Chapter 3. Modeling the Heat and Mass Transfer Phenomena during the Hot-Compression of Wood-Based Composites

Summary

This chapter discusses the development of a two-dimensional mathematical model to describe the heat and mass transfer during the hot-compression of wood-based composite panels. Five primary variables were considered during the model development: air content, vapor content, bound water content, and temperature within the mat, and the extent of the cure of the adhesive system characterized by the cure index. Different heat and mass transfer processes were identified for the transport of the heat and of the moisture phases. The heat was transported by conduction and convection due to a temperature gradient, while the water phases were transported by bulk flow and diffusion due to total pressure and concentration gradients. The resulting differential-algebraic equation system was solved by the finite difference method. The spatial derivatives of the conduction terms were discretized according to a central-difference scheme, while the spatial derivatives of the convection terms were discretized according to the upwind scheme. The resulting ordinary differential equations (ODEs) in the time variable were solved by DDASSL, a freely available differential-algebraic system solver.

The mathematical model predicted temperature, moisture content, partial air and vapor pressures, total pressure, relative humidity, and extent of adhesive cure within the mat structure under a typical hot-compression process. A set of three-dimensional profiles describes the evolution of these variables with time, in the thickness and width dimensions of the mat. The model results allow a better understanding of the interacting mechanisms involved in a complex production process. The model can also assist to optimize the hot-pressing parameters for improved quality of wood-based panel products, while reducing pressing time.
3.1 Introduction

The hot-compression is one of the most important stages of wood-based composite production. The composite panel attains its final characteristics during compression, as the loosely formed flake mat is compressed to its final thickness under elevated temperature and pressure. During the hot-pressing cycle, the internal conditions of the mat change rapidly. Heat is transported by conduction from the hot platens to the mat surface. The abrupt increase of temperature vaporizes the moisture content of the flakes at the surface and increases the vapor pressure. The pressure differential drives the hot vapor to the cooler center of the mat, where it may condense. Therefore, a vertical water vapor flow from the surface of the board towards the center can be observed at the beginning of the press cycle. As the rate of moisture evaporation at the surface declines, the surface temperature quickly reaches the platen temperature. However, it takes a considerable time to increase the centerline temperature of the mat to the local boiling point of water at the given internal pressure. As the center reaches this temperature the water vaporization is accelerated, and the increased pressure in the center of the board will drive the vapor horizontally towards the exposed edges, where it leaves to the environment. The centerline temperature remains nearly constant until the moisture content drops considerably in the mat structure, due to the energy consumed by the vaporization process (latent heat). Consequently, the vertical flow accelerates the temperature rise in the center, while the horizontal flow retards it.

The rate of the vertical and horizontal mass transfer process is controlled by the flow of the water vapor through the porous structure of the mat. During the press closure, the voids between the flakes are eliminated, and the porous structure of the flakes is also compressed. The substantial change in mat structure will affect the rate of the mass transfer through the changing physical mat properties. Therefore, it is crucial to link the mat structural properties to the mat transport and physical properties in the model.

The moisture distribution develops as a response to the temperature gradient. Consequently, the movement of moisture in the form of steam influences the temperature gradient during the press cycle. Therefore, the heat and mass transfer are coupled. Evaporation and condensation of the moisture in the mat will consume or release latent energy, respectively, which contributes to temperature and gas pressure changes. The result of these interacting heat and mass transfer mechanisms is a three-dimensional variation in temperature, moisture content, and pressure within the mat structure. The viscoelastic properties of the flakes, such as the relaxation modulus or compressibility, depend on the moisture content and temperature variation. The rate and extent of the cure of the thermosetting resin is also a function of the mat internal conditions. The production parameters substantially affect the internal environment of the mat and the final characteristics of the manufactured board. The pressing parameters (press
temperature, total press time, press closing time, and ram pressure) and initial mat conditions (initial moisture content and temperature of the flakes) can be controlled during the production process. If the connection between production parameters and the final properties are established, the process operators have a great influence on the ultimate properties of the board. Therefore, it is critical to describe the changes of moisture content and temperature within the flake mat in space and time. The second phase of the research focused on the development of a model to describe the heat and mass transfer phenomena within the board structure during a conventional hot-compression operation.

3.2 Background

Two complementary approaches emerged to find relationships between production parameters and the properties of wood-based composite panels: testing and modeling. A number of investigators studied the hot-compression process based on empirical data collected on a small scale laboratory press (Kelley 1977, Stickler 1959, Maku et al. 1959, Kamke and Casey 1988a, b). Sophisticated experimental designs were constructed to statistically analyze the effect of platen temperature, initial moisture content, panel final density, and other variables on certain board properties. An inherent disadvantage of this approach is that, although general trends can be observed, the data is valid only for the range of testing conditions. In order to remedy the drawbacks of the experimental approach, several numerical models were developed in the last three decades to better understand the transient effects during the hot-compression process of wood-based composites.

One of the earliest attempts to model temperature and moisture distribution in particleboard in two dimensions was that of Bowen (1970). He used measured temperature data and a finite difference model to predict the contribution of conduction and latent (condensation / evaporation) effects on the heat transfer in the mat. He assumed that the latent portion can be calculated by deducting the calculated conduction part from the experimental heat transfer data. Having evaporation and condensation rates, moisture distributions within the mat structure could be effectively calculated at various stages of the press cycle. The energy balance of the hot-compression process was also investigated. Observing differences between calculated and measured energy levels, Bowen concluded that, in addition to the conduction component, the heat of resin polymerization plays an important role. Radiation effects and heat of compaction were also proposed to contribute to the heat transfer and generation. The model was based on a semi-empirical approach. Therefore, the temperature and moisture predictions were valid only for the particleboard under investigation.
An extensive review on the hot-compression of plywood and particleboard was published by Bolton and Humphrey (1988). The primary physical processes and their interactions were identified. A need for the development of a comprehensive hot-compression model was recognized. Several related papers (Humphrey 1989, Bolton et al. 1989a, b, c) described the derivation and validation of the most comprehensive simulation model to date for heat and moisture transfer during the hot-compression of particleboard. Conduction, convection, bulk flow, and water phase change were the heat and mass transfer mechanisms included in the model. The three-dimensional unsteady-state problem was solved by the finite difference method, assuming that steady-state theory adequately describes the behavior of the system during each time increment. Due to unacceptable run times, a cylindrical geometry was considered, essentially reducing the three-dimensional problem to a two-dimensional one. Temperature, steam pressure, and equilibrium moisture content were predicted in the radial and vertical directions. The internal environment at the corner of the board was calculated by interpolating results obtained from inscribed and circumscribed cylinders of the rectangular shape of the board. The model neglected the effect of press closing time and resin cure on the internal environment of the mat. Instead, instantaneous press closing was assumed, and variables were predicted only for the remaining part of the press schedule. The vertical density gradient formation during mat consolidation was not considered, but rather they assumed a stepwise change of the density profile at certain stages of the compression process. Therefore, the transfer properties changed also stepwise in the model, causing some numerical difficulties.

Harless et al. (1987) were among the first who recognized the relationship between the vertical density profile formation and the internal temperature and pressure distribution in the board. A model was developed to simulate the effect of heat and moisture on the density profile. The model, although comprehensive in this respect, had several limitations. To reduce the problem to a one-dimensional one, they assumed that the panel had infinite width and length, essentially disregarding the effects of the surroundings at the edges on the internal environment of the board. They considered only conduction heat transfer effects, neglecting the convection mechanism. Although the gas phase was divided into air and vapor, the only mass transfer mechanism was bulk flow. Diffusion was not included. Furthermore, the latent heat of vaporization was not incorporated in the energy equation, it was only enforced explicitly. The compressibility of the flakes was assumed to be a function of temperature and the plasticization effect of moisture was neglected in the model. The simulated pressing process was terminated as the final thickness of the mat was reached, not accounting for the effect of the differential relaxation of the mat during the remaining part of the press schedule. Additionally, several parts of the model were based on empirical data, therefore it had restricted applicability to predict properties of a wider range of wood products.
Kayihan and Johnson (1983) developed a one-dimensional model for the combined heat and mass transfer in particleboard. Conduction and convection heat transfer, and bulk flow mass transfer were considered together with water phase equilibrium equations in the model. The edge effect, losing moisture and heat at the edge of the board, was taken into consideration by a "leakage term" in the model. It was recognized that the artificial term should be replaced by the incorporation of the lateral heat and mass flow in future models.

Several drying models to describe the heat and mass transfer phenomena were published (Berger 1973, Luikov 1975, Thomas et al. 1980). The most comprehensive model by Stanish et al. (1986) described a detailed one-dimensional drying model for hygroscopic porous media, such as wood. The basis of the model was a set of fundamental one-dimensional transport equations, coupled with a thermodynamic equilibrium equation. The model included five variables: temperature, air content, vapor, bound, and free water content. Different transport mechanisms were established for the separate phases. The heat transfer occurred via conduction and convection. The mass transfer of the gaseous air and vapor was via combined diffusion and bulk (hydrodynamic) flow. The bound water was transported only by diffusion and the free water only by bulk flow. Drying rate experiments established the basic model parameters. Satisfactory agreement was found between model predictions and experimental drying results. A limitation of the model is that it is one-dimensional.

Carvalho and Costa (1998) developed a three-dimensional model for the hot-compression of medium density fiberboard (MDF). The equations were based on the Stanish (1986) drying model, but the physical properties were assessed for fiberboard instead of solid wood. Although the temperature and moisture effects on the physical properties were included, the effect of press closing on the structure, and consequently on the physical properties of the mat, was neglected in the model. The predicted results closely followed general temperature and moisture content trends during a typical hot-compression process, as was demonstrated by comparing the results to other model predictions.

It is clear from the literature review that previous models had inherent limitations; either they were one-dimensional, or gross simplifications were made about the transfer mechanisms. In this work, a general approach was followed during the model development, which allowed a comprehensive description of the heat and mass transfer phenomena during the hot-compression. All conceivable simultaneous heat and mass transfer mechanisms were considered, together with phase balancing sorption isotherms. By numerically solving the governing equations the prediction of the evolution of moisture and temperature profiles in the vertical midplane of the board became attainable. The changing internal environment of the mat allows the assessment of the viscoelastic (time, temperature, and moisture dependent) response of the flakes in the transverse compression part of the model, as is discussed in Chapter 5.
3.3 Model Development

The one-dimensional drying model published by Stanish et al. (1986) was adopted as the basis for further model development. The model was extended to two spatial dimensions, and the transport properties were adapted to incorporate the differences between solid wood and composite mat properties.

3.3.1 Assumptions

Several simplifying assumptions have to be adopted to solve the problem imposed by the coupled heat and moisture transfer mechanisms during hot-compression. These assumptions are:

- the model is two dimensional, with consideration of the thickness and width directions;
- solid and gaseous phases are considered, and these two phases are always in local thermodynamic equilibrium;
- heat and mass transfer between the two phases are instantaneous, therefore any resistance between the solid and gas phase is neglected;
- the gas phase located in the voids is composed of an air-water vapor mixture, and the components follow the Ideal Gas Law;
- air is treated as a single component gas;
- water can be present as bound water in the cell wall or water vapor in the voids, the free water component is ignored due to the low initial mat moisture content typical for wood composite manufacture; future extension of the model may include capillary condensation, and associated free water deposition;
- the bound water in the cell walls is always in local equilibrium with the water vapor in the voids, and the relationship is described by sorption isotherms at the local temperature;
- the heat supply of the process comes from the hot press platens and from the heat of reaction of the resin; the heat of compression of the mat is not considered;
- water produced during the condensation reaction of the resin is neglected;
- the physical and transport properties are functions of temperature, moisture content, density, porosity, and steam pressure, therefore they may vary with respect to space and time;
- the press schedule can include the press closing periods; the porosity and the density of the mat changes continuously during the press closing process, resulting in changes of the physical and transport properties of the mat;
- conditions at the four boundaries are independent of each other, and can vary with time;
- the mechanisms for heat and mass transfer are:

  a.) the heat is transported by conduction due to temperature differential and by convection due to the vapor flow; the conduction follows Fourier's Law;

  b.) the two gas phases (air and vapor) are transferred by bulk flow and diffusion, and follow Darcy's Law and Fick's Law, respectively; the driving force of the bulk flow process is the total pressure differential, while the driving force of diffusion is the partial pressure differential;

  c.) the migration of the bound water occurs by molecular diffusion due to a gradient in chemical potential of the bound water molecules;

  d.) phase change of water from the adsorbed to the vapor phase is implicitly included in the energy equation as latent heat of vaporization.

