed. The model is intended for use by non-point source pollution managers for assessing the relative effectiveness of best management practices (BMPs) on both surface and ground water with a minimum calibration. The model is not intended for making absolute predictions. A finer grid can be used to represent spatial variations of BMPs such as various zones of forest riparian buffer on a smaller watershed. The model can also be run on a field to assess the effectiveness of BMPs in reducing the amount of pesticides reaching the ground water.

System Development
The modeling system consists of databases, newly developed DANSAT and user interface, and existing groundwater models. The model interface accesses the spatial, meteorological, and physical or managerial database and creates input files for DANSAT. MODFLOW and MT3D were selected as ground water models for linkage with DANSAT. DANSAT is the only distributed-parameter, physically-based, continuous-simulation, and multi-soil layer model for simulating the spatial and temporal impacts of BMPs on hydrology, sediment, and pesticide losses at both field-scale and watershed-scale.

Hydrology components include interception, evapotranspiration, infiltration and percolation, overland flow, channel flow, interflow, and baseflow components. The physically-based Green-Ampt equation was used to simulate infiltration considering unsteady rainfall. Soil evaporation and plant transpiration were predicted separately using the Ritchie equation. The capacity-based percolation subroutine was incorporated to simulate the movement of soil water. A kinematic storage model for lateral subsurface flow was adapted into DANSAT to simulate interflow in subsurface areas. A concept similar to the one used in SWAT was selected for simulating baseflow.
Sediment components simulate interrill detachment, rill detachment, channel detachment, transport capacity, overland routing, and channel routing. Physically-based sediment detachment components for overland and channel were adapted. Overland sediment detachment is calculated by separately considering interrill detachment and rill detachment. Available sediments are compared with calculated transport capacity to estimate sediment outflow to the adjacent cells. Yalin's equation was selected to calculate transport capacity for each particle size class. Continuity equation was used to simulate transport of sediment between cells.

The pesticide components simulate pesticide application, degradation, adsorption and desorption, plant uptake, pesticide leaching, pesticide in runoff, interflow, and baseflow. The pesticide component takes into account sediment-bound and dissolved pesticide transport based on the capacity-based approach. Pesticide degradation in the soil or foliage is estimated using first-order kinetics, and the degradation rate for a given compound is adjusted based on soil temperature and soil water content. The simple linear equilibrium isotherm equation is used to simulate the interactions between the pesticide chemical and the soil particle surface. Uptake of pesticides by plants was considered as a part of the overall transpiration process. Pesticide movement by interflow was considered based on the amount of water movement and pesticide concentration, which is updated for changes in soil water using the equilibrium isotherm equation. One dimensional transport of pesticide in ground water was calculated based on the distance from a given cell to the nearest channel cell and travel time, which is required for the pesticide peak to reach the nearest stream segment.

**Model Evaluation**

DANSAT was applied to one field plot (QOB) and two agricultural watersheds in Virginia to evaluate the model components, and its performance in predicting runoff, sediment loss, and pesticide loads. The cell component was calibrated on a corn field with conventional tillage (18m x 27m in size). Capability of hydrology and sediment components for simulating spatially distributed results according to spatially distributed land use practices were evaluated on the Owl Run watershed (1140 ha) using the internal validation approach. Capability of hydrology, sediment, and pesticide components for simulating temporal variations of BMPs were evaluated using the split-sample approach from the QN2 watershed (216 ha in size). The Dual-Simulation (DS) approach was introduced to resolve the problems caused by different temporal scales between DANSAT and MODFLOW within the linked modeling approach. The linked approach
was applied to QN2 and the simulated results were compared with the results from the integrated approach.

DANSAT performed well in predicting total runoff in all cases with a percent error less than 10%, except for a 39.8% of error from an internal subwatershed (QOC) of Owl Run watershed. The model also performed well in predicting temporal variations in runoff with Nash-Sutcliffe model efficiencies of greater than 0.5, except for 0.1 of monthly Nash-Sutcliffe efficiency during the validation period in QN2 watershed. Predicted total sediment yields were within ±35% of observed values in all cases. The poorest prediction occurred in an internal subwatershed (QOC) with a 34.7% of total error. DANSAT performed well in predicting temporal trend of sediment load on Owl Run watershed where flowrate and sediment load have a higher correlation with each other, while the model failed to simulate the temporal fluctuations in monthly sediment loads in QN2 watershed where poor correlations are shown between flow rate and sediment loads. Nash-Sutcliffe model efficiencies for both calibration and validation periods were less than zero. The predicted total pesticide loads were within ±100% of observed values for both calibration and validation periods in QN2 watershed. DANSAT failed to simulate the temporal occurrence of pesticide loads with a 0.42 of maximum daily Nash-Sutcliffe efficiency value for Metolachlor simulation during the calibration period. In addition, movement of infiltrated water and pesticides within a root zone of QNB plot was predicted well by DANSAT with 0.69 and 0.82 of index of agreements for atrazine and metolachlor, respectively, even though the model consistently overpredicted peak pesticide amount within the soil profile. The linked approach was better in predicting the seasonal trend of total runoff with a 0.60 of monthly Nash-Sutcliffe model efficiency, compared to the corresponding value of 0.53 based on the integrated ground water approach.

**Sensitivity Analysis**

Responses of five output variables, including total runoff, sediment loads, pesticides in runoff, ground water recharge, and pesticide flux to the ground water, to the changes in input parameters (watershed-scale parameters, spatially-distributed parameters, and channel related parameters), grid size, and time-step were examined.

Output variables were sensitive to the changes in both watershed-scale parameters and spatially distributed soil parameters such as total porosity and field capacity. Only sediment yield sensitively responded to the changes in channel related parameters. Output variables were more
sensitive to the changes in soil parameters at a cell near stream, compared to the parameter changes at a cell near watershed boundary.

The model response to the different grid sizes in a user-created rectangular watershed showed linear reductions in total runoff and sediment yields as the grid size increased. Total runoff was not sensitive to the changes in grid size, showing a linear decrease of 8% as the grid size increased from 32 m to 120 m. However, pesticide load was sensitive to the changes in grid size, showing 38% decrease in pesticide loads with an increase in grid size from 30 m to 120 m. Sensitivity of DANSAT to different grid size was analyzed on QN2 watershed by considering both parameter impact and model impact. Grid sizes smaller than 100 m were recommended for appropriate representation of spatial distributions of soil, land use, and topographic parameters by analyzing GIS manipulation errors. Total runoff at the watershed outlet positively responded to grid size. The increase in grid size influenced the spatial distribution of recharge and resulted in an increase in baseflow and total runoff. The general trend in sediment yield was similar to that of the hydrology component. However, the sediment yield was sensitive to the changes in grid size.

Sensitivity analyses of DANSAT to different time-steps were conducted on both Owl Run and QN2 watersheds. Both total runoff and sediment yields decreased by 24% and 25%, respectively, in the Owl Run watershed. The increase in time-steps influenced the temporal variation of rainfall intensity, which caused the increase in infiltration and recharge. Total runoff at the watershed outlet increased as the time-step increased in QN2. Daily storm flow sensitively decreased while total runoff was stable, with a slight increase (8%) when the time-steps increased from 1 minute to 60 minutes. Sediment yields were also sensitive to the changes in the shape of the stream cross section. Total pesticide in runoff decreased rapidly and was not stable for time-steps of less than 5 minutes.

**Model Application**

The responses of DANSAT to two different levels of crop rotation information were simulated using three inter-related components such as plant-growth, residue-decomposition, and soil components, which were adapted from WEPP for considering the impacts of temporal changes of BMPs on soil, crop, and surface characteristics. Changes in crop rotation information influenced both surface and subsurface regimes. Even though the differences were not significant, the typical rotation approach showed greater total runoff, ground water recharge, and sediment yields than the dynamic rotation approach. Sediment was more sensitive to the changes in crop rotation information during the wet years. The applications showed that DANSAT is able to consider the

330
impacts of temporal and spatial changes in rotation information on surface and subsurface hydrology and water quality.

**Limitations and Future Works**

The current version of DANSAT contains many limitations because the model was developed based on several assumptions and simplifications of the actual system. Thus, the following limitations could be future research topics for improving the simulation capability of DANSAT.

One of the major limitations of the current version of DANSAT is that the model requires intensive amount of computational time, and the model is not appropriate for long-term simulations at a large watershed. DANSAT cannot be applied to a watershed containing a lake or reservoir, which is greater than a user-defined grid size. DANSAT needs to consider characteristics of outlet structures and emergency spillway as well as reservoir management strategies. Winter hydrology for considering snow accumulation/melting process and freezing/thawing cycle, which are important processes in predicting the gradual release of water during early spring and physical soil properties such as hydraulic conductivity and rill/interrill erodibilities, cannot be simulated in DANSAT. Another important limitation of DANSAT in the assessment of agricultural BMPs is the lack of nitrogen and phosphorus components. Nutrient components could be easily added because a similar procedure and approach for pesticide components can be used to simulate nutrient losses. In addition, there are several components, which DANSAT is not able to simulate, including structural BMP, bacteria, preferential flow, bank erosion, irrigation, point source, urbanization, and subsurface drainage components. These components should be incorporated into DANSAT in the future to enhance applicability of the model. Regarding surface water and ground water interactions, the proposed linked system cannot be used for simulating interactions between surface water and a deep confined aquifer. In addition, DANSAT is not able to simulate upward movement of water and pesticide from a saturated area.

**Conclusions**

The following specific conclusions could be drawn from the study:

- Design concept and structure of the proposed modeling system, including the selected method for newly developed DANSAT, are suitable for considering the impacts of temporal and spatial BMPs and dynamic surface and ground water interactions.
• The performance of DANSAT in predicting the temporal trend of total runoff was reasonable with daily Nash-Sutcliffe model efficiency values of greater than 0.5 at both plot and watershed-scales applications.

• DANSAT performed reasonably well in predicting temporal trend and spatial distribution of sediment loads only when high correlations between flow rates and sediment loads exist.

• DANSAT failed to simulate the temporal trends in pesticide loads at the watershed-scale while it performed well in predicting the movement of pesticides in runoff and soil profile for the plot-scale application.

• The linked approach was better in predicting the seasonal trend of total runoff with a value of 0.60 for monthly Nash-Sutcliffe model efficiency, compared to the values of 0.53 based on the integrated ground water approach.

