Numerical Simulations of Thermo-Fluid Phenomena in Microwave Heated Packed and Fluidized Beds

by

Max Savransky, M.S.

Dissertation submitted to the Faculty of the Virginia Polytechnic Institute and State University in partial fulfillment of the requirements for the degree of

Doctor of Philosophy

in

Mechanical Engineering

James R. Thomas, Jr., Chairman
Clint L. Dancey
Brian Vick
William A. Davis
Lee Johnson

September 2003

Blacksburg, Virginia

Key Words: microwave catalysis, packed beds, fluidized beds

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Max Savransky, Ph.D.
Virginia Polytechnic Institute and State University, 2003
Advisor: James R. Thomas, Jr.,

ABSTRACT

Microwave heating is implemented in various fields such as drying, material processing, and chemical reactors. Microwaves offer several advantages over conventional heating methods: 1) microwaves deposit heat directly in the material without convection or radiation, 2) microwave heating is easy and efficient to implement, and 3) microwave processes can be controlled. In order to understand how to use microwaves more efficiently, we must understand how they affect the material with which they interact. This requires the ability to predict the temperature distribution that is achieved within the material. In recent years packed and fluidized beds have been used as chemical reactors to achieve various tasks in industry. Recent studies have shown that microwave heating offers the potential to heat the bed particles to a higher temperature than that of the fluid. This results in enhanced reaction rates and improves the overall efficiency of the reactor. The focus of this work is to determine the temperature distributions within the packed and fluidized beds, and to determine whether the catalyst particles can be heated to a higher temperature than the gas in catalytic reactions. The beds are modeled with multiphase flow equations. The gas velocity profiles along with the solid and gas temperature profiles for packed and fluidized beds are provided. For the fluidized beds, the hydrodynamics is modeled using FLUENT and the solid velocity profiles are also determined.
Acknowledgments

I would like to thank my advisor, Dr. James R. Thomas, for his patience and guidance. He helped me with problems along the way. I would also like to thank Dr. Clint L. Dancey, Dr. Brian Vick, Dr. William A. Davis, and Dr. Lee Johnson for serving on my committee. Their input was very valuable. I would like to thank my family for their support through this difficult journey. I would like to thank Dr. Peter Menegay. His knowledge of computational fluid dynamics (CFD) was very valuable. I would like to thank the Dupont company and the National Science Foundation (NSF) for partial support of this work. Finally, I would like to thank Dr. Hamid Arastoopour, Dr. Dimitri Gidaspow, and their students for their input. Their knowledge of fluidization was most helpful.

Max Savransky

Virginia Polytechnic Institute and State University

September 2003
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**NOMENCLATURE**