3.3.2 Governing Equations

Calculation of various transport phenomena in two-dimensional heat and mass flow involves the solution of mass and energy conservation equations. The governing equations describe the physical phenomena involved in a conventional hot-compression process. The model equations contain five dependent variables and five governing equations. The five dependent variables are the air density ($\rho_a$), water vapor density ($\rho_v$), bound water density ($\rho_b$), temperature ($T$), and the cure index of the adhesive ($F$). The mass density terms are based on the volume of the mat. The five variables are functions of three independent variables: thickness ($z$), width ($y$), and time ($t$). The five governing equations include two mass balance equations (one for air, and one for the moisture phase), one energy balance equation, one phase equilibrium equation, and one adhesive cure kinetics equation. (The description of variables, subscripts and superscripts in the equations is given in the nomenclature.)
The constitutive equations are the mass conservation equation for air

\[ \frac{\partial}{\partial t} (\rho_a) = -\nabla \cdot n_a , \]  

(3.1)

defined for the water phase

\[ \frac{\partial}{\partial t} (\rho_v + \rho_b) = -\nabla \cdot (n_v + n_b) , \]  

(3.2)

the energy balance equation

\[ \frac{\partial}{\partial t} (\rho_a \cdot h_a + \rho_v \cdot h_v + \rho_b \cdot h_b + C \cdot T) = -\nabla \cdot (n_a \cdot h_a + n_v \cdot h_v + n_b \cdot h_b + q) + G , \]  

(3.3)

the phase equilibrium relation, which is an inverted form of the Hailwood-Horrobin two-hydrate sorption model (Hailwood and Horrobin 1946, Simpson 1971, 1973, 1980),

\[ \rho_v = \rho_v^{\text{sat}} \left( Z_1 + \left( Z_2^2 + \frac{1}{K_1 K_2^2} \right)^2 \right) , \]  

(3.4)

where

\[ K_1 = -45.70 + 0.3216 T - 5.012 \cdot 10^{-4} T^2 , \]
\[ K_2 = -0.1722 + 4.732 \cdot 10^{-3} T - 5.553 \cdot 10^{-6} T^2 , \]
\[ W = 1, 417 \cdot 10^3 - 9.430 T + 1.853 \cdot 10^{-2} T^2 , \]
\[ Z_1 = \frac{1 - Z_2}{2 K_2} - \frac{1 + Z_2}{2 K_1 K_2} , \]
\[ Z_2 = \frac{18}{W \rho_b \rho_d} , \]

and the cure kinetics equation of the adhesive system (Scott 1989, Kiran and Iyer 1994)

\[ \frac{\partial F}{\partial t} = A e^{-\left( \frac{E}{RT} \right)} (1 - F)^n . \]  

(3.5)

This set of coupled differential-algebraic equations form the basis of the hot-compression model. The numerical solution of the system provides the air content, vapor content, bound water content, temperature, and cure index as a function of time and space in two dimensions.
3.3.3 Transport Mechanisms

3.3.3.1 Heat Transfer

The main source of heat is the two hot platens, but the polymerization of the resin and the compaction of the mat also generate heat internally. The generated heat is transported by the combination of three basic mechanisms: conduction, convection, and radiation. Conduction involves energy transfer through the contact of materials of different temperature, convection involves the heat transfer between a surface and a moving fluid at different temperatures, and radiation is the transfer of energy through electromagnetic waves when there is no conveying medium present. Although all three modes are manifested during hot-compression, their relative importance is different and their contribution to heat transfer changes during the pressing cycle.

Conduction is the main mode of heat transfer when surfaces with different temperatures are in close contact. Therefore the majority of heat is transferred by conduction across the hot platen-mat interface. The contribution of conduction to the heat transfer within the mat structure is also relevant and getting larger as the mat is compressed to the target thickness, and the moisture content of the mat is depleted. The conduction is described by Fourier's First Law in the model

\[ q = -k_m \frac{\partial T}{\partial x}. \]  

(3.6)

The rate of the conduction heat transfer for a given temperature differential is determined by the conductivity of the mat \((k_m)\). The conductivity varies with the mat structure (flake density, flake orientation, void fraction) and with the internal environment (moisture content). The exact relationship is derived in the Physical and Transport Properties Section.

Convection has an important role to transport the energy content of the water phases, most importantly the hot vapor phase within the mat structure vertically and horizontally. The magnitude of the convection part of the heat transfer depends on the amount of water available in the structure and the void fraction. The higher the initial moisture content the more water vaporized, increasing the pressure differential and mass flux \((n_p)\), thus increasing the rate of the convective heat transfer. The voids in the structure create a pathway for convection. The larger the proportion of the void volume, the greater the permeability and diffusivity of the mat.
The convection terms in the energy equation are the product of the flux and the enthalpy of the different phases as in

\[ c = n_p \, h_p . \]  

\( n_p \) designates flux terms for air, vapor, and bound water flow, and \( h_p \) is the enthalpy, where the subscript \( p \) is \( a \) (air), \( b \) (bound water), or \( v \) (vapor). The flux and enthalpy terms are defined in detail in the Mass Transfer and Thermodynamic Relationships Sections, respectively.

Radiation transfers heat both from the hot platens to the surfaces and from the edges of the board to the environment. On the surface, radiation has a contribution to heat transfer by warming up the top layer of the mat at the press closing stage of the press cycle. The absorbed radiation energy can cause a non-symmetrical temperature distribution. Keeping the initial press opening close to the mat thickness can substantially reduce the surface radiation effect. On the exposed edges the heat is continuously transported to the surroundings by radiation. According to calculations, the heat loss due to this effect can be as high as 13 %, but the escaping water vapor acts as a reflector with most of the radiation reflected back to the panel (Bowen 1970). The radiation effect is small, especially at low temperatures (below 200 °C), compared to the conduction and convection effects, and can be safely ignored.

Heat is also generated by the heat of compression of the mat, and the exothermic polymerization reaction of the resin. Bowen (1970) derived the relative contribution of these two phenomena; the heat of compression is approximately 2 %, while the polymerization contributes 22 % of the total energy supply. The polymerization, although a contributor to the energy supply, is greatly overemphasized in his calculations. The present model included only the heat supply due to the exothermic reaction of the adhesive incorporated in the generation term of the energy equation as

\[ G = h_g \, \rho_g \, \frac{\partial F}{\partial t} . \]  

\( h_g \, \rho_g \)
3.3.3.2 Mass Transfer

An essential difference between synthetic and wood-based composite materials is the substantial amount of water present in a wood mat structure. Additionally, the water can be in three forms in the mat structure: free (liquid) water partially filling the cell lumens and the space between the flakes, water vapor filling the remaining portion of the cell lumens and the space, and bound water hydrogen-bonded to the cell wall material.

Free water is only present in the structure when the moisture content of wood is higher than the fiber saturation point (FSP). The fiber saturation point is defined as the moisture content where the cells lose all of their liquid water content and the cell cavities are filled with saturated vapor and the cell wall is fully saturated. Typically the FSP of wood is within the range of 20-40 % moisture content depending on temperature and wood species. Because of the low initial moisture content of the strands (maximum 12 %) it is unlikely that free (liquid) water would be present in the voids at the beginning of the compression process, but as the hot vapor reaches the cool center of the mat, it may condense, creating liquid water. Additionally, the resin has typically a 50-55 % water content, therefore introducing a small amount of liquid water to the mat. The presence of liquid water in the mat structure was not accounted for in the model. The assumption of local thermodynamic equilibrium will not allow the presence of liquid water except in extreme cases.

The two main mass phases in the mat are the vapor-air gas mixture in the cell lumens and in the space between the flakes, and the bound water in the cell wall. The transport mechanisms for each of the phases are derived considering the most general case feasible. The gaseous phase (vapor and air) is transported by two mechanisms within the mat and to the surrounding environment; by bulk flow due to total pressure differential and diffusion due to partial pressure differential. The main mechanisms of bulk flow through porous media are laminar (viscous), turbulent, and slip (Knudsen) flow (Siau 1984, 1995). In the case of a large Reynolds number (Re>2300), turbulent flow is present. The slip flow or Knudsen flow exists when the diameter of the pathway is close to the diameter of the fluid molecules. The presence of turbulent flow is only likely during steam-injection pressing and the slip flow is negligible in the case of conventional pressing. Consequently laminar flow is assumed and the other two mechanisms of gas flow were neglected (Kamke and Wolcott 1991). Darcy's Law was used to describe the laminar bulk flow, and the diffusion component was assumed to follow Fick's Law.
Therefore, the transport mechanism for the vapor phase is given by the combination of Darcy's Law and Fick's Law as shown by the general form in one dimension

\[ n_v = -K_m \frac{\partial}{\partial x} (P) - D_m \frac{\partial}{\partial x} \left( \frac{P_v}{P} \right), \]  

(3.9)

where the total pressure is the sum of the air and vapor partial pressures

\[ P = p_a + p_v, \]  

(3.10)

the mat superficial permeability is given by

\[ K_m = \frac{\rho_v K_g}{\zeta_{vm} \eta_g}, \]  

(3.11)

and the mat diffusivity is given by

\[ D_m = \frac{M_v}{\zeta_{vm}} \left( \frac{\rho_a}{M_a} + \frac{\rho_v}{M_v} \right) D_{eff}. \]  

(3.12)

Analogous mechanisms (bulk flow and diffusion) transport the air in the mat structure, therefore the equations are the same, but the subscript \( v \) is interchanged with subscript \( a \).

The rate of the bulk flow and diffusion of vapor or air through the porous structure of the mat is determined by the mat superficial permeability \( (K_m) \) and the mat diffusivity \( (D_m) \), which in turn depend on the specific gas permeability \( (K_g) \) and effective diffusivity \( (D_{eff}) \), respectively. The specific gas permeability \( (K_g) \) and the effective diffusivity \( (D_{eff}) \) are functions of the mat structure, especially the amount of void present in the structure. As a result, the magnitude of these properties vary widely among different types of boards and during the press closure. The derivation of these transport properties are given in the Physical and Transport Properties Section.

The bound water in the cell wall is transported by diffusion as described by Schajer et al. (1984) and follows Fick's Law with chemical potential as the driving force:

\[ n_b = D_b (1 - \zeta_{vm}) \frac{\partial \mu_b}{\partial x}. \]  

(3.13)

Since thermodynamic equilibrium is assumed at every point of the mat, the chemical potential of the bound water \( (\mu_b) \) by definition is equal to the chemical potential of water vapor \( (\mu_v) \):

\[ \mu_b \equiv \mu_v. \]  

(3.14)
From thermodynamic relationships

\[
M_v \frac{\partial \mu_b}{\partial x} = M_v \frac{\partial \mu_v}{\partial x} = -S_v \frac{\partial T}{\partial x} + V \frac{\partial p_v}{\partial x},
\] (3.15)

where the entropy is estimated by

\[
S_v = 187 + 35.1 \ln \left( \frac{T}{298.15} \right) - R \ln \left( \frac{p_v}{101,325} \right).
\] (3.16)

Substituting Eq. 3.15 into Eq. 3.13 gives

\[
n_b = D_b (1 - \zeta_{vm}) \left( - \frac{S_v}{M_v} \frac{\partial T}{\partial x} + \frac{\zeta_{vm}}{\rho_v} \frac{\partial p_v}{\partial x} \right).
\] (3.17)

Simplifying the previous equation yields

\[
n_b = -D_b^T \frac{\partial T}{\partial x} + D_b^\rho \frac{\partial p_v}{\partial x},
\] (3.18)

where

\[
D_b^T = D_b (1 - \zeta_{vm}) \frac{S_v}{M_v},
\] (3.19)

\[
D_b^\rho = D_b (1 - \zeta_{vm}) \frac{\zeta_{vm}}{\rho_v}.
\] (3.20)

Note that in the resulting equation (Eq. 3.18) the driving forces are temperature and partial vapor pressure differentials. These two gradients work against each other. Therefore, the bound water diffusion may move in a direction opposed to the vapor partial pressure differential. The magnitude of the bound water diffusion is small compared to the vapor-air mixture bulk flow and diffusion. The value of the bound water diffusion coefficient is discussed in the Physical and Transport Properties Section.
3.3.4 Sorption Isotherms

Sorption isotherms were established to describe the relationship between the relative humidity of the ambient air and the equilibrium moisture content of solid wood at a certain temperature. Sorption isotherms are well documented at low temperatures (typically below 100 °C) for particular wood species (Wood Handbook 1987). Several theories were developed to describe the sigmoid shape of the sorption isotherm data (Siau 1995, Simpson 1971, 1973, 1980). The most widely used model, based on physical considerations, is the two-hydrate form of the Hailwood-Horrobin equation (Hailwood and Horrobin 1946) with parameters fitted by Simpson (1973) for sitka spruce (*Picea sitchensis*). However, it was demonstrated that the model is not valid above 160 °C.

Data on the high temperature sorption characteristics of wood is limited to that of Lenth (1999), Kauman (1956), and Simpson and Rosen (1981). Lenth confirmed that the sorption characteristics of wood are different at high temperature, however, he collected sorption isotherm data only at 160 °C. Kauman established sorption relationships in the temperature range from 80 °F (26 °C) to 400 °F (204 °C) for solid wood. Several phase equilibrium relations to describe the high temperature sorption behavior of solid wood were proposed (Lenth (1999), Pang (1999)), however these equations are valid only for a certain relative humidity range.

Consequently, an inverted form of the Hailwood-Horrobin two-hydrate model was used to keep the balance between the vapor and the bound water phases below 160 °C (Eq. 3.4), and cubic splines were fit to the data of Kauman (1956) to describe the sorption relationship at high temperature.