• Spatially distributed soil parameters, including total porosity and soil field capacity were revealed as sensitive parameters for the watershed scale application and output variables were more sensitive to the changes in soil parameters at near stream cells than the changes at near watershed boundary cells.

• Sensitivity to different grid sizes and time-steps was the least for hydrology components followed by sediment and pesticide components. Acceptable maximum grid size for appropriately representing spatial distribution of topographic, land use, and soil characteristics was recommended based on GIS manipulation error analysis. Continuous simulation using greater time-step (60 minute) and the appropriate maximum grid size (90 m) dramatically decreased computation time to 2 minutes, compared to 612 minutes of computational time based on smallest time-step (1 minute) and smallest grid size (30 m).

• The capability of DANSAT for predicting the impacts of temporal and spatial changes in crop rotation on both surface and subsurface regimes was judged to be acceptable.
Appendix A: Collecting Soil Parameters
Calculating Total Porosity based on soil survey

Total porosity (TP) was calculated based on bulk density using the equation:

\[ TP = 1 - \frac{BD}{PD} \] \hspace{1cm} (A.9)

Where, BD=bulk density and PD=particle density, which was assumed as 2.65 g/cm³.

Because most soil surveys contain information about the available water capacity (AWC), which is defined as the water held within the pores between field capacity and the wilting point, field capacity (FC) was calculated based on the available water capacity. The assumption was made that approximately one-half of the soil water is not available and field capacity and wilting point were calculated using the equations:

\[ WP = AWC \] \hspace{1cm} (A.10)

\[ FC = 2 \cdot AWC \] \hspace{1cm} (A.11)

Percent passing sieve number of 4, 10, 40, and 200, which respectively correspond to the opening size of 4.7mm, 2mm, 0.42mm, and 0.074mm, were used to estimate total sand percent, very fine sand percent (0.05-0.1 mm), fine and medium sand percent (0.1-0.5 mm), coarse and very coarse sand percent (0.5-0.2 mm), and coarse fragment percent. Percent of soil particles passing 0.05, 0.1, and 0.5 mm of opening size were linearly interpolated using the equations below:

\[ P_{0.05} = \frac{(P_{200} - P_{\text{clay}})}{(0.074 - 0.002)} \cdot (0.05 - 0.002) + P_{\text{clay}} \] \hspace{1cm} (A.12)

\[ P_{0.1} = \frac{(P_{40} - P_{200})}{(0.42 - 0.074)} \cdot (0.1 - 0.074) + P_{200} \] \hspace{1cm} (A.13)

\[ P_{0.5} = \frac{(P_{10} - P_{40})}{(2.0 - 0.42)} \cdot (0.5 - 0.42) + P_{40} \] \hspace{1cm} (A.14)

Where, \( P_{200} \)= Percent of soil particles passing sieve number of 200, which correspond to the opening size of 0.074mm; \( P_{40} \)= Percent of soil particles passing sieve number 40, which correspond to the opening size of 0.42 mm; \( P_{10} \)= Percent of soil particles passing sieve number...
10, which correspond to the opening size of 2.0 mm; P0.05= Percent of soil particles passing 0.05 mm of opening size; P0.1= Percent of soil particles passing 0.1 mm of opening size; P0.5= Percent of soil particles passing 0.5 mm of opening size; and Pclay=clay percent.

Total sand percent, very fine sand percent (Pvfs), fine and medium sand percent (Pfms), coarse and very coarse sand percent (Pcvc), and coarse fragment percent (Pcf) were calculated by the equations below based on the previously interpolated values. Total sand percent was calculated by the equation:

\[ P_{sand} = P_{10} - P_{0.05} \]  
(A.15)

\[ P_{silt} = 100 - P_{clay} - P_{sand} \]  
(A.16)

\[ P_{vfs} = P_{0.1} - P_{0.05} \]  
(A.17)

\[ P_{fms} = P_{0.5} - P_{0.1} \]  
(A.18)

\[ P_{cvc} = P_{10} - P_{0.5} \]  
(A.19)

\[ P_{cf} = P_{4} - P_{10} \]  
(A.20)

Where, \( P_{sand} \)=total sand percent, \( P_{silt} \)=silt percent, and \( P_{4} \)= Percent of soil particles passing sieve number 4.

**Extracting parameters from SSURGO**

Most soil layer parameters can be directly extracted from the SSURGO database file. The exported ascii files including Horizon table (chorizon.txt) and Mapunit table (mapunit.txt) with comma delineated format are used as inputs for the user interface. Mapunit table contains the general soil information, while most of soil layer parameters, except for residual water content and coarse fragment content, can be directly derived from the horizon table. Table A.1 shows the required soil layer parameters in DANSAT and the corresponding column name and column numbers in the horizon table. The interface reads the horizon table file and saves the extracted parameters into the predefined input database file of the interface in Figure 3.18.
Table A.1. Soil layer parameters in DANSAT and corresponding column name and numbers in the horizon table.

<table>
<thead>
<tr>
<th>Soil Parameters</th>
<th>Col. Name(No)</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bottom depth of each layer (m)</td>
<td>hzdepb_r (10)</td>
<td>Distance from the top of the soil to the base of the soil horizon (cm)</td>
</tr>
<tr>
<td>Total porosity</td>
<td>wastiated_r (98)</td>
<td>The estimated volumetric soil water content at or near zero bar tension, expressed as a percentage of the whole soil. (%)</td>
</tr>
<tr>
<td>Field capacity</td>
<td>wthirdbar_r (92)</td>
<td>The volumetric content of soil water retained at a tension of 1/3 bar (33 kPa), expressed as a percentage of the whole soil (%)</td>
</tr>
<tr>
<td></td>
<td>wtenthbar_r (89)</td>
<td>The volumetric content of soil water retained at a tension of 1/10 bar (10 kPa), expressed as a percentage of the whole soil (%)</td>
</tr>
<tr>
<td>Wilting point</td>
<td>wftfteenbar_r (95)</td>
<td>The volumetric content of soil water retained at a tension of 15 bars (1500 kPa), expressed as a percentage of the whole soil (%)</td>
</tr>
<tr>
<td>Residual water</td>
<td>N/A</td>
<td>Estimated in DANSAT</td>
</tr>
<tr>
<td>Bulk density (mg/cm3)</td>
<td>dbthirdbar_r (73)</td>
<td>The oven dry weight of the less than 2 mm soil material per unit volume of soil at a water tension of 1/3 bar.(mg/cm3)</td>
</tr>
<tr>
<td>Soil clay content(%)</td>
<td>claytotal_r (61)</td>
<td>Mineral particles less than 0.002mm in equivalent diameter as a weight percentage of the less than 2.0mm fraction. (%)</td>
</tr>
<tr>
<td>Soil sand content(%)</td>
<td>sandtotal_r (34)</td>
<td>Mineral particles 0.05mm to 2.0mm in equivalent diameter as a weight percentage of the less than 2 mm fraction. (%)</td>
</tr>
<tr>
<td>Soil silt content(%)</td>
<td>siltotal_r (52)</td>
<td>Mineral particles 0.002 to 0.05mm in equivalent diameter as a weight percentage of the less than 2.0mm fraction. (%)</td>
</tr>
<tr>
<td>Soil organic matter content(%)</td>
<td>om_r (67)</td>
<td>The amount by weight of decomposed plant and animal residue expressed as a weight percentage of the less than 2 mm soil material. (%)</td>
</tr>
<tr>
<td>Very fine sand content(%)</td>
<td>sandvf_r (49)</td>
<td>Mineral particles 0.05 to 0.10mm in equivalent diameter as a weight percentage of the less than 2 mm fraction. (%)</td>
</tr>
<tr>
<td>Coarse fragment content(%)</td>
<td>N/A</td>
<td>Estimated in DANSAT</td>
</tr>
<tr>
<td>Saturated hydraulic conductivity (m/h)</td>
<td>ksat_r (83)</td>
<td>The amount of water that would move vertically through a unit area of saturated soil in unit time under unit hydraulic gradient. (um/sec)</td>
</tr>
<tr>
<td>Cation exchange capacity (meq/kg)</td>
<td>cec7_r (127)</td>
<td>The amount of readily exchangeable cations that can be electrically adsorbed to negative charges in the soil, soil constituent, or other material, at pH 7.0, as estimated by the ammonium acetate method. (meq/100g)</td>
</tr>
<tr>
<td>Fine sand content (%)</td>
<td>sandfine_r (46)</td>
<td>Mineral particles 0.10 to 0.25mm in equivalent diameter as a weight percentage of the less than 2 mm fraction. (%)</td>
</tr>
<tr>
<td>Medium sand content (%)</td>
<td>sandmed_r (43)</td>
<td>Mineral particles 0.25mm to 0.5mm in equivalent diameter as a weight percentage of the less than 2 mm fraction. (%)</td>
</tr>
<tr>
<td>Coarse sand content (%)</td>
<td>sandco_r (40)</td>
<td>Mineral particles 0.5mm to 1.0mm in equivalent diameter as a weight percentage of the less than 2 mm fraction. (%)</td>
</tr>
</tbody>
</table>
Appendix B: Interface Manual
Interface Overview

Overview
A modeling system was developed to evaluate the spatial and temporal impacts of BMPs on hydrology and water quality in an agricultural watershed considering the surface and groundwater interaction. A user interface is indispensable to a physically-based, distributed parameter, and watershed scale model that requires intensive spatial and temporal input data. The interface was originally designed to create intensive input data blocks such as cell, rotation, and soil data blocks in the main input file, as well as the break-point rainfall input file. The advantage of using the interface is to avoid errors due to the differences in the input format and to save time for creating the input file.

Menus
Table A.2 shows the hierarchical menu structure of the interface. From this point, bold, underlined, and italic characters indicate main-menu, submenu, and window tabs, respectively. Square brackets indicate buttons in the interface. For example, Activity-Define Activity-Pesticide-[Add] means clicking of [Add] button within the Pesticide tab shown inside the Define Activity window, which can be opened by clicking of Activity → Define Activity within the menu bar. Figure A.1 shows the main window of the interface and the main menus available in the interface.
Figure A.1. Main window of the interface and main menus.