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<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tr>
<td>$D_p$</td>
<td>metallic catalyst particle diameter (m)</td>
</tr>
<tr>
<td>$C_{pf}$</td>
<td>specific heat for the gas phase (J/kg · K)</td>
</tr>
<tr>
<td>$C_{ps}$</td>
<td>specific heat for the solid phase (J/kg · K)</td>
</tr>
<tr>
<td>$d_p$</td>
<td>catalyst pellet diameter (m)</td>
</tr>
<tr>
<td>$E$</td>
<td>electric field (V/m)</td>
</tr>
<tr>
<td>$f$</td>
<td>microwave frequency (Hz)</td>
</tr>
<tr>
<td>$g$</td>
<td>gravitational acceleration (m/s²)</td>
</tr>
<tr>
<td>$h_v$</td>
<td>volumetric coefficient of heat transfer (W/m³ · K)</td>
</tr>
<tr>
<td>$H$</td>
<td>the height of the bed (m)</td>
</tr>
<tr>
<td>$k_f$</td>
<td>conductivity of the gas phase (W/m · K)</td>
</tr>
<tr>
<td>$k_s$</td>
<td>conductivity of the solid phase (W/m · K)</td>
</tr>
<tr>
<td>$K$</td>
<td>permeability of a porous system</td>
</tr>
<tr>
<td>$L$</td>
<td>length of the fluidized bed (m)</td>
</tr>
<tr>
<td>$Nu$</td>
<td>Nusselt number</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandtl number</td>
</tr>
<tr>
<td>$\dot{q}$</td>
<td>rate of heat generated within the solid phase (W/m³)</td>
</tr>
<tr>
<td>$R$</td>
<td>radius of the bed (m)</td>
</tr>
<tr>
<td>$Re_d$</td>
<td>Reynolds number for porous flow</td>
</tr>
<tr>
<td>$T_f$</td>
<td>temperature of the gas phase (K)</td>
</tr>
<tr>
<td>$T_s$</td>
<td>temperature of the solid phase (K)</td>
</tr>
<tr>
<td>$T_\infty$</td>
<td>surrounding temperature of the bed (K)</td>
</tr>
<tr>
<td>$u_D$</td>
<td>dynamic wave velocity (m/s)</td>
</tr>
<tr>
<td>$u_{Dz}$</td>
<td>the gas velocity in a packed bed (m/s)</td>
</tr>
<tr>
<td>$u_K$</td>
<td>kinematic wave velocity (m/s)</td>
</tr>
<tr>
<td>$u_{mf}$</td>
<td>minimum fluidization velocity (m/s)</td>
</tr>
<tr>
<td>$u_f$</td>
<td>x-component of the gas velocity (m/s)</td>
</tr>
<tr>
<td>$u_s$</td>
<td>x-component of the solid velocity (m/s)</td>
</tr>
<tr>
<td>$U$</td>
<td>the overall coefficient of heat transfer (W/m² · K)</td>
</tr>
<tr>
<td>$v_f$</td>
<td>y-component of the gas velocity (m/s)</td>
</tr>
</tbody>
</table>
\( v_s \)  

y-component of the solid velocity (m/s)

Greek Symbols

\( \epsilon_0 \)  

permittivity of free space (f/m)

\( \epsilon \)  

electric permittivity of materials (f/m) or emissivity

\( \epsilon' \)  

dielectric constant (f/m)

\( \epsilon'' \)  

loss factor (f/m)

\( \epsilon''_r \)  

effective relative loss factor

\( \mu_0 \)  

permeability of free space (h/m)

\( \mu \)  

dynamic gas viscosity (N \cdot s/m^2)

\( \rho_f \)  

density of the gas phase (kg/m^3)

\( \rho_s \)  

density of the solid phase (kg/m^3)

\( \sigma \)  

electrical conductivity (S/m)

\( \phi_s \)  

sphericity coefficient

\( \phi_0 \)  

porosity at the center of the bed

\( \phi \)  

porosity in a packed bed

\( \phi_f \)  

volume fraction of the gas in a fluidized bed

\( \phi_s \)  

volume fraction of the solid in a fluidized bed

\( \Phi \)  

volume fraction of catalyst within the pellet
Chapter 1

Introduction

1.1 Prelude

The utilization of microwave energy for heating processes may offer some advantages over conventional heating methods. For dielectric and semi-conducting materials, microwave heating results in better material properties, and time and energy savings. This is because microwaves deposit energy directly in the medium as opposed to conventional heating where heat is delivered by a convective or conductive process. Besides material processing, microwave heating is also utilized in the enhancement of chemical reactions. In some instances, a material that can absorb microwave energy is used to transfer the energy to the reactant because many chemicals cannot absorb the microwave energy directly.

An area where microwave heating offers the advantage of direct heat deposit is chemical catalysis. Several researchers have found that microwave heating brought about an increase in reaction rates and yield over conventional heating. Bond et al. [1] reported that microwave heating reduced catalyst drying time by at least a factor of two while improving their crushing strength. Chemat et al. [2] applied microwave heating to esterification and found increases in reaction rates compared to conventional heating. Kim et al. [3] used a microwave heated fluidized bed reactor for fast pyrolysis of chlorodifluoromethane into tetrafluoroethylene and found that they could achieve yields of more than 80 percent over a temperature range of 700-840 C.
Berlan et al. [4] found that reaction rates in cycloaddition reactions were faster when heated by microwaves than with conventional heating.