3.3.5 Physical and Transport Properties

Material properties in the out-of-plane (thickness) and in-plane (width) directions of the mat necessary for the heat and mass transfer model will be reviewed in the next section. First the transport properties including the thermal conductivity, permeability, and diffusivity of the mat are derived. Then the physical properties of the air-vapor mixture and the specific heat of wood is provided. Finally, the cure characteristics of the adhesive are defined.
3.3.5.1 Transport Properties

An important aspect of the behavior of wood-based composites is that the transport properties of the material are direction dependent. However, three principal axes (in-plane forming and cross-forming directions, and out-of-plane thickness direction) can be identified in an oriented strandboard mat, giving an orthotropic symmetry to the material. This reduces the number of the independent properties to three. A further simplification into a two-dimensional model requires transport properties to be determined only in the out-of-plane (thickness) and in-plane (width) directions of the mat. A considerable improvement on previous models is the inclusion of the press closing in the simulated press schedule since all the mat transport properties are affected by the changing mat structure during this period of the hot-compression. Additionally, the transport properties are a function of the varying temperature and moisture content in the mat structure. The effect of flake orientation on the thermal conductivity of the mat was also included. The transport properties of the mat were estimated using data from the literature for solid wood or particleboard. A sensitivity analysis of the transport properties concluded that the thermal conductivity, and gas permeability of the mat have a substantial effect on the internal environment of composite boards. (see Chapter 4. Validation and Sensitivity Study of the Heat and Mass Transfer Model). The experimental determination of these transport properties can considerably improve the model predictions.

Thermal Conductivity

The density, moisture content, and temperature dependence of thermal conductivity of wood and wood-based composites were demonstrated by several researchers (McLean 1941, Kollmann and Cote 1968, Kollmann and Malmquist 1956, Lewis 1967, Kamke and Zyklowski 1989). The thermal conductivity of compressed panels of different densities was determined experimentally, therefore the presented data are not directly applicable to assess the thermal conductivity of the mat during consolidation. However, the model requires the thermal conductivity of the mat defined in the out-of-plane (z) and in-plane (y) directions as a function of moisture content, mat consolidation, and flake orientation. The approach here was to derive the thermal conductivity of the mat, based on the thermal conductivity of solid wood, the thermal conductivity of air, and the structure of the mat.
The specific gravity and moisture content dependence of the solid wood thermal conductivity in the transverse (radial and tangential) direction is given by Siau (1995) as

\[ k_T = SG (k_{cw} + k_w \cdot M) + k_a \cdot v, \]  

(3.21)

where

- \( SG \) = specific gravity of wood,
- \( k_{cw} \) = conductivity of cell wall substance (0.217 J/m/s/K),
- \( k_w \) = conductivity of water (0.4 J/m/s/K),
- \( k_a \) = conductivity of air (0.024 J/m/s/K),
- \( M \) = moisture content of wood (fraction),
- \( v \) = porosity of wood.

The equation has the following form by substituting model variables:

\[ k_T = \frac{\rho_f}{1000} \left( k_{cw} + k_w \frac{\rho_v + \rho_b}{\rho_d} \right) + k_a \cdot \zeta_{lf}. \]  

(3.22)

The longitudinal thermal conductivity of solid wood is approximately 2.5 times higher than the transverse conductivity (Siau 1995):

\[ k_L = 2.5 \cdot k_T. \]  

(3.23)

It was assumed that the conductivity of the flakes in the two main anatomical directions can be calculated by the corresponding thermal conductivity of solid wood. However, the flakes are intentionally rotated to a certain orientation angle (\( \Theta \)) during the deposition process. Therefore, the magnitude of the thermal conductivity will be between the longitudinal and transverse values in the two perpendicular in-plane board directions. The deposition process is not exact. The orientation angle will fill a range of values, which can be quantified with the degree of alignments (\( \phi_1, \phi_2 \)). The degree of alignment is zero for perfect alignment, when the flakes are positioned at the orientation angle (\( \Theta \)), and increases as the rotation of the flakes deviates from the intended orientation.
The orientation angle ($\Theta$) and degree of alignments ($\phi_1$, $\phi_2$) are depicted in Figure 3.1.

![Figure 3.1. The effect of the orientation angle ($\Theta$), and degree of alignments ($\phi_1$, $\phi_2$) on the thermal conductivity of the flakes at the in-plane direction of the mat.](image)

The dependence of thermal conductivity on the orientation angle and the degree of alignment in the in-plane (y) direction is described by the following function

$$k_f^y = \frac{1}{2} \left( |\cos(\Theta + \phi_1)| k_L + (1 - |\cos(\Theta + \phi_1)|) k_T + |\cos(\Theta + \phi_2)| k_L + (1 - |\cos(\Theta + \phi_2)|) k_T \right).$$

Most of the cases, the orientation angle is 0° or 90° in consecutive layers of a typical oriented strandboard, and the degree of alignments are the same ($\phi_1 = \phi_2 = \phi$). Therefore, the previous equation simplifies to

$$k_f^y = |\cos(\Theta + \phi)| k_L + (1 - |\cos(\Theta + \phi)|) k_T.$$

The thermal conductivity of the flakes in the thickness direction (z) is independent of rotation angle and equal to the conductivity of solid wood in the transverse (radial and tangential) direction (Eq. 3.22).
The loosely formed mat structure consists of flakes and space among the flakes due to the inherent randomness of the mat formation. The magnitude of the space is described by the space fraction of the mat ($\zeta_{sm}$) in the mat formation model. The air-filled space acts as a thermal insulator during the press closure. As the pressing proceeds, the space is eliminated from the structure, and when the mat reaches the target thickness, practically no space remains in the mat.

Therefore, after reaching the target thickness of the panel, the thermal conductivity of the mat will be that of the compressed flakes. It was assumed that the air-filled space and the flakes form a parallel system of thermal resistance in the in-plane, and a serial system of thermal resistance in the out-of-plane directions of the mat as it is shown in Figure 3.2.

![Figure 3.2. The parallel and series arrangement of the flakes and air in the out-of-plane and in-plane mat directions.](image)

Therefore, the thermal conductivity of the mat in two perpendicular directions is given by

\[
k_m^y = k_a \zeta_{sm} + k_f^y (1 - \zeta_{sm}),
\]

\[
k_m^z = \frac{k_a k_T}{k_a (1 - \zeta_{sm}) + k_T \zeta_{sm}}.
\]

These two expressions describe the moisture, flake orientation, and consolidation dependence of the mat thermal conductivity in the model.

Figure 3.3 shows that the thermal conductivity of the mat increases with increasing flake density and moisture content. Figure 3.4 depicts that the consolidation process effectively eliminates the insulating air-filled spaces from the mat structure, which results in increasing thermal conductivity of the mat.
Figure 3.3. The effect of flake density and moisture content on the thermal conductivity of the mat in the out-of-plane ($k_m^z$) and in-plane directions ($k_m^y$) assuming oriented flake deposition ($\Theta=0^\circ$, $\phi_1=-40^\circ$, $\phi_2=40^\circ$) and compressed mat structure ($\zeta_{sm}=0$).

Figure 3.4. The effect of the elimination of the space among the flakes during compaction on the thermal conductivity of the mat, assuming oriented flake deposition ($\Theta=0^\circ$, $\phi_1=-40^\circ$, $\phi_2=40^\circ$) and 450 kg/m$^3$ average flake density. At total compression ($\zeta_{sm}=0$) the mat thermal conductivities in the out-of-plane ($k_m^z$) and in-plane directions ($k_m^y$) are equal to the respective flake conductivities in the transverse ($k_T$) and horizontal ($k_f^y$) directions.
Permeability

Permeability is an important property which determines the rate of fluid flow in the mat structure during hot-compression. Several orders of magnitude difference can be observed in solid wood permeability depending on the anatomical structure. Permeability of wood can not be solely related to porosity but also to the availability of interconnecting pits and perforation plates between the wood cells (Siau 1995). In particulate composites, such as OSB and particleboard, permeability is more closely related to the mat density or porosity. Gaseous flow in the mat is primarily around the wood components rather than through them. In spite of its known effect on the internal environment of the mat, there has not been much research related to permeability of wood composites (Smith 1982, Hata 1993, Hata et al. 1993, Bolton and Humphrey 1994). Only a limited investigation was conducted on the effect of mat density and flow direction on mat permeability (D’Onofrio 1994). Specific permeability data of particleboard in the thickness (out-of-plane) direction as a function of board density was presented by Humphrey (1989).

An exponential curve was fit to the permeability data by Carvalho and Costa (1998), and this equation was used to describe the structure dependence of the specific permeability of the mat in the model in the out-of-plane direction,

\[ K^s_g = 1.74 \cdot 10^{-12} \exp (-8.06 \cdot 10^{-3} \rho_{\text{mat}}). \]

(3.27)

Humphrey (1989) also established a ratio of 59:1 for the permeability parallel to normal to the board plane. The parallel (in-plane) data was based on permeability measurements on extruded particleboards. In the absence of a more reliable relationship, this ratio was considered in the whole density range.
Figure 3.5 shows the permeability of the mat at the in-plane and out-of-plane directions as a function of mat density.

\[ D_{AB} = 2.20 \times 10^{-5} \left( \frac{101,325}{P} \right) \left( \frac{T}{273.15} \right)^{1.75} \]  

(3.28)

Diffusivity

Diffusion occurs due to a partial pressure differential in the mat. The interdiffusion coefficient of an air-vapor mixture (binary gas diffusion coefficient) is calculated by the following semi-empirical relationship (Stanish et al. 1986, Incropera 1996):

\[ D_{rp} = \zeta_{vm}^2 D_{AB} \]  

(3.29)

In the mat the void structure presents a tortuous path for gas flow, which is taken into consideration by an empirical attenuation factor $\alpha$. The attenuation factor was set at a value of 0.5 (Stanish et al. 1986) in both the vertical and horizontal directions, assuming that the pathway is similar for diffusion horizontally and vertically in the mat structure,

\[ D_{eff} = \alpha D_{rp} \]  

(3.30)
Figure 3.6 displays the previous equation. The gas diffusivity decreases as the void is eliminated from the mat during the consolidation process.

![Graph showing the effect of elimination of void on gas diffusivity](image)

**Figure 3.6. The effect of the elimination of the void (ζvm) during compaction on the diffusivity of the mat. (ζvm = 0, when no void present in the mat structure.)**

Bound water diffusivity in solid wood was determined by Stanish et al. (1986). With the lack of more reliable data, the bound water diffusivity was considered to be constant

\[ D_b = 3 \cdot 10^{-13} \, (\text{kg s/m}^3). \]  

(3.31)

### 3.3.5.2 Physical Properties

The specific heat of wood, and its associated moisture content is an integral part of the energy balance equation. The density, temperature, and moisture dependence of the specific heat is given by Skaar (1972):

\[ C = \frac{\rho_d}{1,000} \left( 0.268 + 0.0011 (T - 273.15) + \frac{\rho_v \varphi_p}{\rho_d} \right) \frac{0.293}{0.293}. \]  

(3.32)

The viscosity of the air-vapor mixture is necessary to calculate the superficial gas permeability of the mat. The dependence of viscosity on temperature and partial pressure is given as the linear combination of the component viscosities weighted by the mole fractions in the mixture, resulting in the following equation (Stanish et al. 1986):

\[ \eta_g = \frac{(6.36 \cdot 10^{-6} + 4.06 \cdot 10^{-8} \, T) \, \rho_d + (-1.57 \cdot 10^{-6} + 3.80 \cdot 10^{-8} \, T) \, \rho_v}{P}. \]  

(3.33)
The saturated vapor density is included in the inverted form of the Hailwood-Horrobin model (Eq. 3.4), which was used to calculate the relative humidity within the mat. The temperature dependence of the saturated vapor density is described by an exponential curve fitted to experimental saturated vapor pressure data as follows (Stanish et al. 1986):

\[ \rho_{v,\text{sat}} = \zeta_{v,m} \exp \left( -46.490 + 0.26179 T - 5.0104 \times 10^{-4} T^2 + 3.4712 \times 10^{-7} T^3 \right). \]  

3.3.5.3 Cure Properties of the Adhesive

The adhesive cure kinetics is described by an Arrhenius-type equation (Eq. 3.5). The equation assumes a single step reaction, which is an oversimplification. However it fits experimental data for the cure of thermoset adhesives very well. This equation establishes the relationship between temperature and the extent of the polymerization of the thermosetting resin. The parameters in the equation have to be determined empirically for different adhesive systems. The activation energy of the reaction \( (E) \), the reaction constant \( (A) \), and the order of the reaction \( (n) \) were determined for a phenol-formaldehyde adhesive system by Ahmad (2000) using the same procedure and equipment described by Sernek et al. (2000). The parameters of the Arrhenius-type equation are

\[ A = 0.25 \ (1/\text{s}) , \]
\[ E = 12423.0 \ (1/\text{mol}) , \]
\[ n = 0.587 . \]  

The phenol-formaldehyde adhesive system was a commercial formulation that is commonly used in the face of OSB, and was also used in this study. The heat generated by the curing of the resin has an effect on the generation term of the energy equation (Eq. 3.3). Therefore, the temperature increases more rapidly with an increase of the polymerization reaction of the adhesive.