Table A.2. Hierarchical menu structure of the interface

<table>
<thead>
<tr>
<th>Main-menu</th>
<th>Submenu</th>
<th>Window Tabs</th>
</tr>
</thead>
<tbody>
<tr>
<td>File</td>
<td>Open project</td>
<td>General, Flag</td>
</tr>
<tr>
<td></td>
<td>Save project</td>
<td></td>
</tr>
<tr>
<td>General</td>
<td>General Info</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Create Database</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Create Cell Number</td>
<td></td>
</tr>
<tr>
<td>Input/Output</td>
<td>Parameters</td>
<td>General, Layer, Management, Output, Calibration</td>
</tr>
<tr>
<td></td>
<td>Initial Value</td>
<td></td>
</tr>
<tr>
<td>Cell</td>
<td></td>
<td>Input Files, Channel Type</td>
</tr>
<tr>
<td>Soils</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Activity</td>
<td>Define Activity</td>
<td>Crop, Tillage, Pesticide</td>
</tr>
<tr>
<td></td>
<td>Define Pesticides</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Define Distribution</td>
<td></td>
</tr>
<tr>
<td>Rotation</td>
<td>Define Rotation</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Initial Value</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Rotation Builder</td>
<td></td>
</tr>
<tr>
<td>Weather</td>
<td></td>
<td>Observed Data</td>
</tr>
<tr>
<td>Run</td>
<td>Create Input</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Run DANSAT</td>
<td></td>
</tr>
</tbody>
</table>
General Concepts
Many windows in the interface have common components. Figure A.2 shows the Define Activity window, which is shown by clicking **Activity-Define Activity-Tillage**. Many interface windows have three buttons such as [Save], [Create], and [Cancel] at the bottom of the window. [Save] button updates the selected or changed parameter values into the project file. [Create] button updates the corresponding input data blocks within the main input data file. For example, [Create] button in Figure A.2 will update only three input data blocks of the main input file including Crop, Tillage, and Pesticide input data blocks. [Cancel] button closes the current window without any changes in both the project file and input file. Other commonly used components in many interface windows are DB List box and Input List box, as in Figure A.2. DB List box is linked to the predefined MS Access parameter database file (Input DB in Figure 3.18), which is accessed and manipulated by the interface parameter database file, and all the data names in the database are listed in the DB List component. Figure A.2 shows the available tillage names in the input DB. The user can move items from DB List to Input List by clicking [►] button and remove items from Input List by clicking [◄] button. Numbers before the item names of the Input List box are used as reference numbers in the model input file. If the user wants to change the order, [Up] and [Down] buttons can be used. Specific parameters for each selected item can be reviewed or changed by clicking, [View/Edit] button. Figure A.3 shows the editing windows for the selected Disk_Roll tillage application. In this editing window, the user can delete the record from the database by [Delete] button or change the information by [Update] button. [Add] button in the Define Activity window can be used to add a new tillage application into the parameter database.
Figure A.2. Example of define activity window of the interface.

Figure A.3. Example of Edit Database window (tillage).
Directory structure

The interface requires five directories to create input files for DANSAT and to run DANSAT through the interface. The five directories include database, executable, GIS, model input, and model output directories. Table A.3 shows the required directory names, and the corresponding contents should exist below each directory. The structure and location of the directories are not critical to use the interface and run the model. Arc/View shape files in the GIS directory are optional for displaying the spatial distribution of parameters in the Cell Data Block (Figure A.11). The usage of each content file will be explained in the corresponding section of this manual in detail.

Table A.3 Required directories for the interface and necessary files for each directory.

<table>
<thead>
<tr>
<th>Directory</th>
<th>Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>Database</td>
<td>- Parameter DB file (MS Access format with predefined DB structure)</td>
</tr>
<tr>
<td></td>
<td>- Crop and Tillage database file from WEPP*</td>
</tr>
<tr>
<td></td>
<td>- Pesticide database file from GLEAMS*</td>
</tr>
<tr>
<td></td>
<td>- Soil attribute files (text format) from SSURGO database*</td>
</tr>
<tr>
<td></td>
<td>- Original format of break-point rainfall data files (HAS format only)*</td>
</tr>
<tr>
<td></td>
<td>- ASCII raster files (Arc/View format) for creating cell data input block.</td>
</tr>
<tr>
<td>Executable</td>
<td>- DANSAT executable file (model.exe)</td>
</tr>
<tr>
<td></td>
<td>- MODFLOW executable file (mudflow.exe)</td>
</tr>
<tr>
<td></td>
<td>- MT3D executable file (mt3dms.exe)</td>
</tr>
<tr>
<td>GIS</td>
<td>- Arc/View shape files</td>
</tr>
<tr>
<td>Model Input</td>
<td>- DANSAT input files (main input, weather input, break-point rainfall input, and initial input files)</td>
</tr>
<tr>
<td></td>
<td>- MODFLOW/MT3D input files when the linked GW approach is selected</td>
</tr>
<tr>
<td>Model Output</td>
<td>- Simulation result files will be created in the directory.</td>
</tr>
</tbody>
</table>

*: Files are not necessary when user puts the parameter values one by one using [Add] button.

File

Two submenus are available below the File menu: Open project and Save project. The major function of Save project submenu is to save the user-defined parameters through the interface into the selected project file (extension is prj). The purpose of Open project is to retrieve parameter values from an existing project file to the interface for further editing and model simulations.

General

General main-menu contains three submenus including General Info, Create Database, and Create Cell Number. Through the General Info submenu, the user is able to define the location of the existing five directories and choose the file names of required files for each directory in the Flags tab. Figure A.4 shows the interface window to control “Directory and Input File Name
Block” of the main input file. Simulation description can be added through Title textbox for as many lines as the user wants. Components and output files can be turned on and off in the Flags tab, which is shown in Figure A.5. In addition, different approaches can be selected through the method flag control buttons.

![General Block Generator window](image)

**Figure A.4.** General tab of the General Block Generator window to control directory and file names.
Create Database submenu launches the Create Database Table window, which is shown in Figure A.6. Intensive physically-based input parameters for crop, tillage, and pesticide can be obtained from the database files of existing models. Crop, tillage, and pesticide tables in the parameter database file (MS Access file) can be filled through this interface. Crop and tillage related parameters are read from WEPP database files and saved to the parameter database file of DANSAT. Pesticide parameters are filled based on the GLEAMS database file. Default parameter database file (BMP.mdb) in the DB directory already contains crop, tillage, and pesticide information. Using a copy of the default parameter database file is recommended for a new simulation instead of filling the database file at every model simulation. Using a different database file for each project is recommended because some database tables such as soil and rotation use unique soil types and rotation information.
Cell number ascii raster file in the Arc/View format is one of the input files necessary to create the cell data block of the main input file. Arc/View does not have any spatial analysis function to create appropriate cell numbers for DANSAT. Cell number is used to define calculation order for the overland routing. The user has to create the cell number ascii file based on the flow accumulation ascii file, which can be easily derived using Arc/View. Figure A.7 shows the interface window for creating the cell number ascii file.

**Input/Output**

Input/Output menu contains Parameter and Initial Value submenus. Parameter submenu starts “Input/Output Block Generator” window, which is shown in Figure A.8 and Figure A.9. The interface window consists of five categories such as General, Layer, Management, Output, and Calibration. These interface windows cover general input parameters, output parameter data block, and groundwater data block of the main input. Some parameters such as number of rows and columns, number of soil types, and number of channel types can be input directly by the user or defined based on corresponding ascii raster files by clicking [From DB] button. Output tab of the interface window in Figure A.9 controls the outlet cells, given cells for the vertical distribution and time series output, and cycle of periodic outputs. Periodic outputs include flux files and groundwater output files.
### Figure A.8  General tab of the Input/Output Block Generator interface window.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Starting Date (mm/dd/yyyy)</td>
<td>1/1/1987</td>
</tr>
<tr>
<td>End Date (mm/dd/yyyy)</td>
<td>12/31/1992</td>
</tr>
<tr>
<td>Latitude of watershed (Decimal Degree)</td>
<td>38.5</td>
</tr>
<tr>
<td>Number of Rows</td>
<td>61</td>
</tr>
<tr>
<td>Number of Columns</td>
<td>71</td>
</tr>
<tr>
<td>Number of Active Cells</td>
<td>2333</td>
</tr>
<tr>
<td>Cell width of x-direction (m)</td>
<td>30</td>
</tr>
<tr>
<td>Cell width of y-direction (m)</td>
<td>30</td>
</tr>
<tr>
<td>Number of soil types</td>
<td>8</td>
</tr>
<tr>
<td>Number of Maximu Soil Layers</td>
<td>5</td>
</tr>
<tr>
<td>Number of particle size classes</td>
<td>5</td>
</tr>
<tr>
<td>Number of land use types</td>
<td>13</td>
</tr>
<tr>
<td>Number of Rotations</td>
<td>47</td>
</tr>
<tr>
<td>Max. Number of Application Dates in Rotations</td>
<td>50</td>
</tr>
<tr>
<td>Number of Rain Gages</td>
<td>3</td>
</tr>
<tr>
<td>Number of Channel Types</td>
<td>1</td>
</tr>
</tbody>
</table>
Initial Value submenu covers “Initial Data Block” of the main input file. If the flag is turned on (flag=1), spatial distribution of initial values can be considered based on a separate initial input file. Otherwise, a constant initial value is assigned to every cell. Figure A.10 shows the interface window for creating the initial data block. Even though nitrogen and phosphorus components are not considered in DANSAT, nitrogen and phosphorus components were included in the interface design for future improvements.
Cell

**Cell** menu contains *Input Files* and *Channel Type* tabs without any submenu. *Input Files* tab requires 16 ascii raster files (Arc/View) to create or update the cell data block of the main input file. All ascii files should have the same header to avoid error. [View] button shows Arc/View shape file to the map display area of the main window, only when the shape file has the same file name (030m_rotation.shp) with ascii file (030m_rotation.asc). The shape file should exist in the GIS directory. As mentioned in the overview section, the interface is independent of GIS software. This means that the ascii raster files can be exported by any other GIS software, and
map displaying is not a required function to create the input data block. Required input ascii files for creating the cell data block are shown in Figure A.11. Channel Type tab covers the channel data block of the main input. It also follows the general concepts of the interface, which are mentioned in the overview section. Figure A.12 shows the Edit Channel Database window and available channel types.