Two theories have been suggested as explanations of these phenomena. The first suggests that an increase in the pressure or temperature in the reactor brings about the influence of thermal effects. This is a result of the heat generation that is caused by the interaction between the electromagnetic field and the medium. This interaction may lead to “hot spots” because the electromagnetic field may be locally concentrated in and around the metallic catalyst particles without any noticeable change in the bulk temperature of the system. The second theory suggests the presence of “non-thermal” effects. The idea behind this theory was that microwaves would couple with the desired molecules and alter their rotations, thus increasing yields of the reactions. Stuerga and Gaillard [5] opposed this explanation by showing that such effects are improbable. Despite this fact, many papers have been published successfully demonstrating such effects. In reality, it may be a combination of both that is contributing to the enhancement of the reaction rates, but very little is understood about the microscopic nature of “non-thermal” effects because measurements are very difficult to perform at such a level. This inability in making the appropriate measurements is the reason why the parameters which characterize the “non-thermal” effects have not been quantified. Thus, only the thermal effects will be considered in this work.

1.2 Objectives

A numerical investigation of gaseous flow through packed and fluidized beds in a microwave applicator will be conducted. These can be seen in Fig. 1.1. As the gas is passed through the beds, a fraction of the energy generated by the microwaves is converted into thermal energy by the pellets and transferred to the gas. The desired chemical reaction is then initiated between the gaseous molecules at some optimal temperature, $T_{opt}$. Side reactions may occur if the temperature is sufficiently different from $T_{opt}$. In order to avoid these side reactions, it would be ideal to heat the solids
to a higher temperature than the gas so that the heat supplied by the solids would maintain the gas around $T_{\text{opt}}$. A typical experimental arrangement for a packed bed is shown in Fig. 1.2. The fluidized bed is shown in Fig. 1.3. In this investigation, the packed and fluidized bed was composed of alumina pellets containing nm-sized platinum particles. The packed bed is approximately 1 inch in height and diameter and placed in a glass tube [6]. The fluidized bed container is about 40 cm in length and 60 cm in height and is rectangular [7].

In the packed and fluidized bed setups, we consider the flow of air over alumina/platinum catalysts. Air is a chemically inert gas. The effect of chemical reactions will not be considered because the goal of this work is to determine whether the solids can be heated to a higher temperature than the gas by microwaves. One hypothesis is that the platinum catalyst can achieve significantly higher temperatures than the ceramic support. This phenomenon is known as selective heating and is described in more detail in the section below. If this is true, then the chemical reaction
will be greatly enhanced in the vicinity of the catalyst particles. It is desired to be able to heat the particles without heating the gas so that the desired reaction will take place without any side reactions.

1.3 Selective Heating

In the application of interest in this work, metallic particles are nanometer-sized particles attached to a ceramic support. These particles are believed to couple better with the microwave energy than the support and hence achieve significantly higher temperatures, approximately 200 – 300°C. The electrical conductivity becomes significantly smaller than the bulk conductivity for nanometer-sized particles, as reported by Nimtz et al. [8], allowing the microwaves to couple with the metallic catalysts. The bulk conductivity of the catalyst particles may still be higher than that of their ceramic support. For particles whose diameter is less than 500 nm, the conductivity may be represented approximately by [8]

$$\sigma_{eff} = \left( \frac{D_p}{5 \cdot 10^{-6}} \right)^3 \sigma_b,$$

where $D_p$ is the particle diameter (m) and $\sigma_b$ is the bulk conductivity of the metal. The catalyst particles thus behave as dielectrics.

1.4 Numerical Model

A thermal model assuming a constant and attenuated electric field in the packed and fluidized beds is developed. The thermal model for the packed bed and fluidized beds provide temperature distributions for the bed particles. The packed bed model also provides the velocity profile of the gas, but the velocity profiles are obtained with the aid of FLUENT [9], a commercial computational fluid dynamics (CFD) software package, for the fluidized bed. The velocity profiles determine the rates at which the gas removes heat from the particles and the electric field determines the rate of heat generation within the particles. The temperature distribution of the gas will
determine the extent to which the reaction will be enhanced. Also, the temperature difference between the gas and solid phases will serve as an indicator of whether selective heating is likely to occur. A moderate temperature difference between the gas and solid indicates that selective heating is possible while a very small temperature difference does not reveal anything about selective heating.