3.3.6 Thermodynamic Relationships

For the air, vapor, bound water, and adhesive phases within the mat an enthalpy function was defined (Stanish et al. 1986).

The enthalpy of air was determined to be only a function of temperature:

\[ h_a = C_a (T - 273.15) , \]  

where

\[ C_a = \text{air heat capacity} \ (1,000 \ J/\text{kg}/\text{K}) . \]
The enthalpy of water vapor was calculated as the sum of the enthalpy of the liquid phase of water, heat of vaporization, and enthalpy of the gas phase of water as:

\[ h_v = C_{lw}(T_{dp} - 273.15) + \lambda_{dp} + C_{gw} \left( T - T_{dp} \right), \quad (3.37) \]

where

- \( C_{lw} \) = liquid water heat capacity (4, 180 J/kg/K),
- \( C_{gw} \) = vapor heat capacity (1, 950 J/kg/K).

Heat of vaporization data from steam tables was fitted to a polynomial as a function of temperature (Stanish et al. 1986):

\[ \lambda = 2.792 \cdot 10^6 - 160 T - 3.43 T^2. \quad (3.38) \]

Dewpoint temperature as a function of partial vapor pressure was described by:

\[ T_{dp} = 230.9 + 2.10 \cdot 10^{-4} p_v - 0.639 \sqrt{p_v} + 6.95 \sqrt{p_v^3}. \quad (3.39) \]

After substituting Eq. 3.38 into Eq. 3.37 and Eq. 3.37 into Eq. 3.36, the enthalpy of water vapor is given by:

\[ h_v = 1.65 \cdot 10^6 + 1, 950 T - 2, 070 T_{dp} - 3.43 T_{dp}^2. \quad (3.40) \]

The differential enthalpy of bound water is equal to free water enthalpy less the differential heat of sorption. The differential heat of sorption decreases quadratically with increasing bound water content. At zero bound water content (\( \rho_b = 0 \)) it was considered to be 40% of the heat of free water vaporization (Stanish et al. 1986):

\[ h_b = C_{lw} \left( T - 273.15 \right) - 0.4 \lambda \left( 1 - \frac{\rho_b}{\rho_{fspb}} \right)^2, \quad (3.41) \]

where

- \( C_{lw} \) = liquid water heat capacity (4, 180 J/kg/K),
- \( \rho_{fspb} \) = bound water density at fiber saturation.

According to the previous relationship, at full saturation (\( \rho_b = \rho_{fspb} \)) the differential enthalpy of bound water reaches a maximum, and decreases as the bound water is depleted. The heat capacities (\( C \)) were considered to be constant in the previous relationships; in future models the temperature dependence of the heat capacities can be included if necessary.
The heat of reaction of the adhesive system was taken from the literature (Myers et al. 1991, Holopainen et al. 1997). Differential scanning calorimetry (DSC) data describes the energy generation of the exothermic reaction during the polymerization of the thermosetting resin. This data shows distinct peaks as the reaction enters different stages. Therefore a total heat of reaction value was calculated, which was determined as the area under the DSC curve,

\[
h_g = 3 \cdot 10^5 \text{ (J/kg)}.
\]  

(3.42)

These enthalpy relations and heat of reaction were used in the energy balance equation (Eq. 3.3) to describe the energy content of the different phases.

### 3.3.7 Partial Pressures

The driving force in the diffusion flux equation (Eq. 3.9) is the partial air and vapor pressure differential. Therefore, the phase densities \(\rho_p\) have to be related to the partial pressures \(p_p\). The partial pressure calculations in the mat are based on the assumption that air and water vapor behave as ideal gases. The air and vapor partial pressure at the prevailing temperature can be calculated from the air and vapor densities with the Ideal Gas Law as follows:

\[
p_a = \frac{\rho_a R T}{\xi_{vm} M_a},
\]

(3.43)

\[
p_v = \frac{\rho_v R T}{\xi_{vm} M_v}.
\]

(3.44)
3.3.8 Initial and Boundary Conditions

Solution of the mass conservation and energy balance equations (Eq. 3.1-3.5) requires one initial and four boundary conditions. The initial and boundary conditions are depicted in Figure 3.7.

\[ T(y, z, 0) = T^0, \]
\[ \rho_a(y, z, 0) = \rho_a^0, \]
\[ \rho_v(y, z, 0) = \rho_v^0, \]
\[ \rho_b(y, z, 0) = \rho_b^0. \]

Figure 3.7. Interpretation of the initial and the boundary conditions. The vertical midplane of the board where the model predicted results are calculated is also depicted.

From the initial moisture content of the mat and the temperature of the ambient air, the initial conditions are calculated by satisfying the local thermodynamic and phase equilibrium constraints,
The boundary conditions are obtained from the heat and moisture transfer phenomena between the surfaces and edges of the board and the external environment. The boundary conditions for the four surfaces are independent of each other and they can vary with time in the model. Although this assumption increases computational time, it also allows the simulation of nonsymmetrical boundary conditions, and the simulation of industrial press closure, where the bottom and top surfaces will experience different time-temperature histories due to the press daylight, where "daylight" refers to the gap between the top of the mat and the top platen at the beginning of the press cycle. The following equations specify the boundary heat and mass fluxes at the top and bottom surfaces and left and right edges of the mat.

The heat transfer at the boundaries were assumed to follow Newton's Law of cooling:

\[ q^j = -H^j (T^{j,\infty} - T^b), \]  \hspace{1cm} (3.49)

where \( j \) refers to the top, bottom, left, or right boundary.

The mass transfer of the gas phase (air and water) is a combination of bulk flow and diffusion, due to total pressure and partial pressure difference between the surface of the board and the ambient environment:

\[ n_a^j = -\rho_a \frac{K^j}{\eta_g} (P^{j,\infty} - P^b) - M_a \left( \frac{\rho_a}{M_a} + \frac{\rho_v}{M_v} \right) D^j (p_a^{j,\infty} - p_a^b), \]  \hspace{1cm} (3.50)

\[ n_v^j = -\rho_v \frac{K^j}{\eta_g} (P^{j,\infty} - P^b) - M_v \left( \frac{\rho_v}{M_v} + \frac{\rho_a}{M_a} \right) D^j (p_v^{j,\infty} - p_v^b). \]  \hspace{1cm} (3.51)

The bound water flux is zero at the boundary:

\[ n_b^j = 0. \]  \hspace{1cm} (3.52)

Setting the bound water flux to zero at the boundary implies that the water in the bound phase can not leave the mat structure; it has to be vaporized before it can escape to the environment. The boundary temperatures \( (T^{j,\infty}) \) are that of the hot plate temperature on the surface (top and bottom) boundaries and the ambient air temperature on the edge (left and right) boundaries of the mat. Variation of surface temperature of the hot platen, due to nonuniform heating, and variation of temperature at the edges of the mat, due to the effect of the escaping hot vapor, might be present during the hot-compression. This may be simulated in the model, but these effects are assumed to be negligible. The total pressure \( (P^{j,\infty}) \) was considered to be constant at 101,325 Pa.
The partial air and vapor pressures \( (p_a^{j,\infty}, p_v^{j,\infty}) \) of the ambient air-vapor mixture were calculated from the total pressure \( (P^{j,\infty}) \) and relative humidity of the environment \( (RH^{j,\infty}) \) as:

\[
p_{v}^{j,\infty} = p_{v}^{\text{sat}} \frac{RH^{j,\infty}}{100},
\]

\[
p_{a}^{j,\infty} = P^{j,\infty} - p_{v}^{j,\infty}.
\]

By adjusting the external heat and mass transfer coefficients \( (\mathcal{H}^j, \mathcal{K}^j, \mathcal{D}^j) \), the rate of temperature change at the boundaries and the amount of water leaving the mat can be controlled. The heat transfer is fast from the hot platens to the surface of the mat, which is indicated by high external heat transfer coefficients. However, only a small amount of water can leave the mat towards the metal plates. Therefore, low external mass transfer coefficients are assumed at the platen. The contrary is true for the edge boundaries, where the heat transfer is slower, and the mass transfer is far faster, indicating that the majority of the water vapor leaves the mat through the edges.

The governing equations of the heat and mass transfer of hot-compression (Eq. 3.1 - 3.5) and all the terms in the equations have been identified. The next section will introduce the numerical technique used for the solution of the equations.
3.4 Numerical Solution

The analytical solution of the previously described unsteady-state, two-dimensional, coupled algebraic-differential equation system (E.q. 3.1.-3.5.) is not possible. However, the equations possess a common form. Once the form is recognized, a numerical method can be developed to solve the general equation in the common form. The method of lines with finite differences in space was chosen for solution of the equation system, because it is especially efficient when the model has regular geometry with simple boundary conditions. The partial differential equations (PDEs) were discretized in the spatial variables using a control volume formulation as shown in Figure 3.8. The central-difference scheme was applied for the discretization of the conduction terms and an upwind scheme for the convective terms as described in detail by Patankar (1980).

3.4.1 Discretization at the Internal Points

The partial differential equations can be written in short-hand form, using the tensor product notation, the mass balance equation is

$$\sum r \rho_p \frac{\partial h_p}{\partial t} = -\nabla \cdot n_p \rho,$$

and the energy equation is

$$\frac{\partial}{\partial t} (\rho_p h_p + C T) = -\nabla \cdot (n_p h_p) - \nabla \cdot q + G,$$

where $\rho_p h_p$ means $\sum \rho_p h_p$, $n_p h_p$ means $\sum n_p h_p$, and subscript $p$ designates different phases (air, water vapor, and bound water).

After expansion, the energy equation takes the following form:

$$\rho_p \frac{\partial h_p}{\partial t} + h_p \frac{\partial \rho_p}{\partial t} + C \frac{\partial T}{\partial t} + T \frac{\partial C}{\partial t} = -\nabla \cdot (n_p h_p) - \nabla \cdot q + G.$$

Assuming that the enthalpy terms ($h_p$) and the specific heat of wet wood ($C$) can be considered constant within a short time step, the energy equation simplifies to the following common form:

$$h_p \frac{\partial \rho_p}{\partial t} + C \frac{\partial T}{\partial t} = -\nabla \cdot (n_p h_p) - \nabla \cdot q + G$$

The left-hand-side of the energy equation (Eq. 3.58) is referred to as the unsteady term, and the three terms in the right-hand-side are the convection, conduction, and generation terms, respectively.
The following discussion will demonstrate the finite difference formulation for the energy balance equation in one dimension. The two dimensional extension is straightforward and will be summarized at the end of the section. The same discretization method can be directly applied to the mass conservation equations.

![Finite difference mesh in one dimension.](image)

Integrating Eq. 3.58 over the control volume shown in Figure 3.8a gives

\[
\int_{w}^{e} h_p \frac{\partial \rho P}{\partial t} \, dy + \int_{w}^{e} C \frac{\partial T}{\partial t} \, dy =
- \int_{w}^{e} \frac{\partial}{\partial y} (n_p \cdot h_p) \, dy - \int_{w}^{e} \frac{\partial q}{\partial y} \, dy + \int_{w}^{e} G \, dy ,
\]

after discretization

\[
h_p \frac{\partial \rho P}{\partial t} \Delta y + C \frac{\partial T}{\partial t} \Delta y = -(n_{p,e} \cdot h_{p,e} - n_{p,w} \cdot h_{p,w}) - (q_e - q_w) + G \Delta y ,
\]

dividing both sides by \( \Delta y \)

\[
h_p \frac{\partial \rho P}{\partial t} + C \frac{\partial T}{\partial t} = - \frac{1}{\Delta y} (n_{p,e} \cdot h_{p,e} - n_{p,w} \cdot h_{p,w}) - \frac{1}{\Delta y} (q_e - q_w) + G .
\]

The discretization of the conduction term follows the central difference scheme

\[
- \frac{1}{\Delta y} (q_e - q_w) =
\]

\[
\frac{1}{\Delta y} \left( \left( k \frac{\partial T}{\partial y} \right)_e - \left( k \frac{\partial T}{\partial y} \right)_w \right) = \frac{1}{\Delta y} \left( \frac{k_e (T_e - T_P)}{\delta y_e} - \frac{k_w (T_P - T_W)}{\delta y_w} \right) ,
\]

where the value of the thermal conductivity at the interface is defined as

\[
k_e = \frac{2 k_p k_E}{k_p + k_E} .
\]
This is the harmonic mean of $k_P$ and $k_E$ instead of the arithmetic mean. This formulation has several advantages. For example, if one of the faces is an insulator, implying that $k_P = 0$, then this formulation will give the correct answer (0) for the conduction term, while the arithmetic mean would allow a certain amount of heat flow. Although an iteration scheme can be set up for nonlinear situations, when $k$ is function of the dependent variables, in this formulation it was assumed that the thermal conductivity is constant between two time steps, and the values were recalculated after each iteration. Given the uncertainty in establishing the value of $k$ and the small magnitude of the time steps, this assumption will not induce significant error in the solution.