Figure A.11 Required input ascii files for creating cell data block.
Soils

Soils menu pop up the Soil Block Database interface window. This interface covers three different types of soil information including 1) particle class information, 2) general soil information, and 3) soil layer information, all of which are included in the Soil Data Block of the main input file. Even though DANSAT is able to consider different numbers of particle classes, the number of particle classes in the interface was fixed as 5 and the particle size for each class was decided based on USDA classification. Particle table in the default parameter database was already filled with information, which is shown in Figure A.13. However, if the user copied the default parameter database file (BMP.mdb), the soil and soil layer tables are currently empty. The user can fill the soil and soil layer table in two different ways. If the new version of SSURGO data is available for the watershed study, the user can easily fill soil related tables by locating two soil attribute files and clicking [Create DB] button shown in Figure A.13. The required two soil attribute files are mapunit.txt and chorizon.txt. Both files should be converted from tab delimited to semicolon delimited text files for the interface to recognize soil parameters correctly. In case only old soil survey data is accessible, the required soil parameter for the interface should be derived based on other existing parameters such as sieve analysis results. Calculated soil parameter data should be input in the database by clicking [Add] button shown in
The procedure to derive soil parameters based on an old soil survey report is explained in Appendix A. SSURGO soil data covers just around the root zone area. Note that the user should add more than one soil layer to cover soil layers between the root zone and saturated zone.

![Figure A.13 Soil Block Generator interface window.](image)

**Activity**

**Activity** menu contains three submenus including Define Activity, Define Pesticides, and Depth Distribution. Activity menu covers the Land Use Data Block, Tillage Data Block, Pesticide Data Block, and Distribution Data Block of the main input file. Figure A.14 shows the overall linkage between the interface windows, which are contained within the **Activity** menu.
Click of Activity-Define Activity opens Define Activity window shown in Figure A.14. Even though Define Activity window contains 6 tabs, only 3 tabs including Crop, Tillage, and Pesticide are active. Each [View/Edit] button on Crop, Tillage, and Pesticide tabs opens Edit Crop window, Edit Tillage window, and Edit Pesticide Application window, respectively. If table approach is selected for predicting LAI in the General menu, [View LAI Table] button is visible in the Edit Crop window. Clicking this button opens the Edit LAI Table window. Figure A.15 shows the Edit LAI Table window, which shows the LAI ratio (LAI divided by maximum LAI for each fraction of growing season) with a maximum value 1 for selected crop in the Edit Crop window.
About the pesticide application, Edit Pesticide window is linked to the [View Pesticide] button within the Edit Pesticide Application window, and Edit Depth Distribution window is linked to the [Distribution] button within the Edit Pesticide window. Edit Pesticide window and Edit Depth Distribution window can be directly accessed through the Define Pesticides and Depth Distribution submenus, as shown in the Figure A.14. The user can choose depth distribution factors for half-life in soils, partitioning coefficient, and water solubility parameters. If depth distribution type is not selected in the pesticide data block of the main file, same values of half-life, partitioning coefficient, and solubility parameters, which are given in the same data block, are used for every soil layer. If the user wants to consider different pesticide characteristics depending on soil depth, fraction values in Figure A.16 will be multiplied to the user given parameters value and an adjusted value will be used for each soil layer. Figure A.16 shows the Edit Depth Distribution window.
Every window mentioned here also follows the general concept of the interface. So, a detailed explanation to show how to use each interface window will be excluded in this section.

**Rotation**

Rotation menu contains Define Rotation, Initial Value, and Rotation Builder submenus. Rotation data block is one of the most complicated data blocks in the main input file because crop, tillage, and pesticide application information should be combined in this block. In the interface, two different approaches are available to combine management information and save it to the rotation table in the parameter database file: 1) individual inserting and 2) block inserting. At first, individual inserting through the interface is recommended in the case that the user has very specific actual rotation information. Figure A.17 shows the component of the Generate Rotation Data Block window. In order to add new rotation into the database, the user needs to put basic information including rotation name, rotation cycle, and descriptions in the corresponding textboxes, which are shown in Figure A.17 and click [Add] button. The user needs to select the application type in the Land Use, Pesticide, and Tillage list boxes and click [>] button to insert
information to the spreadsheet on right side. Then, the user has to put specific information for the date, type, and variable fields manually. Define Activity window covers Rotation Data Block in the main input file. After defining rotation through Define Rotation submenu, the user has to provide the initial values for each selected rotation type by clicking the Rotation-Initial Value. Figure A.18 shows the Initial Value for each rotation window for updating initial values for daily changing variables. This window overwrites the Daily Changing Variable Block in the main input file by clicking [Create] button.

If the user has typical rotation information for the watershed study, the block inserting approach through Excel spreadsheets, which will be referred to as Rotation Builder, are recommended. The user will be prompted to select the locations of the Excel executable file and workbook file by clicking the Rotation Builder submenu. Figure ** shows the control panel and rotation spreadsheet of the Rotation Builder file. Detailed instructions for showing how to use the Excel file is not included in this section.
Figure A.17 Generate Rotation Data Block window for individual inserting of management information.
Figure A.18 Rotation Initial Value window.
Figure A.19 Control panel and spreadsheet of Rotation Builder Excel workbook.

Weather

Weather menu opens Generate Break Point Rainfall Data window (Figure A.20). This routine is available only for the HAS format of the BSE department at Virginia Tech. The break point input file for DANSAT is generated through two steps. At first, break point rainfall data with irregular time-step (Basic format of HAS) are used to generate the break point rainfall data with one minute timestep by the [Create] button within the Input Files frame. Second, created temporal break point rainfall files (1 minute time-step) are combined into the final break-point input file depending on the storm event time-step. Thiessen averaging is not considered in the routine.
Run menu contains Create Input and Run DANSAT submenus. Although, the Show Output submenu, which opens post-processor window, will not be mentioned in this manual because there is still a practical problem in importing output files to the result database file: it takes too long to import output files to the database file.

Create Input submenu creates new DANSAT input file or updates all data blocks in the existing main input file. DANSAT can be run within the interface by clicking the Run DANSAT submenu.
Appendix C: Recommendations for future research
The following list of recommendations was developed to have a better overview of what needs to be done in the future to make DANSAT a part of a comprehensive decision support system (DSS). The long-term goal of the DSS is to evaluate the impacts of spatially and temporally changing BMPs using physically-based and distributed nonpoint source (NPS) mode, DANSAT. Figure A.21 shows major challenges to be considered in developing the proposed DSS.

In the figure, challenges were categorized into five tasks including 1) searching appropriate watersheds and collecting the necessary data; 2) searching appropriate analytical methods including statistical and geographical approaches to understand the responses of the watershed to the different placement and time of BMP implementation; 3) developing an interface and database; 4) improving distributed, physically-based, and continuous NPS model, DANSAT; and 5) developing supportive models or developing an interface for existing supportive models such as economical, biological, and statistical sub-models. Specific lists for each category will be discussed in the following sub-sections.
Watersheds

Selection of appropriate watersheds is critical for success in developing and validating a new model. A model developer complains about a lack of dataset for model validation. Appropriate watersheds need to have a sufficient period of records including 1) weather and BMP implementation history; 2) water quality and quantity data; and 3) watershed characteristics such as soil, topological, and geo-hydrologic data. Nomini Creek (NC) and Owl Run (OR) watersheds, which are included in this dissertation, seem to be appropriate for validating hydrology and sediment components of DANSAT. However, the two watersheds are not suitable for the validation of pesticide and surface-groundwater interaction components. Well organized watershed data with quality control (QC) will save a lot of time required to assemble the information from the watershed by each model developer. In addition, nation-wide watershed DB containing watershed-scale monitored data based on standardized format will be very useful for validating the newly developed model in different hydrologic conditions.

Analytical Methods

Development of new model components is impossible without understanding the real world because modeling should simplify and imitate the real world based on reasonable assumptions. Difficulties in understanding the real world exist due to the following reasons: 1) interactions among practices and biophysical setting, 2) lag time in water quality responses, 3) complexities of watersheds, and 4) surface and ground water interactions.

Collaborating with researchers in different area such as hydrology, statistics, and GIS are necessary to identify suitable analytical methods.

Interface and Database

Recommendations for the interface are classified into three different categories. The first category contains recommendations for the current version of the interface in which GIS processes are not included. The second and third categories describe expecting interfaces, which can be accomplished in a short-term and long-term time schedule, respectively, depending on the selected linkage approach between the model and GIS.

First, the current version of the interface for DANSAT is independent of GIS software even though format of the ascii files, which are used to transfer data between GIS and DASAT, is
based on Arc/View. The following list of recommendations was developed to make the interface more user-friendly.

**Post-processor:** The current approach to handle the simulation output files is based on a pre-defined format of a result database (Result.mdb) and Excel workbook for each different type of output. The way of transferring the simulated results from output files to the pre-defined MS Access database was selected because of line limitation in the spreadsheet of the Excel workbook. However, there is a critical limitation in the procedure because it takes so long time to transfer necessary output files to the database. As a result, another reasonable approach is necessary as a post-processor of the interface.

**Error checking subroutines:** The interface does not have a function to screen out the input parameters, which are outside of possible data ranges. Incorporating error checking routines into the current version of the interface will be useful for preventing unexpected simulation.

**Weather and break-point input generator:** The interface does not generate the weather input file. And, the break-point rainfall input can be created only if HAS format of observed data is available. Adding a function of creating weather input file will be very useful for running DANSAT, especially if there is no observable break-point rainfall data. A climate generator, which creates break-rainfall data based on long-term weather station statistics, will be very helpful for extending the model applicability.

**Soil input generator:** The current version of the interface has the fixed number of particle classes and particle size classes based on USGS classification, even though DANSAT has the capability to consider variable particle classes and sizes. For the flexibility of the model application, variable number of particle classes and flexible particle sizes for each class should be considered in the interface. In addition, routines for extracting required soil parameters for DANSAT from the soil database are based on a recent version of SSURGO. Many required soil parameters for DANSAT are not included in old soil survey data. In Appendix A, procedures for extracting soil parameters from old soil survey data was explained. So, the procedure needs to be coded in the interface.