Thus far, microwave effects on packed and fluidized beds have been studied by Lanz [10] and Faucher [11] respectively. Both have developed one-dimensional heat transfer models to analyze the temperature distributions and both have assumed constant gas velocity and zero solid velocity. Hence, Faucher’s model does not account for the motion of the solids and the expansion of the bed while Lanz’s model does not account for the radial variation in gas velocity which can produce temperature gradients in that direction. These limitations are removed in the current model.
Figure 1.2: Packed bed setup.
Figure 1.3: Fluidized bed setup.
Chapter 2

Literature Review

2.1 Increased Reaction Rates Via Hot Spots

Several researchers have concluded that the enhancement of reaction rates under microwave irradiation is due to the presence of “hot spots”. Chemat et al. [2] deduced the existence of a temperature difference in liquid phase chemical reactions under the influence of microwaves through thermodynamic calculations. They used 3 to 5 mm montmorillonite clay pellets with $Fe_2(SO_4)_3$ catalyst particles. The temperature differences between the reactant and the catalyst pellets were estimated to range from 9-18 C. It was concluded that the temperature difference and the increase in yields were due to microwave heating.

Using a lumped-capacitance model and a kinetic theory description of the heat transfer coefficient, Thomas [12] showed that the catalyst particles can be heated to higher temperature than the support into which they are imbedded when the gas pressure is reduced to 0.1 atm.

2.1.1 Increased Selectivity

The investigation of chemical reactions under the influence of microwaves has been studied since the 1970s. As mentioned earlier, microwaves have the advantage of delivering heat directly within the catalyst as opposed to conventional heating where
the heat is delivered to the catalyst by a heat exchanger by convection and possibly radiation. Several authors reported increased selectivity when the reactor was heated by microwaves.

Ioffe et al. [13] emphasized that irradiation time is crucial to the observed increases in selectivity. He used radio frequency and microwave heating to produce acetylene from methane and hydrogen.

Roussy et al [14] reported much higher selectivities in isomerization of 2-methylpentane. However, the higher yields were due to subjecting the catalyst to an electromagnetic field prior to utilization in a chemical reactor. Also, the nature of the catalyst particle added to the $\gamma$-alumina played an important role in the increased selectivity. Wan [15] used microwave heating to produce hydrocarbons from water and carbon. He emphasized the importance of the catalysts used in the reaction and observed that catalysts serve a dual purpose; 1) increase the chemical reactivity, and 2) convert microwave energy into chemical energy.

### 2.1.2 Modeling Efforts

Multiphase flow problems arise in many areas in engineering such as chemical reactors, conveyers of solid materials, and heat exchangers. Therefore, correct prediction of the flow and thermal behavior in these various devices is important in their design. Several approaches have been used to solve the fluid mechanics portion of the multiphase flow problem.

The first approach is based on empirical methods [16,17]. The resulting equations derived based on this approach are restricted in their application by the parameters of the particular system to which they are applied.

A second approach is based on the continuum mixture theory [18,19] in which the phases are assumed to exist as overlapping continua over the entire region of interest. Each variable is expressed as the sum of the volume fractions of the variable for each phase. Only a single conservation of mass, momentum, and energy equation is written to describe the state of the system.

A third approach which has been utilized with much success by Kawaguchi
et. al [20] is the discrete element method (DEM). It is assumed that the fluid phase is viewed as a continuum while the particles are treated discretely. The fluid phase variables are described by volume-averaged continuity and Navier-Stokes equations while the state of the solid phase is governed by Newton’s laws. The relationship for the drag force between the solid and fluid states is determined empirically.

Kawaguchi used the DEM to simulate the behavior in a two-dimensional fluidized bed in which particle motion was restricted by parallel plates inserted inside the bed. The disadvantage of this approach is that it is difficult to implement it to fine-particle systems because the computational capabilities are insufficient for this method to be applied to systems with a large number of particles.

A fourth approach is based on the method of local volume averaging [21]. Each phase is treated as an interpenetrating continuum and occupies a different portion of the region of interest. Each phase is also assumed to be separated by irregular surfaces. Conservation laws are written for each phase with appropriate boundary conditions at the interphases. However, since the boundaries undergo changes in their size and shape with space and time, solving these equations is an overwhelming task. Hence, the field variables are averaged over a representative control volume which is large in comparison to the control volume for a single phase and yet small in comparison to overall dimensions of the region of interest. A resulting set of differential equations is developed for each phase.