The discretization of the convection term follows the upwind scheme. Patankar (1980) discusses the rationale and several benefits of this formulation. The upwind scheme discretization of the convection terms is more stable, and always gives physically meaningful results contrary to the central-difference scheme. The basic premise of the upwind scheme is that the value of the enthalpy ($h$) at the interface is always equal to the value of the enthalpy at the grid point on the upstream side of the interface, more precisely:

$$h_{p,e} = h_{p,P} \text{ if } n_{p,e} > 0,$$

$$h_{p,e} = h_{p,E} \text{ if } n_{p,e} < 0,$$

similarly,

$$h_{p,w} = h_{p,P} \text{ if } n_{p,w} < 0,$$

$$h_{p,w} = h_{p,W} \text{ if } n_{p,w} > 0.$$  

The conditional statements can be more compactly written with a standard notation:

$$n_{p,e} \cdot h_{p,e} = h_{p,P} \cdot (n_{p,e})_+ - h_{p,E} \cdot (n_{p,e})_-,$$

$$n_{p,w} \cdot h_{p,w} = h_{p,W} \cdot (n_{p,w})_+ - h_{p,P} \cdot (n_{p,w})_-,$$

where

$$(n_{p,e})_+ \text{ is the greater of } n_{p,e} \text{ or } 0,$$

$$(n_{p,e})_- \text{ is the greater of } -n_{p,e} \text{ or } 0.$$

After substitution, the discretized form of the convection term becomes

$$-\frac{1}{\Delta y} (n_{p,e} \cdot h_{p,e} - n_{p,w} \cdot h_{p,w}) =$$

$$-\frac{1}{\Delta y} (h_{p,P} \cdot (n_{p,e})_+ - h_{p,E} \cdot (n_{p,e})_- - h_{p,W} \cdot (n_{p,w})_+ + h_{p,P} \cdot (n_{p,w})_-).$$  

(3.68)
The vapor flux through the interface \((n_{v,e})\) is calculated from the partial vapor and the total pressures at the grid points by

\[
n_{v,e} = -K_m \frac{\partial}{\partial y} P - D_m \frac{\partial}{\partial y} \left( \frac{p_v}{P} \right) \approx
- \frac{K_{m,e}}{\delta y_e} (P_E - P_P) - \frac{D_{m,e}}{\delta y_e} \left( \left( \frac{p_v}{P} \right)_E - \left( \frac{p_v}{P} \right)_P \right).
\]

The same equation applies for the air gas phase transport, only the subscript \(v\) is interchanged with subscript \(a\).

The bound water flux through the interface \((n_{b,e})\) is calculated from the partial vapor pressure and temperature at the grid points by

\[
n_{b,e} = -D_T \frac{\partial T}{\partial y} + D_p \frac{\partial p_v}{\partial y} \approx - \frac{D_{b,e}}{\delta y_e} (T_E - T_P) + \frac{D_{b,e}}{\delta y_e} (p_{v,E} - p_{v,P}).
\]

The air and vapor partial pressures were derived from the phase densities and temperature at the mesh points according to Eq. 3.43 and Eq. 3.44. The total pressure was the sum of the two partial pressures. The transport properties at the interface, such as the mat permeability \((K_{m,e})\), mat diffusivity \((D_{m,e})\), and bound water diffusivities \((D_{b,e}^T, D_{b,e}^p)\) were calculated the same way as the thermal conductivity \((k_e)\), according to Eq. 3.63.
Figure 3.8b. The finite difference mesh superimposed on the vertical midplane of the board (φ designates any dependent variable at the mesh point).

The equations in two spatial dimensions were discretized on the domain shown in Figure 3.8b as follows:

the air mass balance equation

\[
\frac{\partial \rho_a}{\partial t} \approx -\frac{1}{\Delta y} (n_{a,e} - n_{a,w}) - \frac{1}{\Delta z} (n_{a,n} - n_{a,s}),
\]

(3.71)

the water phase mass balance equation

\[
\frac{\partial \rho_v}{\partial t} + \frac{\partial \rho_b}{\partial t} \approx
-\frac{1}{\Delta y} (n_{v,e} - n_{v,w}) - \frac{1}{\Delta y} (n_{b,e} - n_{b,w}) - \frac{1}{\Delta z} (n_{v,n} - n_{v,s}) - \frac{1}{\Delta z} (n_{b,n} - n_{b,s}),
\]

(3.72)
and the energy equation

\[ h_a \frac{\partial \rho_a}{\partial t} + h_v \frac{\partial \rho_v}{\partial t} + h_b \frac{\partial \rho_b}{\partial t} + C \frac{\partial T}{\partial t} \approx \]

\[ \frac{1}{\Delta y} \left( h_{a,P} \cdot (n_{a,e})_+ - h_{a,E} \cdot (n_{a,e})_- - h_{a,W} \cdot (n_{a,w})_+ + h_{a,P} \cdot (n_{a,w})_- \right) \]

\[ - \frac{1}{\Delta y} \left( h_{v,P} \cdot (n_{v,e})_+ - h_{v,E} \cdot (n_{v,e})_- - h_{v,W} \cdot (n_{v,w})_+ + h_{v,P} \cdot (n_{v,w})_- \right) \]

\[ - \frac{1}{\Delta y} \left( h_{b,P} \cdot (n_{b,e})_+ - h_{b,E} \cdot (n_{b,e})_- - h_{b,W} \cdot (n_{b,w})_+ + h_{b,P} \cdot (n_{b,w})_- \right) \]

\[ - \frac{1}{\Delta z} \left( h_{a,P} \cdot (n_{a,n})_+ - h_{a,N} \cdot (n_{a,n})_- - h_{a,S} \cdot (n_{a,s})_+ + h_{a,P} \cdot (n_{a,s})_- \right) \]

\[ - \frac{1}{\Delta z} \left( h_{v,P} \cdot (n_{v,n})_+ - h_{v,N} \cdot (n_{v,n})_- - h_{v,S} \cdot (n_{v,s})_+ + h_{v,P} \cdot (n_{v,s})_- \right) \]

\[ - \frac{1}{\Delta z} \left( h_{b,P} \cdot (n_{b,n})_+ - h_{b,N} \cdot (n_{b,n})_- - h_{b,S} \cdot (n_{b,s})_+ + h_{b,P} \cdot (n_{b,s})_- \right) \]

\[ - \frac{1}{\Delta y} (q_e - q_w) - \frac{1}{\Delta z} (q_n - q_s) + G. \]

After substitution of the discretized heat and mass flux terms (Eq. 3.62, Eq. 3.69, Eq. 3.70) into Eq. 3.71 - 3.73, the second order PDEs become a set of ordinary differential equations (ODEs) in implicit form, where the right-hand-sides of the equations are functions of the dependent variables at the actual and the four surrounding mesh points.

The fourth equation in the system, the algebraic sorption equation, does not require special treatment. The fifth equation, for the adhesive cure kinetics, is already a first order ODE. In this form it is directly solvable by the time integrator. The three discretized partial differential equations, the sorption equation, and the adhesive cure kinetics equation describe the heat and mass transfer and resin cure at all internal points of the grid.
3.4.2 Discretization at the Boundary Points

The following section describes the methods used to discretize the equations at the boundary points. The discussion will follow the one-dimensional case at the left-side boundary, the extension to two dimensions and other boundaries is straightforward.

The same mass balance and energy equations were applied at the boundary points as at the internal points. The differences are that the heat and mass flux between the surrounding environment and the surface of the board is described with Eq. 3.48 - 3.51, and the control volume has half of the width. Therefore integrating the general form of the energy equation over the control volume (Figure 3.8a) will yield the following result after discretization:

\[
\begin{align*}
    h_p \frac{\partial \rho_p}{\partial t} + C \frac{\partial T}{\partial t} &\approx - \frac{1}{\Delta y} \left( n_{p,e} \cdot h_{p,e} - n_{p,w} \cdot h_{p,w} \right) - \frac{1}{2 \Delta y} \left( q_e - q_w \right) + G .
\end{align*}
\] (3.74)

The heat flux was calculated according to

\[
q_w^l = -\mathcal{H}^l \left( T^{l,\infty} - T^B \right) .
\] (3.75)

The left edge vapor boundary flux is calculated as follows,

\[
n_{v,w}^l = -\rho_a \frac{\mathcal{K}^l}{\eta_g} \left( P^{l,\infty} - P^B \right) - M_a \left( \frac{\rho_a}{M_a} + \frac{\rho_v}{M_v} \right) \mathcal{U}^l \left( P_v^{l,\infty} - P_v^B \right) ,
\] (3.76)

where the partial vapor pressure \( \rho_v \) and the total pressure \( P \) is defined in Eq. 3.44, and Eq. 3.10 respectively. Analogous mechanisms (bulk flow and diffusion) transport the air between the board boundaries and the ambient environment. Therefore, the equations are the same, but the subscript \( v \) is interchanged with subscript \( a \).

The bound water flux

\[
n_{b,w}^l = 0 ,
\] (3.77)

implying that the water can not leave the mat structure in bound water form, it has to be vaporized before it can escape to the environment.

In two dimensions, the same equations (Eq. 3.75 - 3.77) describe the heat and mass fluxes at the boundary points. However, the flux calculations and the size of the control volume have to account for differences in points positioned at the corner or at other boundary points of the two dimensional mesh.
3.4.3 Solution of the ODE-Algebraic Equation System

The resulting ODE's, the algebraic sorption equation, and the adhesive cure kinetics equation were solved by an algebraic-differential time integrator, called DDASSL developed by Petzold (1998). DDASSL is a specialized initial value, ordinary differential equation system solver, which can handle algebraic equations in the system. The solver accepts the equations in implicit form. Another advantage of DDASSL is that the internal time steps are adjusted automatically depending on the convergence and stability criteria of the problem. In the case of fast convergence, the internal time steps are increased, essentially reducing the computational time. The solver uses backward differential formulas, and the Jacobian matrix is approximated internally. The solution requires the calculation of the right-hand-side of the equations with a programmer-supplied subroutine. The main program calls the solver with the specified output time when values of the dependent variables are required. The main program flow diagram is depicted in Figure 3.9a, and the flow diagram of the calculation of the right-hand-side of the equations is depicted in Figure 3.9b.

The main program reads in the mat formation data, then the input routine asks for the initial conditions, boundary conditions, and the press schedule. The following loop calls the time integrator DDASSL for each of the time values in the press schedule when output data is required by the user. The COMPRESS routine recalculates the mat physical properties, such as the different void fractions, and mat and flake densities, as the press schedule progresses. Finally, all the dependent variable data is written to separate files at the times defined by the user. The finite difference discretization of the spatial variables of the three PDEs are calculated by the programmer-supplied RHS (Right-Hand-Side) subroutine (Figure 3.9b). The RHS routine walks through all the mesh points in the superimposed grid (Figure 3.8b). The routine identifies whether the mesh point is positioned at the boundary or at the interior of the mat. The fluxes from the surrounding mesh points to the actual mesh point are calculated. In the case of an interior point, the heat flux \( q \) is calculated according to Eq. 3.62, the air and vapor fluxes \( n_a, n_v \) according to Eq. 3.68, and the bound water flux \( n_b \) according to Eq. 3.70. In the case of a boundary point, Eq. 3.75, Eq. 3.76, and Eq. 3.77 are used. During the assembly of the right-hand-side of the PDEs at the boundary points, the half size of the control volume is also taken into consideration.

The vertical midplane of the board was discretized to 361 mesh points, 19 at each direction in the following case study. Although the problem is two-dimensional, nonlinear, and the number of equations is quite high, a solution was reached on a DEC Alpha workstation within 1.5 hours. The computer used was a Digital Personal Workstation 500au, with a 500-MHz Alpha processor, 2-MByte of cache, 512-MByte of main memory, and running Digital Unix V4.0E.
Figure 3.9a. Flow diagram of the hot-compression module (GX is grid points in the x direction, GY is grid points in the y direction).
SUBROUTINE RHS

DO (GY)

DO (GX)

CALL PROPS (AP)
Actual Point (AP) transport properties

Calculate position of
Surrounding Points (SP)

DO (SP)

IF (Boundary) True
CALL BCONDS (SP)
boundary transport properties

False
CALL PROPS (SP)
internal transport properties

END DO

CALL FLUX
Fluxes w/ Finite Difference Scheme

Assemble Right Hand Side (RHS) of the
Partial Differential Equations (PDEs)

END DO

END DO

RETURN

Figure 3.9b. Flow diagram of the right-hand-side routine.
3.5 Results of a Simulation Run

The previously described model can predict the evolution of temperature, moisture content, total pressure, partial air and vapor pressures, relative humidity, and extent of cure of the adhesive with time in the vertical midplane of the mat. Several simulations were completed under hypothetical pressing conditions to test the robustness of the program. It performed well over a wide range of input parameters.