Second, the model-based loose coupling approach is recommended in the short-term. In the approach, GIS and the model have a separate user interface, and ASCII or binary files are used to transport data between GIS and the model. This approach may be the most realistic method for
developing GIS-model interface because this approach requires minimum modification of GIS software and DANSAT. The major modification will be added to the GIS side by developing automatic procedures for manipulating GIS data.

Third, the model-based tight coupling approach is recommended in the long-term. The interface is expected to cover DANSAT and other supporting submodels based on a common spatial and attribute database. Subinterfaces, which create input files for both DANSAT and other submodels and analyze the output files, can be treated as a module within the overall functionality of the interface. Development of the common database for the interface requires defining the database structure based on required input parameters for each submodel by preventing overlapping of the parameters.

**DANSAT**

The major component of the proposed DSS is to develop an appropriate NPS model as an analytical engine. DANSAT must be improved by adding new components in order to consider major water quality problems in the watershed scale. The following are necessary components that should be added in the future.

**Nutrient:** The current version of DANSAT does not consider nitrogen and phosphorus movement, even though arrays and a part of the input structure are defined for adding nutrient related components in the future. Nutrient components should be included in DANSAT before other components because impairment of streams and reservoirs by nutrients is one of the major water quality problems in agricultural watersheds.

**Bacteria:** The structure of DANSAT has more advantages compared to the existing semi-distributed conceptual models such as HSPF and SWAT in considering the movement of bacteria at a watershed scale. Those semi-distributed models have difficulties in tracking the movement of bacteria from the source to the streams because of the general size of the subwatershed, which is usually used by a semi-distributed model that is too big to consider bacteria detachment, deposition, and die-off. As a result, the lumped approach, which calculates bacterial load from an overland area to streams using a spreadsheet outside of the model, is used to predict the overland areas, and the model considers the movement of bacteria in streams based on overland
input. DANSAT, however, simulates water and sediment movement from the watershed boundary to streams based on topography, land use, and soil characteristics. Movement of bacteria can be directly simulated within the model based on the results of hydrology and sediment components, as well as physically based land use and soil characteristics.

Reservoir: If the watershed study contains a reservoir or ponds inside, the impacts of reservoir on hydrology and water quality should be considered by the model. The reservoir may decrease flow peak and sediment loads at the watershed outlet by storing storm waters and slowly releasing the stored water after storms. Decrease of flow peak and sediment deposition in the reservoir may reduce the sediment loads at the watershed outlet. DANSAT needs to consider characteristics of outlet structures and emergency spillway as well as reservoir management strategy such as timing and amount of releasing water. Hydrology should be predicted based on that information and the deposition of sediment and sediment-bound nutrients should be calculated considering the results of hydrology and soil particle characteristics.

Winter hydrology: Winter hydrology components are required for watersheds where snow accumulation and melting processes occur during winter and early spring, respectively. This is an important part of the hydrology. Without winter hydrology components, it is difficult to simulate high flow rates occurring in early spring when there is no storm event. Freezing and thawing cycles also should be considered in predicting physical soil properties such as hydraulic conductivity and rill/interrill erodibilities. The current version of DANSAT assumes soil temperature is the same as air temperature. In order to consider freezing and thawing processes in the soil profile, a component for predicting soil temperature based on available input parameters seems to be necessary. Expecting winter hydrology can consist of three components including 1) component to simulate snow accumulation in each cell based on air temperature, 2) component to predict amount of melting snow from snow pack, and 3) component to consider freezing and thawing impacts on soil properties.

Preferential flow: The current version of DANSAT considers the impacts of conservation tillage by changing the soil and residue characteristics such as effective hydraulic conductivity and residue covers based on the application method. Some field scale research reports that long term no-till application may quicken the movement of infiltrated water and increase the movement of agri-chemicals to the shallow groundwater due to the development of preferential flow. In that case, DANSAT needs to consider water and agri-chemical movement through a bypass mechanism in a soil profile with a different approach compared to the regular percolation based
approach. Addition of preferential flow component to DANSAT will allow users to consider realistic tillage management and surface-groundwater interaction at the watershed scale.

Urbanization: Urbanization impacts are considered in DANSAT using percent of impermeable area as a crop parameter. For example, agricultural grass area, low-density developed area, and high-density developed area can be simulated using a different percent of impermeable area (0%, 20%, and 50%, respectively) without changing other crop parameters. If the impermeable percent is greater than zero, DANSAT does not calculate infiltration and percolation in that area and all precipitation amounts are used to calculate the outflow to the adjacent cell. However, new subroutine for atmospheric deposition of pollutant and subroutine for washoff by precipitation should be considered in DANSAT.

**BMP:** Agricultural BMPs can be classified into specific categories of vegetative, management, and structural BMP. Vegetative and management BMPs are relatively easy to consider in DANSAT compared with structural BMPs. Vegetative BMPs such as changes of cropping sequence can be considered in DANSAT by changing the crop parameters. Management BMPs such as tillage practice and pesticide and nutrient management practice can be considered in DANSAT by changing the application method, application time, and application rate. However, structural BMPs such as terraces, filter strip, and sediment control basins should be considered in a separate BMP component. Regarding the filter strip, if the grid size is small enough to consider a buffer strip near the stream, changing vegetative parameters can be used to consider the filter strip. A similar approach with reservoir components can be used for structures such as sediment control basins and dry/wet pond.

**Point source:** Concentration based regulations have been replaced by load based regulations. Total Maximum Daily Load (TMDL) is a calculated maximum amount of the pollutant that can be received by a water body without violating the water quality standards. TMDL is allocated to the contributing pollutant sources including point and nonpoint sources. DANSAT can be used in the agricultural watershed where no point sources are available as a tool for TMDL allocation. However, if DANSAT is applied to a watershed that contains point sources such as waste water treatment plant and springs, DANSAT needs to consider additional point source of water and pollutant at a specific location. In contrast, a sudden sink of water and pollutant at a Karst area should be considered in DANSAT.

**Irrigation:** DANSAT needs to contain irrigation components to be used in an arid area where irrigation is an indispensable agricultural management practice for crop growth. Even though
the current version of DANSAT has some irrigation parameters in the main input file, the actual code is not developed for an irrigation component. Two different application methods can be considered in DANSAT: manual irrigation and automatic irrigation. Manual irrigation can be considered in the rotation data block by defining application date, application rate, and irrigation sources such as stream, reservoir, and groundwater for each rotation type. Automatic approach can be considered for each grid by starting and stopping the application of water when soil moisture reaches user-defined minimum and maximum levels, respectively.

**Tile drainage**: Horizontal movement of water in the soil profile is considered by interflow components of DANSAT based on saturated hydraulic conductivity and surface slope. To simulate tile drainage in DANSAT, two separate routines should be considered in the model: 1) cell drainage component and 2) routing component. At first, the cell drainage component needs to predict the drainage time required to remove excessive water from the soil layer to tile drains based on tile drains’ characteristics such as depth from the surface, density of drains within a cell, hydraulic conductivity of drains, etc. One more data field may be necessary in the Cell Data Block of the main input to define spatial distribution of the tile drainage network in the watershed scale. The routing component needs to calculate the water and chemical movement through tile drains to streams. A similar approach with the interflow component can be used.

Several components, which are already considered in DANSAT, are necessary to be modified in order to improve the accuracy of model simulation and enlarge the model applicability. The following are recommended components that should be modified in the future.

**Channel component**: The current version of DANSAT does not consider channel evolution according to the bank erosion. In the case that bank erosion is a major source of sediment load compared to the sediment detachment from the stream bed, bank erosion subroutine should be incorporated into DANSAT. Detailed in-stream processes for nutrients and bacteria should be included in the model. Even though DANSAT is able to consider two different channel shapes such as rectangle and triangle shapes, the model needs to consider other shapes of channels and complex floodplains.

**Overland flow routing component**: Overland flow routing in the model is based on storage based equations, which consist of the spatially uniform and temporarily variable continuity
equation and a stage-discharge equation. To satisfy the assumption of the routing approach, a small time-step is necessary for the stable stream flow output during storm events. Solving other equations such as diffusive wave equations and kinematic wave equations using numerical methods may increase the minimum time-step for storm event simulations.

**Multi-layer based interflow component:** Soil water, which exceeds field capacity in each soil layer within the user-defined interflow depth, is lumped into the interflow pool, which is defined in each cell. Interflow routing is calculated based on the lumped interflow pool. Lumped water should be redistributed into soil layers in order to be considered in the evapotranspiration (ET) calculation. Simulating interflow using multi-soil layers without lumping process will be more realistic and improve the model accuracy.

**PET Methods:** Four different approaches are available for potential evapotranspiration (PET) prediction depending on the available weather data. However, only the Priestly-Taylor method was validated and other methods need to be validated. In the future, Penman method (Penman, 1948) is recommended to be added into DANSAT as an original combination based model.

**Partial leakage through impermeable layer:** No percolation is considered through the impermeable soil layer such as bed lock in the current version of DANSAT. When the user wants to consider partial leakage through the impermeable soil layer, one more parameter, which defines a fraction of total available soil water, should be included in the model.

Variable Manning’s Roughness Coefficient: Manning’s roughness coefficient is an important parameter used to predict travel time from one cell to an adjacent cell during the overland flow routing process. Conceptually, roughness coefficient in a cell is expected to temporally change depending on percent of impermeable area, soil disturbing operations such as tillage, crop type, and percent of residue cover. DANSAT, however, simulates overland flow using the constant Manning’s roughness coefficient throughout the simulation period without considering the relationship between daily changing surface conditions and Manning’s roughness coefficient. An array for the roughness coefficient value of crop was assigned in General Crop Data Block, but it is not used in the current version. An equation for predicting roughness coefficient of bare soil based on soil characteristics and residue cover is needed. Roughness coefficient for impermeable area can be treated as a constant value. Finally, daily average may be calculated based on three different roughness coefficients.
Variable Rill Space: Rill and interrill detachment is calculated based on total overland flow rate. If rill space increases with the same flow rate, flow rate per rill contributing area increases and flow depth also increases in spite of a slight increase of rill width. Rill detachment capacity by flow can increase due to the increased flow depth. Even though the rill space is a very sensitive parameter for sediment simulation, DANSAT uses a constant value as a calibration parameter. Like other parameters, rill space may be predicted based on soil characteristics, percent residue cover, and total flow rate etc.