Local volume averaging was first employed by Anderson and Jackson [22] to describe the fluid mechanics in a fluidized bed. Drew and Segel [23] applied the same technique to study fluidized beds and foams. Hassanizadeh and Gray [21] developed a generalized approach to multiphase flow systems without considering any particular applications. Bogere [24] later applied a more rigorous form of the generalized approach to derive the governing equations in gas-solid fluidized beds. Gidaspow et. al [25,26] used volume-averaged Navier-Stokes equations to analyze bubbling flow in fluidized beds. They also validated the kinetic theory approach which is used to determine the solids particle viscosity. Arastoopour et. al [27,28] used the volume-averaging capabilities of FLUENT and CFX, another CFD software package, to study
the solids motion in circulating fluidized beds (CFB).

Another possible approach is to compute the desired quantities directly without approximation at each location and at each time step in the system. One possible way to accomplish this would be to combine the portion of the DEM method for the solid phase used in [20] with the direct solution of the Navier-Stokes equations for the fluid on a domain which consists of the interior of the container with volumetric voids induced by the occupation of the solid particles. The DEM method would then provide the location and the velocity of the solid particles which could then be used to identify the geometry of the fluid and the boundary condition at the interface between the solid particle and the gas for the solution of the Navier-Stokes equations. The magnitude of the $x$, $y$, and $z$-component of velocity of the solid particle is the boundary condition which is implemented in the $x$, $y$, and $z$-component of the Navier-Stokes equations respectively. The problem with this method is that when the particles change location, a new grid is required for the solution of the Navier-Stokes equations which means that a new grid is required at every time step of the solution. Such a method is impractical with current computational capabilities.

Several researchers have also used the first four of the above approaches to study the thermal problem in packed and fluidized beds. Thomas and Faucher [29], used the volume-averaged energy equations to study packed and fluidized beds. The packed bed was modeled by an approach which was based on the work of Choudhury [30] while the fluidized bed was modeled in a similar manner except with a different correlation for the heat transfer coefficient between the solid and gaseous phases. Zahavi [31] used the energy equations to study liquid-solid fluidized beds. He considered the motion of the solid particles but used a mixture approach instead of the two-phase approach used by Thomas and Faucher. Chen and Wang [32] derived a simplified one-dimensional steady-state model for a gas-solid fluidized bed. They wanted to study the effects of the fluidization on the temperature and saturation within a single particle. The particle was assumed to be representative within the fluidized bed. The governing differential equations with the appropriate boundary conditions for the temperature and saturation were provided. The same authors [33] used a
similar approach to study fluidized bed drying with microwave heating. The heat generation within a particle was modeled as a constant times the square of the electric field. The electric field was assumed to be constant. Minoura et al. [34] used the volume-averaged energy and mass transfer equations to develop a three-dimensional multiphase model which describes the temperature and oxygen concentration distributions in a fluidized bed refuse incinerator. However, they assumed constant velocities for all phases. Roussy et al [35] developed a two-phase two-dimensional model to predict the heat transfer in a fluidized bed which was placed in a multimode rectangular cavity. They assumed the particles were stationary and that the gas velocity was constant. Also, the model is one-dimensional in each phase. They found that the electric field is strongly dependent on the motion of the solid in a multimode cavity.

Several organizations have conducted experiments on microwave-heated fluidized beds [36,37]. In their setups, the solids are initially fed into the bed until the desired solid capacity is attained. The solids entrance valves are then closed and the measurements are taken. Unfortunately, the results presented in these papers are very difficult to compare with the current model since the geometry of the system is different and not all of the necessary input data is provided.
Chapter 3

Interactions Between Materials and Electromagnetic Waves

3.1 Introduction

Microwave processes involve the generation and transmission of electromagnetic energy to some particular system. The microwave system consists of three main components; the generator, the transmission line, and the applicator [6]. In low power applications, transmission lines are employed instead of waveguides. In high power applications, waveguides are preferred because transmission lines yield large conductor losses.