The basic capabilities of the model will be demonstrated on a single-layer strandboard hot-compression simulation for one type of mat and press schedule specification. The next chapter will compare the model predictions with experimental data among a wide range of pressing schedules. The structure of the mat was recreated by using the mat formation model. The mat was built up from one type of strand (face) with dimensional characteristics given in Table 2.1. The target density of the finished board was 610 kg/m$^3$. The number, cumulative thickness, and weight of the overlapping flakes in the simulated mat were calculated at 19 mesh points in the width and length directions. The simulated mat was positioned in the "virtual hot press" to further analyze the temperature, moisture and internal gas pressure distribution in the vertical midplane of the panel. For the simulation run, the platen temperature, the temperature at the edge of the board, the relative humidity of the surrounding air, the initial moisture content and temperature of the board, and the press schedule were specified. These parameters, together with other simulation input parameters, are given in Table 3.1. In the following discussion the results of the simulation were analyzed in two different ways. First a qualitative overview of the process is given. Secondly, a detailed analysis was performed.

3.5.1 The Dynamic Nature of Hot Compression

The following discussion gives insight into the dynamic nature of the hot-compression process. The time dependent changes of the thermodynamic variables (temperature, moisture content, total pressure, relative humidity) and adhesive kinetics (cure index) can not be considered in isolation, because of their interaction. Several three-dimensional profiles of the basic variables were created at certain stages of the hot-compression simulation to characterize the profound changes taking place in the internal environment of the mat. These profiles are largely qualitative, but provide a good graphical presentation of the time-dependent variations in the spatial conditions. The plots were generated by Mathematica software (Wolfram Research, Inc., Champaign, IL), which has been adapted for easy input of the data files. The evolution of temperature and moisture content in the vertical midplane of the panel is depicted in Figure 3.10. Figure 3.11 gives the variation of total pressure and relative humidity at certain stages of the pressing schedule. Additionally, the two components of the total pressure, the air and vapor partial pressures, are shown in Figure 3.12. Figure 3.13 summarizes the cure index data.
Table 3.1. Hot compression parameters used in the simulation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dry wood density</td>
<td>$\rho_d$</td>
<td>466</td>
<td>(kg/m$^3$)</td>
</tr>
<tr>
<td>Initial Temperature</td>
<td>$T_0$</td>
<td>25</td>
<td>(°C)</td>
</tr>
<tr>
<td>Initial Moisture Content*</td>
<td>$M.C._0$</td>
<td>5</td>
<td>(%)</td>
</tr>
<tr>
<td>Permeability of the mat</td>
<td>$K_g$</td>
<td>$1.74 \cdot 10^{-12}$</td>
<td>(m$^2$)</td>
</tr>
<tr>
<td>Permeability Ratio ($K_{g, l}/K_g$)</td>
<td>$KRatio$</td>
<td>59</td>
<td></td>
</tr>
<tr>
<td>Diffusion attenuation factor</td>
<td>$\alpha$</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>Bound water diffusivity</td>
<td>$D_b$</td>
<td>$3 \cdot 10^{-13}$</td>
<td>(kg s/m$^3$)</td>
</tr>
<tr>
<td>Cell wall thermal conductivity</td>
<td>$k_{cw}$</td>
<td>0.217</td>
<td>(J/m/s/K)</td>
</tr>
<tr>
<td>Moisture thermal conductivity</td>
<td>$k_w$</td>
<td>0.4</td>
<td>(J/m/s/K)</td>
</tr>
<tr>
<td>Air thermal conductivity</td>
<td>$k_a$</td>
<td>0.024</td>
<td>(J/m/s/K)</td>
</tr>
<tr>
<td>Surface temperature</td>
<td>$T^{\infty, o}$, $T^{\infty, b}$</td>
<td>200</td>
<td>(°C)</td>
</tr>
<tr>
<td>Surface relative humidity</td>
<td>$RH^{\infty, o}$, $RH^{\infty, b}$</td>
<td>35</td>
<td>(%)</td>
</tr>
<tr>
<td>Surface total pressure</td>
<td>$p^{\infty, o}$, $p^{\infty, b}$</td>
<td>1</td>
<td>(bar)</td>
</tr>
<tr>
<td>Surface heat trans. coeff.</td>
<td>$H^o$, $H^b$</td>
<td>85</td>
<td>(J/m$^2$/s/K)</td>
</tr>
<tr>
<td>Surface bulk flow coeff.</td>
<td>$K^o$, $K^b$</td>
<td>$3.3 \cdot 10^{-13}$</td>
<td>(m)</td>
</tr>
<tr>
<td>Surface diffusion coeff.</td>
<td>$\mathcal{D}^o$, $\mathcal{D}^b$</td>
<td>$0.5 \cdot 10^{-6}$</td>
<td>(m/s)</td>
</tr>
<tr>
<td>Edge temperature</td>
<td>$T^{\infty, o}$, $T^{\infty, b}$</td>
<td>100</td>
<td>(°C)</td>
</tr>
<tr>
<td>Edge relative humidity</td>
<td>$RH^{\infty, o}$, $RH^{\infty, b}$</td>
<td>35</td>
<td>(%)</td>
</tr>
<tr>
<td>Edge total pressure</td>
<td>$p^{\infty, o}$, $p^{\infty, b}$</td>
<td>1</td>
<td>(bar)</td>
</tr>
<tr>
<td>Edge heat trans. coeff.</td>
<td>$H^o$, $H^b$</td>
<td>0.35</td>
<td>(J/m$^2$/s/K)</td>
</tr>
<tr>
<td>Edge bulk flow coeff.</td>
<td>$K^o$, $K^b$</td>
<td>$1 \cdot 10^{-6}$</td>
<td>(m)</td>
</tr>
<tr>
<td>Edge diffusion coeff.</td>
<td>$\mathcal{D}^o$, $\mathcal{D}^b$</td>
<td>1.5</td>
<td>(m/s)</td>
</tr>
<tr>
<td>Board width</td>
<td>$L_y$</td>
<td>609.6</td>
<td>(mm)</td>
</tr>
<tr>
<td>Board final thickness</td>
<td>$L_z$</td>
<td>19.05</td>
<td>(mm)</td>
</tr>
<tr>
<td>Press closing time</td>
<td>$Pct$</td>
<td>60</td>
<td>(s)</td>
</tr>
<tr>
<td>Press opening time</td>
<td>$Pot$</td>
<td>480</td>
<td>(s)</td>
</tr>
<tr>
<td>Total press time</td>
<td>$Ptt$</td>
<td>540</td>
<td>(s)</td>
</tr>
<tr>
<td># of mesh points @ Y direction</td>
<td>$Nmp_Y$</td>
<td>19</td>
<td></td>
</tr>
<tr>
<td># of mesh points @ Z direction</td>
<td>$Nmp_Z$</td>
<td>19</td>
<td></td>
</tr>
<tr>
<td>Reaction constant</td>
<td>$A$</td>
<td>0.25</td>
<td>(1/s)</td>
</tr>
<tr>
<td>Activation energy</td>
<td>$E$</td>
<td>12423.0</td>
<td>(J/mol)</td>
</tr>
<tr>
<td>Order of the reaction</td>
<td>$n$</td>
<td>0.587</td>
<td></td>
</tr>
<tr>
<td>Resin content**</td>
<td>$\rho_g$</td>
<td>24.4</td>
<td>(kg/m$^3$)</td>
</tr>
<tr>
<td>Resin average enthalpy</td>
<td>$h_g$</td>
<td>$3 \cdot 10^5$</td>
<td>(J/kg)</td>
</tr>
</tbody>
</table>

* includes water content of the resin

** resin solid / compressed volume of the mat
Figure 3.10. Predicted temperature and moisture profiles during the hot-compression of a single-layer strandboard. The moisture content is the sum of the vapor and bound water content within the mat. The Y and Z coordinates designate the width and the thickness of the mat respectively. The boundary conditions are also depicted in the profiles. (Same interpretation of Y and Z, and the boundary conditions are also shown from Figure 3.11 to Figure 3.13.)
Figure 3.11. Predicted total pressure and relative humidity (P, RH) profiles during the hot-compression of a single-layer strandboard. Total pressure is the sum of the partial air ($p_a$) and vapor ($p_v$) pressures. The relative humidity is calculated from the vapor pressure and the saturated vapor pressure at the given temperature.
Figure 3.12. Predicted partial air and vapor pressure ($p_a$, $p_v$) profiles during the hot-compression of a single-layer strandboard. The pressures are calculated according to thermodynamic relationships (Eq.3.43, 3.44).
Figure 3.13. Predicted adhesive cure index ($F$) profiles during the hot-compression of a single-layer strandboard. Cure index 1 designates the complete cure of the adhesive.
At the commencement of the hot-compression (0 s) the profiles show the defined initial and boundary conditions. The temperature of the mat is a uniform 25 °C, and the high 200 °C platen temperature at the surface and somewhat lower 100 °C ambient temperature at the edge boundary of the board also can be observed. The moisture content is a uniform 5 % within the mat structure, and very low (~0 %) at the boundaries because of the specified low relative humidity and high temperature of the ambient environment (Figure 3.10). The total pressure inside of the mat is in balance with the atmospheric pressure at the beginning of the compression process. The relative humidity is approximately 25 % within the mat structure and approximately ~2 % at the boundaries (Figure 3.11). Note, that the main component of the gas phase in the mat initially is air. The vapor content is very low, indicated by the high air and low vapor partial pressures in the vertical midplane of the mat (Figure 3.12). The adhesive reaction is not initiated, the cure index is 0 everywhere in the cross section of the mat (Figure 3.13).

During the press closing period, the temperature increases sharply at the top and bottom surface of the board. It reaches a value close to the hot platen temperature soon after the press closing time (60 s). However, the center temperature is still low, forming a large temperature gradient in the vertical direction. The temperature gradient initiates conduction heat transport vertically from the hot platens to the cooler center. At this stage of the press schedule the horizontal temperature differential is insignificant, resulting in only convection heat transfer in the lateral direction. Notice, the effect of the environment surrounding the edge of the board on the temperature distribution. The lower ambient temperature at the edge retards the temperature increase, essentially creating a lower edge than center temperature within the board (Figure 3.10). Closest to the hot platens the temperature increases high enough, that the activation energy of the polymerization reaction is reached and the adhesive cure begins to accelerate (Figure 3.13). It is apparent in Figure 3.12 that the growing temperature close to the hot platens will vaporize the moisture of the strands and will increase the partial vapor pressure considerably. The air component of the gas phase is forced out from the board as indicated by the sudden decrease in partial air pressure at the face location of the mat. The net effect is that the total pressure increases above the atmospheric pressure close to the hot platens (Figure 3.11). The total pressure differential drives the vapor normal to the surface of the board. Except for a small fraction, the hot vapor can not escape towards the metal caul plates, but rather migrates vigorously by bulk flow and diffusion towards the center due to the total and partial vapor pressure gradient in the vertical direction (Figure 3.11, Figure 3.12). The movement of the water vapor front towards the center of the board can be traced on the relative humidity profile. The relative humidity gradually increases towards the center, and can reach high values (~60%) at certain locations (Figure 3.11). An additional consequence of the quickly moving hot vapor is that the convection mechanism plays a more significant role in the vertical heat transfer at this stage of the press schedule. The majority of the moisture is transported in the vapor phase.
Nonetheless, a small (almost negligible) part of the vertical moisture movement is due to bound water diffusion in the cell wall of the strands, where the driving force is also the vertical temperature and vapor partial pressure gradient. The initial stage of the hot-compression is characterized by very intense vertical movement of heat and moisture.

Typical internal environment conditions are depicted in the middle of the press schedule (240 s). The surface temperature of the mat is getting closer to the hot platen temperature asymptotically, and the center temperature gradually reaches the boiling point of water at the prevailing total pressure (Figure 3.10). This triggers an intensive vaporization in the center location of the board. The partial pressure profiles (Figure 3.12) confirms this phenomena, where the vapor partial pressure increases sharply in the center location creating large pressure differentials between the center and the edges of the panel. The air partial pressure is low, implying that the majority of the air fraction of the gas phase is depleted. The total pressure increases far above the atmospheric pressure in the center of the panel (Figure 3.11). The high total and partial vapor pressure differential drives the moisture horizontally towards the edges of the board, effectively reducing the moisture content (Figure 3.10). The adhesive cure reaction is initiated through the whole cross section of the board, and is quite advanced at the surfaces (Figure 3.13). The middle stage of the hot-compression is characterized by moderate vertical movement of heat and moisture and steady horizontal migration of moisture.