Infiltration Representative Depth: To calculate infiltration rate using the Green-Ampt equation in DANSAT, effective matrix potential based on volumetric soil water content of representative soil layer should be calculated. DANSAT is a multi-soil layer model and soil water content should be averaged within the user-defined soil layer depth, infiltration representative depth (IRD). IRD was revealed as one of the sensitive parameters for hydrology simulation. As a result, a reasonable way to decide the IRD is necessary for users to use DANSAT with minimum calibration in the ungaged watershed.

Hydraulic Conductivity: In the dynamic approach for the hydraulic conductivity based on WEPP model, DANSAT calculates the conductivity value using daily rainfall amount as one of the input parameters. The simulated storm peak based on temporally changing hydraulic conductivity could not mimic the observed flow when daily rainfall amount was used without adjustment. In the current version of DANSAT, a rainfall adjustment factor was included to increase or decrease the impact of rainfall amount on hydraulic conductivity values. Considering hydraulic conductivity is a very sensitive parameter in hydrology; more reasonable approaches are recommended.

In addition to the development of new components and modification of existing components, adding more intensive error checking routines into DANSAT and providing a detailed user’s manual in depth are necessary for DANSAT to be more user-friendly.

Supporting Models
In addition to the improvement in water quality, BMPs should be economically feasible and well suited to a particular site. Several factors should be considered, such as crop yields, implementation and administrative cost, flexibility related to the cost of reversibility, and additional effects. Appropriate collaboration with economists, ecologists, and social scientists is
necessary for the development of a comprehensive DSS. DANSAT can be linked with other supporting models with additional interface components. The current version of DANSAT considers dynamic surface-groundwater interaction by linkage with existing groundwater models such as MODFLOW and MT3DMS. For the application of DANSAT to basin scale watersheds, linkage with an existing river model such as WASP and QUAL2E is recommended. For example, several DANSAT applications for every subwatershed simulate flow rate and pollutant loads at the subwatershed outlet, and WASP or QUAL2E simulate changes of water quality through the main river to the basin outlet. Linkage between existing ecological models is also possible.
Appendix D: Input Files
Plot-Scale Validation
QNB - Conventional Tillage

*** Directory and Input File Name Block
InputDir  D:\DANSAT\Validation\QNB-CT\Input
OutputDir D:\DANSAT\Validation\QNB-CT\Output
ExeDir    D:\DANSAT\EXE
Weather   Weather.inp
BrkPoint  Break_Point.Inp
Initial   Initial.Inp
End Directory and Input File Name Block ****

*** Flag and General Input Parameter Block
### Component flags (1: On, 0: Off)
# Unit: Flag for unit (not used)
# Sur: Flag for different surface components (not used)
# Usat: Flag for different unsaturated components (not used)
# Sat: Flag for saturate component (0: Integrated, 1: Linked approach)
# Sed: Flag for sediment component
# N: Flag for nitrogen component (not used)
# P: Flag for phosphorus component (not used)
# Pest: Flag for pesticide component (1: On, 0: Off)
# Irr: Flag for irrigation component (not used)
# Till: Flag for tillage component (1: On, 0: Off)
# BMP: Flag BMP component (not used)
# Urb: Flag for urban component (not used)
# Unit Sur  Usat Sat  Sed  N    P    Pest Irr  Till BMP  Urb
0     1     1     0     1     0     1     0     1     0     0  ### Output flags (1: On, 0: Off)
# FlgSOE: Storm event output at specific outlets
# FlgSOD: Daily output at specific outlets
# FlgFSR: Flux from Surface to Root zone
# FlgFRI: Flux from Root zone to Intermediate zone
# FlgFIG: Flux from Intermediate zone to Groundwater zone
# FlgUGC: Vertical distribution and Time series at a give cell
# FlgGAP: Ground water table and concentration
# FlgSGI: Interaction between Stream and Groundwater
# FlgMsg: Message output
# FlgChk: Check files(Infiltration, Soil, Daily changing variables)
# SOE  SOD  FSR  FRI  FIG  UGC  GAP  SGI  Msg  Chk
#     0     1     1     1     0     1     0     0     1     1

### Method flags
# FlgPET: Potential ET
#    1: Pan ET value
#    2: Prestly-Taylor
#    3: Jensen and Haise
#    4: Hamon
# FlgEHC: Effective Hydraulic Conductivity
#    1: Model calculation(Variable Ke value during simulation)
#    2: Constant Ke value during simulation
#    3: Combination of 1 and 2
# FlgLAI: Leaf Area Index
#    1: Model calculation(WEPP approach)
#    2: Pre-defined value(LAI table)
# FlgKIB: Baseline Interrill Erodibility (KiBase)
#    1: Model calculation
#    2: Default base value (5300000 kg-s/m4)
# FlgKRB: Baseline Rill Erodibility and Critical Shear Stress
#    1: Model calculation
#    2: Default base value (0.0115 s/m), (3.1 pascals)
# PET  EHC  LAI  KIB  KRB
#    2     1     1     1     1

# General Parameters follows  | Start from 52th column
Beginning day of simulation (mm dd yyyy)--------- 01 01 1990
End day of simulation (mm dd yyyy)-------------- 12 31 1990
Latitude of watershed (Decimal Degree)--------- 38.5
Number of Rows ----------------------------- 1
Cell width of x-direction (meters) ----------- 18
Number of Columns ---------------------------- 1
Cell width of y-direction (meters) ----------- 27
Number of Cells ----------------------------- 1
Number of Maximum Soil Layers ----------------- 7
Number of soil types -------------------------- 1
Number of particle size classes --------------  5
Number of land use types --------------- 1
Number of Rotations ---------------------- 1
Max. Number of Application Dates in each Rotn --- 8
Number of Rain Gages ------------------------ 2
Number of Channel Types ---------------------- 1
  
  # Parameters for Root Zone
  Time step during Rainfall Event (min) -------- 1
  Number of Root Zone Layers ------------------ 12
  
  # Parameters for Unsaturated Zone Simulation
  Number of Unsaturated Zone Layers ---------  4
  
  # Parameters for Linked Groundwater Approach
  Time step of saturated zone component (Day) -- 0
  Number of saturated zone layers -------------  0
  File name of MODFLOW/MT3D simulation --------- Non
  
  # Tillage information
  Number of tillage Type ----------------------- 2
  
  # Parameters for Fertilizer Application
  Number of Fertilizer Application Methods ---- 0
  
  # Parameters for Pesticide Application
  Number of applied pesticide type -------------- 2
  Number of Pesticide Application Methods ------- 2
  
  # Parameters for Depth Distribution
  Number of Depth Distribution Type ------------ 2
  
  # Automatic and Manual Irrigation
  # Automatic Irrigation
  Fraction of the Maximum Available Water ------- 0
  Flag for interception by canopy --------------- 0
  Amount of water to leach salts out of root zone - 0
# Manual Irrigation

Number of Irrigation type ---------------  0
#

# BMP information

Number of Structural BMP Type ---------------  0
#

# General Calibration Parameters

Convergence condition for the end of storm ------  0.007
Effective soil depth for infiltration (meters)---  0.3
Rainfall adjustment factor for Keff --------------  0.01
Rill space (Rills/meter)-------------------------  0.06
Manning's n in the rill ------------------------  0.015

Fraction of dissolved chemical avail for runoff -  1.0
Considering depth for interflow calculation (m) -  0
Anisotropic factor for interflow (K_hor/K_ver) --  0
Length for rill detachment calculation (m)------  10.0
Length for channel detachment calculation(m)-----  10.0

End Flag and General Input Parameter Block ***

*** Output Parameter Data Block

# Maximum outlet cell is 10

Number of Outlets -----------------------------  1

Cycles of Storm Event Outlet files (min) --------  15
# First line: cell number, Second Line: Area(ha)
# CN_01

  1

  0.049

# Maximum given cell number is 10

Number of given cell ---------------------------  1
# CN_01

  1

# Cycles of periodic output files

# FSR, FRI, FIG ==> -3:Simulation period, -2:Yearly, -1:Monthly, 0:Not consider, 5:Every 5 days
# GAP, SGI ==> Repeated every # of Saturated zone time step

# FSR   FRI   FIG   GAP   SGI


### Groundwater Data Block

- **GwCoeff**: Specific yields
- **GwKsat**: Saturated hydraulic conductivity (m/h)
- **K_Base**: Baseflow coefficient

<table>
<thead>
<tr>
<th>GW</th>
<th>GwKsat</th>
<th>GwCoeff</th>
<th>GwPower</th>
<th>GwSlope</th>
<th>GwInterg</th>
<th>GwThresh</th>
<th>GwBD</th>
<th>GwTPor</th>
<th>GwEffDep</th>
<th>Dispersivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.000000</td>
<td>0.7</td>
<td>0.24</td>
<td>0.32</td>
<td>0.7</td>
<td>1800.0</td>
<td>0.3</td>
<td>5</td>
<td>0.1</td>
<td>1</td>
</tr>
</tbody>
</table>

### Cell Data Block

- **Row**: Row Number
- **Col**: Column Number
- **CellN**: Cell Number (minus indicates outlet)
- **RgN**: Raingage Number
- **SoN**: Channel Soil number + Overland Soil Number (3 digit)
- **RtN**: Channel type + Rotation Number (minus indicates channel)
- **Cslp**: Slope of channel (%)
- **Sslp**: Slope of surface (%)
- **Asp**: Aspect from north on clockwise (Degree)
- **ManN**: Manning’s roughness coefficient for overland flow calculation
- **Elev**: Surface Elevation from the sea level (m)
- **DX.EDI**: Channel segment length (m). Effective Depth of Interaction (m)
- **D2GW**: Depth to the ground water table from surface (m)

<table>
<thead>
<tr>
<th># Cmmt</th>
<th>Row</th>
<th>Col</th>
<th>CellN</th>
<th>RgN</th>
<th>SoN</th>
<th>RtN Cslp</th>
<th>SSlp</th>
<th>Asp</th>
<th>ManN</th>
<th>Elev</th>
<th>DX.EDI</th>
<th>D2GW</th>
<th>SubWS</th>
<th>FDir</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>2.0</td>
<td>180.0</td>
<td>0.08</td>
<td>34.3</td>
<td>0.01</td>
<td>9.0</td>
<td>1</td>
</tr>
</tbody>
</table>