Several devices are employed as microwave generators. Some of the common sources include traveling wave tubes (TWT), Gunn diodes, klystrons, and magnetrons. In most microwave applications, the generator is a magnetron tube which consists of a cathode/anode system. The cathode is heated to a sufficiently high temperature and then set to a higher negative potential than the anode. The electrons are boiled off from the cathode and propagate towards the anode in a spiral, thus generating an electric field. The magnetron is simple, reliable, efficient, and cost-effective as opposed to the other devices. Typical commercial magnetrons are designed to be operated in a $TE_{10}$ launcher $^1$.

$^1$This notation describes the specific electromagnetic field mode in the waveguide. Additional
A waveguide provides a coupling between the generator and the applicator. It is a long hollow conductor of constant cross-sectional dimension such that its dimensions are at least a quarter of the operational wavelength. This size is substantially larger than that of a comparable transmission line, and hence the losses will be drastically reduced. The appropriate electric field determines the dimensions of the waveguide. Rectangular waveguides are most commonly used and are usually operated in the \( TE_{10} \) mode.

An applicator is needed to produce desired electromagnetic field distributions within the object to be heated. The design of the applicator is highly influenced by the dimensions of the object to be heated by the electromagnetic field. This implies that microwaves are appropriate for small objects and RF is appropriate for large ones. The frequency range is also affected by the total power to be applied. For applications in which the power is greater than 200 kW, RF systems are usually employed. For applications in which the power is between 1 and 20 kW, microwaves are preferred. For intermediate power applications, (1-100 kW), the frequency is determined by thermal and electrical properties and the geometry of the object. Hence, the applicator design is a compromise between the way in which the electromagnetic field interacts with the object to be heated and the advantages and disadvantages of different applicator-workpiece combinations.

### 3.2 Electric Field

The electromagnetic energy is carried by a traveling electromagnetic wave and interacts with the system in a way which is characterized by the electric conductivity, \( \sigma \), the electric permittivity, \( \epsilon \), and the magnetic permeability, \( \mu \) of the system. The energy can be dissipated or absorbed by the system. The system properties relate the electric field strength, through constitutive relations, to quantities which appropriately describe the relationship between the system and the electromagnetic energy. The force exerted on a test charge \( Q \) by another point charge at rest is expressed explanation is given in [38].
by Coulomb’s Law [39],

$$\vec{F} = \frac{1}{4\pi \epsilon_0} \frac{qQ}{r^2} \vec{r},$$  \hspace{1cm} (3.1)

where $\epsilon_0$ is the permittivity of free space, $r$ is the distance between the two charges, and $q$ is the magnitude of an arbitrary point charge.

Now, suppose there are $n$ point charges $q_1, ..., q_n$, at distances $r_1, ..., r_n$ from the test charge $Q$. The total force on $Q$ is the sum of the forces of the individual $n$ point charges given by,

$$\vec{F} = Q\vec{E},$$  \hspace{1cm} (3.2)

where

$$\vec{E}(\vec{r}) \equiv \frac{1}{4\pi \epsilon_0} \sum_{i=1}^{n} \frac{q_i}{r_i^2} \vec{r}_i.$$  \hspace{1cm} (3.3)

Here, $\vec{E}$ is called the electric field, and is a measure of the amount of force exerted by the discrete point charges on a test charge as indicated by equation (3.2). The electric field strength is the magnitude of the electric field.

### 3.3 Constitutive Relations

The constitutive relations indicate that the current density, the electric flux density, and the magnetic flux density are proportional to the electric field [39].

The electric field, $\vec{E}$, is related to the electric conductivity and to the current density, $\vec{J}$, by:

$$\vec{J} = \sigma \vec{E},$$  \hspace{1cm} (3.4)

where $\sigma$ and $\vec{E}$ are defined as above. The current density is measured in amperes per square meter, $(A/m^2)$ and is a representation of the amount of current passing through a surface.