The last 240 seconds of the pressing cycle is less dynamic. At 480 seconds the end of the pressing period is reached and the venting begins in the hot-compression schedule. The surface of the board almost reached the platen temperature. The heat slowly migrates towards the center of the mat, mainly by conduction. The initially vigorous heat convection, due to the flow of hot vapor, ceases in the vertical direction, because there is no gradient in pressure (Figure 3.11, 3.12). The vaporization of the remaining water in the center is still active, which creates high relative humidity at this location (Figure 3.11). The vapor generation can not keep up with the vapor losses at the edges, and both the partial vapor pressure and the total pressure drop in the center, diminishing the initially large pressure differential in the horizontal direction. Therefore, the migration of vapor towards the edges gradually slows down, together with the moisture escape from the board. Note, that although the moisture is completely depleted at the surface of the board, there is still a considerable amount of water remaining in the center location (Figure 3.10). Only a far longer simulated pressing period (~750 s) would be able to completely consume this moisture, and eliminate the pressure in the center of the board. However, at the end of a typical pressing schedule simulation the final total pressure in the center is around 1.3 bar, which if equilibrated too quickly, can result in a panel blow. An adequate venting period is crucial to eliminate the delamination of the panel. The polymerization reaction of the adhesive is still not complete (Figure 3.13). The last stage of the hot-compression is characterized by very slow vertical movement of heat and moisture and diminishing horizontal migration of moisture.
The three-dimensional profiles are powerful graphical tools to have a better understanding of the relative magnitude and interaction of the different physical processes during the hot-compression. However, it is difficult to analyze them in a quantitative manner. In the following section the profiles were cut with an imaginary plane in the middle, either vertically or horizontally, creating projections of the variables. This allows a more detailed analysis of several crucial phenomena during the hot-compression.

3.5.2 Detailed Analysis

The hot-compression simulation provides a large amount of detailed information about the modeled process. The information can be presented in many different ways. The most typical ones either display the variables as a function of time, using space as the parameter, or as a function of space using time as the parameter. The two approaches, although representing the same data, can emphasize completely different aspects of the mechanisms involved. Therefore, the profiles were further analyzed and the predicted temperature, moisture content, total pressure, and relative humidity are shown as a function of time at the center location of the board at various vertical positions (Figure 3.15), and at the middle location of the board at various horizontal (Figure 3.16) positions. Interpretation of the center location and the middle location is given in Figure 3.14. The previous variables are also depicted as a function of vertical position at the center location of the board (Figure 3.18) and as function of horizontal position at the middle location of the board (Figure 3.19) at different times. Additionally, the partial air and vapor pressures are depicted as a function of time in Figure 3.17 and as a function of space in Figure 3.20.

![Diagram 3.14](image.png)

*Figure 3.14. The vertical midplane of the board where the predicted results are calculated, showing the interpretation of middle and center locations together with the mesh point numbering scheme.*
3.5.2.1 Time Analysis

The occurrence of the events were investigated in the time analysis. Figure 3.15 shows the evolution of the dependent variables (temperature, moisture content, total pressure and relative humidity) in the center of the vertical midplane. Figure 3.16 shows the evolution of the dependent variables in the middle of the horizontal midplane of the mat. The air and vapor partial pressures are depicted in Figure 3.17 as a function of time in the two perpendicular directions. The numbers designate mesh points in the thickness or width direction, where 1 refers to the surface or edge of the board respectively and 10 refers to the center of the board. Therefore, location 10 in both cases is the geometric center of the panel, and at this location the variables will show the same values and shapes either in the vertical or horizontal direction. To accomplish the analysis in an ordered fashion the press schedule was subdivided to certain well defined time periods depending on the behavior of the center temperature curve (Figure 3.15a position 10).

The first period is characterized with no temperature rise in the center of the board, called the "vertical shock" phase. The phase coincides with the time period from the initiation of the press closing until the press is closed to the target thickness of the board, which was 60 s in the present simulation run. In the vertical direction the temperature starts to rise sharply on the surface of the board as soon as the hot platens make contact with the mat (Figure 3.15a location 1). However, it takes approximately 60 s for the heat front to reach the center of the board (Figure 3.15a location 10). During this period a tremendous temperature gradient builds up in the vertical direction which drives the heat towards the center by conduction. However, the mat is compressed gradually in this period of the pressing schedule, and at the beginning of the compression the thermal conductivity of the mat is low due to the large amount of air-filled spaces in the structure. The conduction component of the heat transfer in the vertical direction gets progressively more important, as the mat is compressed to its target thickness, effectively eliminating the insulating air spaces. Humphrey (1989) hypothesized that any change in temperature will affect the equilibrium moisture content of wood, and therefore, the partial vapor pressure. In other words, vapor generation commences as soon as the temperature increases in any location of the mat. The vapor generation greatly accelerates when the boiling point of water is reached at the prevailing total pressure. The surface of the mat quickly reaches the boiling point of water, approximately 20 s into the press schedule. This results in an increase in the partial vapor pressure and the total pressure at the surface location in this early stage of the compression process (Figure 3.17c Figure 3.15c location 1). The boiling point of water is reached gradually at locations towards the center of the board. Consequently, at the end of the period, a vertical total and partial vapor pressure differential is formed, which is apparent in Figure 3.15c and Figure 3.17c. The vertical pressure gradient drives the hot vapor from the press platens to the middle of the mat by bulk flow and diffusion.
Figure 3.15. Evolution of temperature (a.), moisture content (b.), total pressure (c.) and relative humidity (d.) in the vertical midplane of the board with time for several positions in the vertical direction. The vertical positions are numbered from the surface of the board (1) to the center of the board (10) in the thickness direction. The lighter grayscale of the lines corresponds to increasing mesh point numbers from 1 to 10.
Figure 3.16. Evolution of temperature (a.), moisture content (b.), total pressure (c.) and relative humidity (d.) in the vertical midplane of the board with time for several positions in the horizontal direction. The horizontal positions are numbered form the edge of the board (1) to the center of the board (10) in the width direction.
Figure 3.17. Evolution of partial air (a., b.) and partial vapor (c., d.) pressures in the vertical midplane of the board with time for several positions in the vertical (left) and horizontal (right) direction. The vertical positions are numbered from the surface of the board (1) to the center of the board (10) in the thickness direction. The horizontal positions are numbered from the edge of the board (1) to the center of the board (10) in the width direction.
Both of the mass transport processes are fast because the permeability and diffusivity of the mat are high due to the large amount of voids in the structure. The fast vertical migration of the hot vapor has three major effects. First, a substantial amount of heat is transported by convection from the surface of the board to the cooler center. Second, the moisture content of the surface decreases considerably as moisture moves towards the center of the board in vapor form, and third, the air content of the gas phase is gradually replaced by vapor. The first effect is clearly manifested by the progressive increase in temperature at each vertical location as the end of the press closing period is approached (Figure 3.15a.). The second effect can be traced in Figure 3.15b, where the moisture content of the surface layer (location 1) drops from 5 to almost 0 %, while at position 3, the moisture content increases, indicating that the moisture migrates towards the center. The third effect is obvious in Figure 3.17a, where the air partial pressure decreases considerably at the two mesh points closest to the surface (locations 1 and 3).

In the horizontal direction in the middle of the board, nothing particularly interesting is happening in the first period. The temperature stays at the initial value, except at the edge of the board where a temperature increase can be observed (Figure 3.16a). The edge effect can be attributed to convection heat transfer between the hotter surroundings and the edge of the board. This was also detected experimentally by Bowen (1970). The partial air pressure increases slightly (Figure 3.17b) together with the total pressure (Figure 3.16c). The increase in air partial pressure and total pressure in the middle of the board was ascribed to the compression of the air-filled spaces in the mat structure (Kamke and Casey 1988a, b).

The second period is initiated at the moment when the press is closed to the target thickness of the panel and finishes at 180s. This period is characterized with a rapid temperature rise in the center of the board and is called the "vertical acceleration, horizontal initiation" phase. In the vertical direction all the previously described heat and mass transport processes are accelerated. The most substantial and most prolonged temperature gradient can be observed between the surface and the center of the board (Figure 3.15a), resulting in the fastest conduction heat transfer. The conduction heat transfer is further enhanced by the high thermal conductivity of the mat, as nearly all the air-filled spaces between the flakes have been eliminated from the structure. The vigorous temperature increase generates a large amount of vapor at every location in the mat. Consequently, the partial vapor pressure increases (Figure 3.17c). The partial air pressure decreases (Figure 3.17a) abruptly, and at the end of the period, the majority of the air is replaced by water vapor. The total pressure starts to increase at every location, but the steepest rise occurs in the center of the board. At the end of the period, the vertical total pressure differential disappears, replacing the emphasis from bulk flow to diffusion as the main mass transfer mechanism in the vertical direction (Figure 3.15c). The total pressure differential, although diminished, is still significant (Figure 3.15c), and the largest partial vapor pressure differential can be observed during this period (Figure 3.17c). The permeability and diffusivity
of the mat has been reduced, due to the elimination of the free pathway of gas flow (voids) from the mat during the consolidation. Therefore, the vapor transfer continues from the surface towards the center of the board, but at a lower rate. The hot vapor migrating from the surface to the core transfers its heat content by convection, amplifying the temperature rise in the center of the mat. The moisture, mainly in vapor form, continuously moves towards the center, as is apparent from Figure 3.15b. The moisture content of the surface is completely depleted and the inner points reach a moisture content as high as 7.5%.

Events in the horizontal direction become more energetic during this period. The most important change occurs when the heat front reaches the middle of the board and the temperature increases sharply (Figure 3.16a). This results in a considerable magnitude of vapor generation in the center, and consequently, lateral vapor flow is initiated towards the edges. The heat front reaches the middle of the board at the same time (except at the edge). The temperature difference between the interior points is insignificant, resulting in a negligible horizontal conduction heat transfer (Figure 3.16a). The vapor generation becomes extensive with the increasing temperature, which is manifested in the sharp increase of the partial vapor pressure (Figure 3.17d) and relative humidity (Figure 3.16d). The increasing amount of vapor replaces the air, and the partial air pressure is substantially reduced (Figure 3.17b). The net effect is that the total pressure begins to increase and a horizontal, gradually expanding pressure differential builds up (Figure 3.16c). The total pressure gradient drives the hot vapor towards the edges of the mat by bulk flow. At this stage of the compression process, there is no horizontal partial vapor pressure differential in the interior of the mat. Consequently, the diffusion part of the mass transfer is not significant (Figure 3.17d). As in the vertical case, the hot vapor transports its heat content towards the edges of the board by convection, which essentially reduces the temperature of the core of the board.

The third period (180-270 s) is characterized with the leveling off of the temperature in the center of the board, and is called the "vertical deceleration, horizontal acceleration" phase. The temperature differential between the surface and the center of the board becomes nearly constant at the end of the period. Heat migrates steadily from the hot platens to the interior of the panel by conduction. The continuous heat supply vaporizes the moisture in the interior of the mat, further increasing the partial vapor pressure (Figure 3.17c), together with the relative humidity (Figure 3.15d). The air is completely depleted at the end of the period (Figure 3.17a). Although the magnitude of the total pressure gradually increases to its peak value (~1.3 bar), there is only a small gradient, resulting in a minute vertical bulk flow. The vapor is mainly transported by the sluggish diffusion mechanism, which further slows down as the partial vapor pressure differential diminishes during the period (Figure 3.17c). Actually, the vertical movement of the vapor almost ceases at the end of this pressing period. The moisture content of the center of the board also reaches its maximum value at about 8% (Figure 3.15b).
In the horizontal direction events just started to accelerate. The temperature in the middle of the panel gradually increases to a value close to 110-118 °C, and stabilizes at the end of the period (Figure 3.16a). A small temperature difference (~5 °C) is formed in the interior of the board giving rise to conduction heat transfer from the interior towards the edges. The increase of the partial vapor pressure, together with the total pressure, accelerates. Vapor is continuously lost to the environment, resulting in lower pressure values closer to the mat edge (Figure 3.17d, Figure 3.16c). The progressively increasing total and partial vapor pressure differential in the horizontal direction drives the vapor at an increasing pace to the edges. Vapor at the edges continuously leaves to the environment, taking its heat content, and effectively cooling the center of the mat. The total pressure increases until the end of the period, indicating that the generation of vapor within the mat is faster than the vapor loss at the edges. The temperature also increases during the period, implying that the vertical conduction heat transfer can keep up with the horizontal convection heat losses. However, the water supply, and the necessary heat supply for vaporization, are gradually exhausted at the end of the period.

The fourth period (270-360 s) is characterized with no temperature rise in the center of the board. This is the "vertical stagnation, horizontal deceleration" phase. A fine balance is formed between the normal and lateral flow of heat and moisture. The water is completely depleted in the surface of the mat (Figure 3.15b position 1), thus nothing remains to be vaporized. The surface temperature asymptotically increases to the platen temperature. At this stage there is a steady heat migration from the hotter surface towards the center of the panel by conduction. The moisture content is still high in the center (Figure 3.15b) and this heat supplies the necessary energy (latent heat) for vaporization. A small total pressure and partial vapor pressure difference exists in the vertical direction, which slowly transports the vapor to the center. To summarize, the moisture slowly continues to flow towards the center by bulk flow and diffusion, and the heat flows by conduction. Therefore, the water content in the middle of the panel is continuously replaced, vaporized and migrates towards the edges. The relative magnitude of the normal to the lateral flow will determine the behavior of the core temperature.

The bulk flow and diffusion of the hot vapor from the center to the edges also continues, because a substantial total and partial vapor pressure differential exists in the horizontal direction during the rest of the press schedule (Figure 3.16c, Figure 3.17d). The magnitude of the pressures declines at every point in the mat (Figure 3.15c, Figure 3.16c, Figure 3.17c and d), indicating that the horizontal flow of vapor is faster than the vertical replacement of moisture. The moisture content declines rapidly everywhere in the panel (Figure 3.15b).