### Channel Data Block

- **CName**: Channel Name
- ** CType**: Channel type (1: Rectangle, 2: Triangle)
# Width: Width of channel (m: only for rectangle channel)
# BSlope: Bank slope of channel (only for triangle channel)
# ManN: Manning's roughness coefficient
# FUES: Fraction of Unerodible channel Soil, or erosion resistant
# Cndt: Streambed hydraulic conductance (not used)

<table>
<thead>
<tr>
<th>CName</th>
<th>CType</th>
<th>Width</th>
<th>BSlope</th>
<th>ManN</th>
<th>FUES</th>
<th>HyCndt</th>
</tr>
</thead>
<tbody>
<tr>
<td>QNB-Str</td>
<td>1</td>
<td>2.0</td>
<td>0.0</td>
<td>0.03</td>
<td>0.0</td>
<td>0.0006</td>
</tr>
</tbody>
</table>

End Channel Data Block *****

*** Soil Data Block

# Particle Class Information
# PSize: Particle diameter (mm)
# SGrav: Specific gravity
# FVel: Fall velocity (m/sec)
# SSurf: Specific surface area for each particle (m²/g)
# WFlag: Washload flag (0: no washload, 1: Washload, 2: Automatic)

<table>
<thead>
<tr>
<th>Part_1</th>
<th>PSize</th>
<th>SGrav</th>
<th>FVel</th>
<th>SSurf</th>
<th>WFlag</th>
</tr>
</thead>
<tbody>
<tr>
<td>Part_2</td>
<td>0.02</td>
<td>2.75</td>
<td>0.0</td>
<td>800.0</td>
<td>1</td>
</tr>
<tr>
<td>Part_3</td>
<td>0.05</td>
<td>2.65</td>
<td>0.0</td>
<td>1.0</td>
<td>0</td>
</tr>
<tr>
<td>Part_4</td>
<td>0.1</td>
<td>2.65</td>
<td>0.0</td>
<td>0.5</td>
<td>0</td>
</tr>
<tr>
<td>Part_5</td>
<td>0.5</td>
<td>2.65</td>
<td>0.0</td>
<td>0.16</td>
<td>0</td>
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<tr>
<td>Part_6</td>
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<td>2.65</td>
<td>0.0</td>
<td>0.1</td>
<td>0</td>
</tr>
</tbody>
</table>

# General Information for Each Soil Type
# Ptcl_X: Particle_X content of the top soil (%)
# TSSurf: Total Specific Surface Area (m²/g)
# Ke: Effective Hydraulic Conductivity (m/h)

<table>
<thead>
<tr>
<th>SName</th>
<th>Ptcl_1</th>
<th>Ptcl_2</th>
<th>Ptcl_3</th>
<th>Ptcl_4</th>
<th>Ptcl_5</th>
<th>TSSurf</th>
<th>Ke</th>
<th>Albedo</th>
<th>Kirill</th>
<th>Krill</th>
</tr>
</thead>
<tbody>
<tr>
<td>QNB</td>
<td>11.7</td>
<td>26.4</td>
<td>10.3</td>
<td>20.5</td>
<td>30.7</td>
<td>0.0</td>
<td>0.00613</td>
<td>0.1</td>
<td>300000</td>
<td>0.03</td>
</tr>
</tbody>
</table>

# Layer Information for Each Soil Type
# Depth: Bottom depth of each layer from ground surface(m)
# TPor: Total porosity
# FCap: Field capacity
# WPnt: Wilting point
# RsWC: Residual water content
# BDens: Bulk density (mg/cm³)
# Clay: Soil clay content(%)  
# Sand: Soil sand content(%)  
# Silt: Soil silt content(%)  
# OM: Soil organic matter content(%)  
# VFSand: Very fine sand content(%)  
# CFrag: Coarse fragment content(%)  
# Ks: Saturated hydraulic conductivity (m/h)  
# CEC: Cation exchange capacity (meq/100g)

<table>
<thead>
<tr>
<th>LName</th>
<th>Depth</th>
<th>TPor</th>
<th>FCap</th>
<th>WPnt</th>
<th>RsWC</th>
<th>BDens</th>
<th>Clay</th>
<th>Sand</th>
<th>Silt</th>
<th>OM</th>
<th>VFSand</th>
<th>CFrag</th>
<th>Ke</th>
<th>CEC</th>
</tr>
</thead>
<tbody>
<tr>
<td>QNB-1</td>
<td>0.15</td>
<td>0.387</td>
<td>0.192</td>
<td>0.056</td>
<td>0.0</td>
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<td>11.7</td>
<td>61.5</td>
<td>26.4</td>
<td>0.94</td>
<td>0.0</td>
<td>11.7</td>
<td>5.8</td>
<td>6.8</td>
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<tr>
<td>QNB-2</td>
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<td>0.37</td>
<td>0.224</td>
<td>0.070</td>
<td>0.0</td>
<td>1.64</td>
<td>14.8</td>
<td>60.4</td>
<td>24.8</td>
<td>0.55</td>
<td>11.5</td>
<td>0.0</td>
<td>0.00369</td>
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</tr>
<tr>
<td>QNB-3</td>
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<td>0.369</td>
<td>0.241</td>
<td>0.080</td>
<td>0.0</td>
<td>1.64</td>
<td>16.7</td>
<td>63.9</td>
<td>19.5</td>
<td>0.42</td>
<td>11.5</td>
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<td>0.00359</td>
<td>6.8</td>
</tr>
<tr>
<td>QNB-4</td>
<td>0.6</td>
<td>0.402</td>
<td>0.197</td>
<td>0.073</td>
<td>0.0</td>
<td>1.67</td>
<td>12.6</td>
<td>76.1</td>
<td>11.4</td>
<td>0.32</td>
<td>15.2</td>
<td>0.0</td>
<td>0.00356</td>
<td>1.8</td>
</tr>
<tr>
<td>QNB-5</td>
<td>0.75</td>
<td>0.41</td>
<td>0.127</td>
<td>0.059</td>
<td>0.0</td>
<td>1.67</td>
<td>6.8</td>
<td>86.2</td>
<td>7.1</td>
<td>0.23</td>
<td>15.2</td>
<td>0.0</td>
<td>0.00613</td>
<td>1.8</td>
</tr>
<tr>
<td>QNB-6</td>
<td>0.9</td>
<td>0.41</td>
<td>0.127</td>
<td>0.059</td>
<td>0.0</td>
<td>1.67</td>
<td>5.5</td>
<td>90.8</td>
<td>3.8</td>
<td>0.23</td>
<td>15.2</td>
<td>0.0</td>
<td>0.00613</td>
<td>1.8</td>
</tr>
<tr>
<td>QNB-7</td>
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<td>0.127</td>
<td>0.059</td>
<td>0.0</td>
<td>1.67</td>
<td>5.5</td>
<td>90.8</td>
<td>3.8</td>
<td>0.23</td>
<td>15.2</td>
<td>0.0</td>
<td>0.00613</td>
<td>1.8</td>
</tr>
</tbody>
</table>

End Soil Data Block

*** Land Use Data Block

# General Information for each Crop Type
# ImpA: Percent of Impervious Area (%)  
# ManN: Maning's N for the surface (not used)  
# E2Bm: Crop parameter for converting energy to biomass (kg/MJ)  
# CrWC: Critical soil water content below which plant growth is subjected to water stress(m3/m3)  
# Tbase: Base temperature (no growth occurs at or below Tbase) (C)  
# Topt: Optimum temperature (C)  
# PMat: The amount of the crop's growth period required for the crop to reach full size(NOD: 0-1)  
# MRtD: Maximum Rooting Depth (m)  
# MHt: Maximum plant canopy height (m)  
# MLAI: Maximum Leaf Area Index  
# RPR: Root to shoot ratio (0-1)  
# CoefCC: Parameter for canopy cover equation  
# CoefCH: Parameter for canopy height equation  
# Fbs: Fraction of above-ground biomass remaining after senescence (0-1)  
# Fcs: Fraction of canopy cover remaining after senescence (NOD:0-1)  
# SPrio: Number of days between the beginning and end of leaf drop
# PHUnit: Potential Heat Units to crop maturity (C)
# DLAI: Fraction of groq
# CF: parameter for flat residue cover equation (m2/kg)

<table>
<thead>
<tr>
<th>Line-1</th>
<th>ImpA</th>
<th>ManN</th>
<th>E2Bm</th>
<th>CrWC</th>
<th>Tbase</th>
<th>Topt</th>
<th>PMat</th>
<th>MRtD</th>
<th>MHt</th>
<th>MLAI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Line-2</td>
<td>RPR</td>
<td>CoefCC</td>
<td>CoefCH</td>
<td>Fbs</td>
<td>Fcs</td>
<td>SPrio</td>
<td>PHUnit</td>
<td>DLAI</td>
<td>CF</td>
<td></td>
</tr>
<tr>
<td>Corn</td>
<td>0.0</td>
<td>1</td>
<td>35.0</td>
<td>0.25</td>
<td>10.0</td>
<td>25.0</td>
<td>1.0</td>
<td>1.52</td>
<td>2.6</td>
<td>3.5</td>
</tr>
<tr>
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<td>0.25</td>
<td>3.6</td>
<td>3.0</td>
<td>0.98</td>
<td>0.65</td>
<td>30.0</td>
<td>1700</td>
<td>0.82</td>
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</tr>
</tbody>
</table>

# Leaf Area Index
# MLAI: Maximum Leaf Area Index (m2/m2)
# CName | MLAI | Fraction of growing season (0.0-1.0)
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Corn</td>
<td>3.50</td>
<td>0.0</td>
<td>0.105</td>
<td>0.21</td>
<td>0.28</td>
<td>0.56</td>
<td>1.365</td>
<td>3.465</td>
<td>3.5</td>
</tr>
</tbody>
</table>