The fifth period (360-480 s) is characterized with the slow increase of the temperature in the center of the board, called the "drying-out" phase. The most important change in the process is that the moisture content declines at every point in the mat (Figure 3.15b, Figure 3.16b). The moisture is largely depleted. The movement of mass is mainly a slow, steady horizontal
migration from the core towards the periphery of the panel at this stage of the press schedule.

In the vertical direction the heat is mainly transported from the hot platens to the core by conduction, due to the stabilized temperature difference (Figure 3.15a). There is a small total or partial pressure gradient. Therefore, there is only a small vertical heat transport by convection and mass transport by bulk flow or diffusion (Figure 3.15c, Figure 3.17c). Only a minute bound water diffusion endures normal to the surface. There is a linear drop in total and partial vapor pressures, indicating that the vapor leaves the mat at a steady fashion from the edges (Figure 3.15c, Figure 3.17c). The temperature in the center starts to rise because less vapor is generated, and less energy is consumed as latent heat. The result of the retarded vapor generation is that the relative humidity in the center decreases substantially (Figure 3.15d), together with the moisture content (Figure 3.15b).

In the horizontal direction there is still a substantial and prolonged total and partial vapor pressure gradients between the core and the periphery of the panel (Figure 3.16c, Figure 3.17d). The pressure differentials ceaselessly drives the vapor towards the edges, continuously reducing the moisture content of the mat until the press cycle ends (Figure 3.16b). At the beginning of the venting period the total pressure in the center of the panel (~1.25 bar) is still 25 % higher than the atmospheric pressure (Figure 3.16b). Therefore, during the venting, the press has to be opened slowly to release this pressure and evade a panel blow.

The previous "Time Analysis" can be performed using various board characteristics or pressing parameters. Investigation of the effect of the model parameters on the length of the five pressing periods can result in a better understanding of the heat and mass transfer phenomena during hot-compression.
3.5.2.2 Spatial Analysis

The location of events were investigated in the spatial analysis. Figure 3.18 shows the evolution of the dependent variables (temperature, moisture content, total pressure and relative humidity) in the vertical direction in the center of the vertical midplane of the mat. Each line represents a selected time that corresponds to the time periods discussed in the previous sections. Figure 3.19 shows the evolution of the dependent variables in the horizontal direction. The air and vapor partial pressures are depicted in Figure 3.20 as a function of the vertical and horizontal positions in the center and middle locations of the mat. The outer two mesh points, designating the edge and the surface of the board, showed distinctly different behavior than the rest of the points.

In the following discussion, the spatial differences of the variables are investigated. The magnitude of the gradients can be related to the rate of heat or mass flow in a particular direction. Each variable behavior is analyzed in the two perpendicular directions.

The temperature gradient is connected to the rate of heat conduction in the mat. The temperature in the vertical direction changes very rapidly during the press closure, and the largest temperature gradient is formed between the surface and the center of the mat at 60 s in the press schedule (Figure 3.18a). The conduction mechanism is most effective at this period. As time progresses the temperature of the center gradually increases, diminishing the temperature differential between the surface and the center of the board. The gradient almost remains the same after 270 s, indicating a continuous, steady, heat conduction in the vertical direction during the rest of the press schedule.

In the horizontal direction there is negligible temperature difference between the internal points (Figure 3.19a). Therefore, the conduction mechanism is not significant. Note, that the temperature stays almost constant between 10 and 60 s. All the temperature increase happens between 60 and 180 s, and only a minute temperature increase can be observed thereafter. The environment has a pronounced effect on the edge temperature of the mat.
Figure 3.18. Vertical profiles of temperature (a.), moisture content (b.), total pressure (c.) and relative humidity (d.) in the vertical midplane of the board for different times during the press schedule, varying from 10 to 480 s. The vertical positions are numbered from the surface of the board (k=1) to the center of the board (k=10) in the thickness direction.
Figure 3.19. Horizontal profiles of temperature (a.), moisture content (b.), total pressure (c.) and relative humidity (d.) in the vertical midplane of the board for different times during the press schedule, varying from 10 to 480 s. The horizontal positions are numbered from the edge of the board ($j=1$) to the center of the board ($j=10$) in the width direction.
Figure 3.20. Vertical (left) and horizontal (right) profiles of partial air (a., b.) and partial vapor (c., d.) pressures in the vertical midplane of the board for different times during the press schedule, varying from 10 to 480 s. The vertical positions are numbered from the surface of the board (k=1) to the center of the board (k=10) in the thickness direction. The horizontal positions are numbered from the edge of the board (j=1) to the center of the board (j=10) in the width direction.
The total pressure gradient is connected to the rate of bulk flow, and the air and vapor partial pressures to the rate of diffusion of the gas phase in the mat. Substantial total pressure differential exists in the vertical direction only in the first 60 s (Figure 3.18c). From this time forward the bulk flow component of the vertical mass transfer almost ceases to exist.

In the horizontal direction total pressure differential builds up continuously between the center and the edge of the board (Figure 3.19c). The total pressure differential is highest at 270 s, and steadily diminishes until the end of the pressing period. Therefore, the contribution of the bulk flow component to the lateral mass transfer is continuously increasing until 270 s, and it decreases thereafter.

The partial pressure gradients show interesting behavior in the vertical direction only in the first 270 s of pressing time. At the initiation of the compression process the vapor content of the gas phase in the mat is very low (Figure 3.20c). As the temperature front moves towards the center, the vaporization becomes more intense at the high temperature locations of the mat. Consequently, the partial vapor pressure gradually increases, first at the surface, then at inner locations of the mat (Figure 3.20c). A large vertical partial vapor pressure gradient builds up, which drives the hot vapor to the center by diffusion. The vertical partial vapor pressure differential diminishes as the vaporization becomes more intense in the center of the board, and disappears at 270 s. The air partial pressure behaves in the opposite way as air is replaced by water vapor. The relatively high partial air pressure diminishes, first at the surface, then gradually at inner points (Figure 3.20a). The pressure drops to 0 at 270 s, indicating that the air is completely replaced by vapor (Figure 3.20a). Gas phase diffusion contributes to vertical mass transfer only in the first 270 s, then the vertical diffusion ceases.

In the horizontal direction the partial vapor pressure gradient starts to increase around 60 s, and continues to do so until 360 s, at which time it begins to slowly decrease. (Figure 3.20d). Vapor is transported in the lateral direction by diffusion after the press closing period. The air was depleted quickly in the interior of the mat, but the air partial pressure is still high at the edge of the mat, implying that the high air content of the surrounding gas phase is nearly at equilibrium with the outer points of the mat (Figure 3.20b).

The moisture and relative humidity fronts are related to the amount of water moving in vapor or bound form in the mat. The water moves continuously from the surface to the center of the board. The moisture content and relative humidity at the inner points of the mat gradually increase as the pressing process progresses (Figure 3.18b, 3.18d). The locations close to the surface of the board are practically dry, while the center moisture content is still high (4.5 %) at the end of the hot-compression.

In the horizontal direction in the middle of the mat the moisture and relative humidity show an even distribution at the interior points (Figure 3.19b, d). The edge of the board (location
1) starts to dry-out early in the pressing process, after about 60 s. The center starts to loose moisture at about 270 s and continues until the end of the press schedule.

### 3.6 Conclusions

The comprehensive experimental characterization of the heat and mass transfer process during hot-pressing is a formidable task due to the large number of interacting variables. A realistic mathematical model of the phenomena can make the task manageable. A one-dimensional drying model of hygroscopic porous materials was extended to two dimensions and adapted to include all the relevant heat and mass transfer mechanisms to simulate the hot-compression of wood-based composite panels. The model is capable of simulating the change of the internal environment within the vertical midplane of the flake mat in order to characterize the rapid moisture and temperature gradient development, and the extent of the adhesive polymerization reaction in two dimensions.

The model is robust enough to simulate industrial pressing situations, including the press closing time and asymmetric boundary conditions. Events happening in the vertical direction are directly applicable to industrial board production, because they are not sensitive to the lateral size of the panel. However, predictions in the horizontal direction, especially at the edges, are dependent on the lateral dimension. The edge to surface area ratio is even smaller in the case of commercial boards, further reducing the losses at the edges. Generally, the relationship between the behavior of laboratory-size panels and full-scale panels is still not understood. The model, with slight modifications, is capable of predicting events happening in a full-size composite panel during the hot-compression, and direct comparison of the results becomes viable.

The model was extended to include the third dimension. However, the model execution time became prohibitively long. Actually, the information gained by the three-dimensional model were irrelevant, when symmetrical boundary conditions were assumed. Assigning different transport properties at certain mesh points, the simulation of the hot-compression of a multi-layer board is also attainable.

The heat and mass transfer part of the hot-compression model allows one to do "what-if" analysis using the same mat structure. Process operators can gain insight into the effect of certain production parameters on the internal environment of the mat, thus allowing them to make more informed decisions about the production process.
Nomenclature

Constants

\( R \) = universal gas constant \( 8.31696 \, (J \, mol^{-1} \, K^{-1}) \)
\( M_a \) = molar weight of air \( 0.028968 \, (kg \, mol^{-1}) \)
\( M_v \) = molar weight of vapor \( 0.018016 \, (kg \, mol^{-1}) \)

Basic Variables

Independent variables
\( t \) = time (s)
\( y \) = horizontal coordinate in the width of the board
\( z \) = vertical coordinate in the thickness of the board

Dependent variables
\( \rho_a \) = density of air \( (kg \, m^{-3}) \)
\( \rho_v \) = density of vapor \( (kg \, m^{-3}) \)
\( \rho_b \) = density of bound water \( (kg \, m^{-3}) \)
\( T \) = temperature \( (K) \)
\( F \) = extent of reaction (cure index)

Symbols

\( A \) = reaction constant
\( C \) = specific heat of wet wood \( (J \, m^{-3} \, K^{-1}) \)
\( C_p \) = heat capacity \( (J \, kg^{-1} \, K^{-1}) \)
\( D_{AB} \) = binary gas diffusivity for air–vapor mixture \( (m^2 \, s^{-1}) \)
\( D_{eff} \) = effective gas diffusivity \( (m^2 \, s^{-1}) \)
\( D_m \) = mat gas diffusivity \( (kg \, m^{-1} \, s^{-1}) \)
\( D_b \) = bound water diffusivity \( (kg \, s^{-3} \, m^{-3}) \)
\( E \) = activation energy \( (J \, mol^{-1}) \)
\( G \) = heat generation \( (J \, m^{-3}) \)
\( K_g \) = specific gas permeability of dry wood \( (m^3 \, m^{-1}) \)
\( K_m \) = mat superficial gas permeability \( (s) \)
\( L \) = board dimension \( (m) \)
\( P \) = total pressure \( (Pa) \)
\( S \) = entropy \( (J \, mol^{-1} \, K^{-1}) \)
\( c_p = \) heat convection flux (J / m\(^2\) / s)
\( h_p = \) enthalpy (J / kg)
\( k = \) thermal conductivity
\( n_p = \) mass flux (kg / m\(^2\) / s)
\( n = \) order of reaction
\( p = \) partial pressure (Pa)
\( q = \) heat conduction flux (J / m\(^2\) / s)

\( \alpha = \) attenuation factor for vapor diffusivity in the flakes
\( \Theta = \) rotation angle (deg)
\( \phi_1, \phi_2 = \) degree of alignment (deg)
\( \eta = \) viscosity (kg / m / s)
\( \lambda = \) heat of vaporization (J / kg)
\( \mu = \) chemical potential (J / kg)
\( \rho_d = \) density of dry wood (kg / m\(^3\))
\( \zeta_{lf} = \) lumen fraction in the flakes
\( \zeta_{sm} = \) space fraction in the mat
\( \zeta_{vm} = \) void (space + lumen) fraction in the mat
\( \zeta_{lm} = \) lumen fraction in the mat

\( \mathcal{H}^l = \) external heat transfer coefficient (J / m\(^2\) / s / K)
\( \mathcal{K}^l = \) external bulk flow coefficient (m)
\( D^l = \) external diffusion coefficient (m / s)

**Superscripts**

\( B = \) boundary point
\( b = \) bottom boundary
\( j = \) represents boundaries (top, bottom, left, right)
\( l = \) left boundary
\( r = \) right boundary
\( t = \) top boundary
\( \infty = \) environment
Subscripts

E = east from the actual point
L = longitudinal anatomical direction in solid wood
N = north form the actual point
P = actual point
S = south from the actual point
T = transverse (radial and tangential) anatomical direction in solid wood
W = west from the actual point
a = air
b = bound water
cw = cell wall
d = dry wood
dp = dew point
e = east interface
f = flake
fsp = fiber saturation point
g = gas phase (air + vapor)
l = lumen (hole in the flake)
m = mat
n = north interface
p = phase (air, vapor, bound water)
s = space (hole in the mat)
s = south interface
sat = saturation
v = vapor
v = void (space + lumen)
w = water
w = west interface
References


Mahoney, R. J. 1980 Physical changes in wood particles induced by the particle board hot-pressing operation.