End Land Use Block *****

*** Tillage Data Block
# RR0: Random roughness immediately after tillage (m)
# Tds: Fraction of soil surface disturbed by the tillage implement (0-1)
# RH0: Ridge height immediately after tillage (m)
# RInt: Ridge interval (m)
# TDep: Mean tillage depth associated with each implement (m)
# TName | RR0 | Tds | RH0 | RInt | TDep |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Ch-Plow</td>
<td>0.02</td>
<td>1.0</td>
<td>0.05</td>
<td>0.36</td>
<td>0.15</td>
</tr>
<tr>
<td>Disk</td>
<td>0.03</td>
<td>1.0</td>
<td>0.05</td>
<td>0.3</td>
<td>0.08</td>
</tr>
</tbody>
</table>

End Tillage Data Block *****

*** Pesticide Data Block
### General Pesticide Information
# WFrac: Washoff fraction (0-1)
# H-foli: Foliar residue half-life (days)
# H-soil: Soil half-life (days)
# Koc: Partitioning coefficient (ml/g)
# Sol: Water solubility (mg/l)
# Dst: Distribution number for Half-Life on Soil
# Dst: Distribution number for Koc
# Dst: Distribution number for Solubility (not used)
# PName | WFrac | H-Foli | H-Soil | Koc | Sol | Dst | Dst | Dst | Dst |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Atrazine</td>
<td>0.5</td>
<td>5.0</td>
<td>90.0</td>
<td>140.0</td>
<td>33.0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.0</td>
</tr>
<tr>
<td>Dual</td>
<td>0.6</td>
<td>5.0</td>
<td>50.0</td>
<td>110.0</td>
<td>530.0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.0</td>
</tr>
</tbody>
</table>
### Pesticide Application Information

- **Pest:** Pesticide Number
- **Mthd:** Application Method (1:Foliage, 2:Soil, 3:Incorporated, 4:Injection)
- **ADepth:** Application Dept (m)
- **AEff:** Application efficiency (0-1)
- **PFoli:** Partitioning coefficient to foliage (0-1)

<table>
<thead>
<tr>
<th>Name</th>
<th>Pest</th>
<th>Mthd</th>
<th>ADepth</th>
<th>AEff</th>
<th>PFoli</th>
</tr>
</thead>
<tbody>
<tr>
<td>S-Atra</td>
<td>1</td>
<td>2</td>
<td>0.01</td>
<td>0.548</td>
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<td>S-Dual</td>
<td>2</td>
<td>2</td>
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<td>0.403</td>
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End Pesticide Data Block *****

### Distribution Data Block

- **Line-1:** Depth
- **Line-2:** Multipling Factor

<table>
<thead>
<tr>
<th>DName</th>
<th>Dep_1</th>
<th>Dep_2</th>
<th>Dep_3</th>
<th>Dep_4</th>
<th>Dep_5</th>
<th>Dep_6</th>
<th>Dep_7</th>
<th>Dep_8</th>
<th>Dep_9</th>
<th>Dep_10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atra_02</td>
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<td>0.3</td>
<td>0.45</td>
<td>0.6</td>
<td>0.75</td>
<td>0.9</td>
<td>1.5</td>
<td>5.0</td>
<td>10.0</td>
<td>15.0</td>
</tr>
<tr>
<td></td>
<td>1.1</td>
<td>1.0</td>
<td>0.9</td>
<td>0.8</td>
<td>0.7</td>
<td>0.6</td>
<td>0.5</td>
<td>0.4</td>
<td>0.3</td>
<td>0.1</td>
</tr>
<tr>
<td>Sim_01</td>
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<td>0.3</td>
<td>0.45</td>
<td>0.6</td>
<td>0.75</td>
<td>0.9</td>
<td>1.5</td>
<td>5.0</td>
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<td>15.0</td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>0.9</td>
<td>0.8</td>
<td>0.7</td>
<td>0.6</td>
<td>0.5</td>
<td>0.4</td>
<td>0.3</td>
<td>0.2</td>
<td>0.1</td>
</tr>
</tbody>
</table>

End Distribution Data Block *****

### Initial Data Block

- **Root:** Initial soil water content (0-1) for root zone layers
- **USat:** Initial soil water content (0-1) for unsaturated zone layers
- **GWStr:** Initial groundwater storage depth (mm)
- **Hydro Flag Root USat GWStr**

<table>
<thead>
<tr>
<th>Wcontent</th>
<th>Dep_1</th>
<th>Dep_2</th>
<th>Dep_3</th>
<th>Dep_4</th>
<th>Dep_5</th>
<th>Dep_6</th>
<th>Dep_7</th>
<th>Dep_8</th>
<th>Dep_9</th>
<th>Dep_10</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.30</td>
<td>0.30</td>
<td>4.00</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **Nitro Flag Root USat Sat**

| LOrgN    | 0    | 0.34  | 0.23  | 0.14  |
| SOrgN    | 0    | 0.35  | 0.24  | 0.15  |
| DNH4      | 0    | 0.36  | 0.25  | 0.16  |
| SNH4      | 0    | 0.37  | 0.26  | 0.17  |
| DNO3      | 0    | 0.38  | 0.27  | 0.19  |

- **Phos Flag Root USat Sat**

| LOrgP    | 0    | 0.31  | 0.20  | 0.10  |
| SOrgP    | 0    | 0.32  | 0.21  | 0.11  |
| LSPO4    | 0    | 0.33  | 0.22  | 0.12  |
SSPO4  0  0.34  0.23  0.13
DPO4   0  0.35  0.24  0.15
# DPest: Desolved Pesticide (ug/l)
# SPest: Sediment bound pesticide (ug/kg)
# Pest01 Flag  Root  USat  Sat
DPest01 0  0.00  0.00  0.00
SPest01 0  0.00  0.00  0.00
# Pest02 Flag  Root  USat  Sat
DPest02 0  0.00  0.00  0.00
SPest02 0  0.00  0.00  0.00
End Initial Data Block ****

*** Daily Changing Variable Block

##### Variables for residue decomposition (crop specific value but use avg value)
# CF: Parameter for flat residue cover equation (m2/kg)
# ARate: Optimum decomposition rate for the above ground part of a residue type
# RRate: Optimum decomposition rate for the dead roots of a residue type
# CF  ARate  RRate
4.0  0.009  0.009

##### Initial values
# RotN: Rotation number
# BmTot: Cumulative total biomass (kg/m2)
# ResSt: Cumulative standing biomass (kg/m2), actually not used
# ResFl: Cumulative flat biomass (kg/m2)
# ResBu: Cumulative buried biomass (kg/m2)
# ResDR: Cumulative dead root biomass in the 0-0.15m depth(g/cm2)
# RRou: Random roughness immediately after tillage (m)
# RHei: Ridge height immediately after tillage (m)
# BDen: Bulk density immediately after tillage (m)
# CuRf: Cumulative rainfall since last tillage (m)
# CuKE: Cumulative kinetic energy since last tillage (J/m2)
# CuDay: Cumulative number of days since last tillage
# RotName  BmTot  ResSt  ResFl  ResBu  ResDR  RRou  RHei  BDen  CuRf  CuKE  CuDay
QNB  1.851  0.0   1.096  0.329  0.425  0.012  0.025  1510.0  0.614  30.34  267
End Daily Changing Variable Block ****

*** Rotation Data Block
<table>
<thead>
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<th>MM</th>
<th>DD</th>
<th>YY</th>
<th>Type</th>
<th>AppN</th>
<th>Var</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Disk</td>
<td>03</td>
<td>25</td>
<td>01</td>
<td>0</td>
<td>02</td>
<td>0.00</td>
</tr>
<tr>
<td>2</td>
<td>Ch-Plow</td>
<td>03</td>
<td>25</td>
<td>01</td>
<td>0</td>
<td>01</td>
<td>0.00</td>
</tr>
<tr>
<td>3</td>
<td>Corn</td>
<td>04</td>
<td>23</td>
<td>01</td>
<td>1</td>
<td>01</td>
<td>0.00</td>
</tr>
<tr>
<td>4</td>
<td>S-Dual</td>
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<td>25</td>
<td>01</td>
<td>4</td>
<td>02</td>
<td>2.24</td>
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<tr>
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<td>25</td>
<td>01</td>
<td>4</td>
<td>01</td>
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<tr>
<td>6</td>
<td>Corn</td>
<td>10</td>
<td>09</td>
<td>01</td>
<td>8</td>
<td>01</td>
<td>30.0</td>
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</tbody>
</table>

End Rotation Data Block *****
Appendix F: Source Codes
Source codes are included in the compressed file (Appendix_F.zip) as a digital format. The file contains four folders including DANSAT, Interface, FluxOut2AView, and QualLoad. Brief descriptions for the source codes in each folder are described in Figure A.21.

**Table A.4. Descriptions for the source codes included in the compressed file.**

<table>
<thead>
<tr>
<th>Folder Name</th>
<th>Descriptions</th>
</tr>
</thead>
<tbody>
<tr>
<td>DANSAT</td>
<td>This folder contains the source codes for DANSAT. The code was developed using Digital Fortran based on fortran 90. Global variables are defined in “ModVariables.f90” and the descriptions for each subroutine can be searched using “* SUBROUTINE”.</td>
</tr>
<tr>
<td>Interface</td>
<td>This folder contains the source codes of the interface for DANSAT. The codes were developed using Visual Basic 6.0.</td>
</tr>
<tr>
<td>FluxOut2AView</td>
<td>This folder contains a utility program that converts the flux output files to the Arc/View ascii files. The code requires two files including flux output file and sample Arc/View ascii file as input files. Sample input files and output file are included in the folder</td>
</tr>
<tr>
<td>QualLoad</td>
<td>This folder contains a utility program, which calculates the flow-weighted daily sediment loads based on the HAS format of measured flow rates and sediment concentrations. The code requires three input files such as flow input, water quality concentration input, and storm input files. Storm input, which defines the starting and ending time of each significant storm event, is created based on hydrograph manually. Sample input files and output files are included in the folder.</td>
</tr>
</tbody>
</table>
Vita

Jaepil Cho was born on March 14, 1971, in Puyo, South Korea. In 1995, he graduated with his B.S. degree in Agricultural Engineering from Seoul National University in South Korea. He earned his M.S. degree in Agricultural Engineering in 1998 from the same school. Before he started his Ph.D. in the U.S., he worked at Auburn University as a visiting scholar from May to December 1999. He began his Ph.D. at Virginia Tech in the Department of Biological Systems Engineering in February 2000. After earning his Ph.D. degree in April 2007, he will begin work at the University of Georgia as a post-doctoral fellow.