The electric field, $\vec{E}$, is related to the electric permittivity and to the electric flux density, $\vec{D}$, by:

$$\vec{D} = \epsilon \vec{E},$$  \hspace{1cm} (3.5)

15
where $\epsilon$ is a complex quantity whose real part represents the amount of electromagnetic energy stored within the material and whose imaginary part represents the amount of electromagnetic energy which can be converted into thermal energy and is written as:

$$
\epsilon = \epsilon' - j \epsilon''.
$$

(3.6)

The permittivity of free space is denoted $\epsilon_0$, and its value is $8.85 \times 10^{-12}\text{C}^2/(\text{N} \cdot \text{m}^2)$. It is often convenient to represent the real and imaginary parts of the permittivity in nondimensional form relative to $\epsilon_0$ as,

$$
\epsilon'_r = \frac{\epsilon'}{\epsilon_0},
$$

(3.7)

and

$$
\epsilon''_r = \frac{\epsilon''}{\epsilon_0}.
$$

(3.8)

The magnetic field, $\vec{H}$, is related to the electric permeability and to the magnetic flux density, $\vec{B}$, by,

$$
\vec{B} = \mu \vec{H},
$$

(3.9)

where $\mu$ is a complex quantity whose real part represents the amount of magnetic energy stored within the material and whose imaginary part represents the amount of magnetic energy which can be converted into thermal energy and is written as,

$$
\mu = \mu' - j \mu''.
$$

(3.10)

### 3.4 Dielectric Losses

Dielectric materials can be classified as semiconductors. The atomic and molecular forces which bound the electrons in these materials are sufficient to conduct some electricity but not to the same extent as in metals. When these materials are irradiated by an electric field, their dominant electric charges tend to align with the field.
The direction of the field turns out to be the vector from the negative to the corresponding positive charges. There is an energy loss due to interatomic friction forces which results during this alignment. If the field is alternating, the electron alignment is also alternating, thus causing electric energy to be converted into molecular kinetic energy.

In general, it is the valence electrons of the material that are most affected by the electric field. These electrons can exist only in discrete energy levels. In order for them to pass from one energy level to another, they must emit or absorb an exact amount of energy. The applied electric field supplies the energy which is required to alternate the valence electrons from one state to another. Materials which couple strongly with the electric field are called lossy materials. The electric energy within the material is dissipated as thermal energy and the dissipation is described by the dielectric loss of the material.

The power absorbed by an object is the difference between the entering and exiting electromagnetic fields and is given by [6]

$$\int_{S} \frac{1}{2} (E \times H^*) \, ds = \int_{V} \frac{1}{2} (E \cdot J) \, dV + \frac{j \omega}{2} \int_{V} \frac{1}{2} (B \cdot H^* - E \cdot D^*) \, dV. \quad (3.11)$$

where $S$ is the surface area of the object, $V$ is the volume of the object, and $^*$ indicates complex conjugation. Applying the constitutive relations to equation (3.11) yields

$$- \int_{S} (E \times H^*) \, dS = \int_{V} \sigma |E|^2 \, dV + \frac{1}{2} \omega \int_{V} (\varepsilon'' |E|^2 + \mu'' |H|^2) \, dV \quad (3.12)$$

The first integral on the righthand side represents the amount of energy dissipated due to conduction losses while the second integral on the right represents the amount of energy dissipated due to dielectric and magnetic losses. The final integral represents the net amount of electric and magnetic energy stored, but does not cause any heating of the object. Equation (3.12) is a generalization of the power loss that occurs within the material. Some simplifications will be made to describe the heat generation accurately without resorting to the complexities of implementation of equation (3.12).
In the development of a model for the heat generation, it is assumed that the magnetic permeability contributes very little in comparison with the electric permittivity to the amount of heat dissipated inside the material. For our purposes, the losses due to conduction are also negligible and only the second term on the right side of equation (3.12) is important. Hence, equation (3.12) reduces to

\[ P_{\text{ave}} = \omega \epsilon_0 \epsilon'' r E_{\text{rms}}^2 V, \]

(3.13)

where \( \omega \) is the frequency, \( V \) is the volume of the material, and \( E_{\text{rms}}^2 \) is the root mean square of the electric field, or \( 1/\sqrt{2} \) times the peak value. The heat generated per unit volume within the material can now be determined by substituting \( \omega = 2\pi f \), and dividing both sides of equation (3.13) by \( V \) giving:

\[ \dot{q} = 2\pi f \epsilon_0 \epsilon'' r E_{\text{rms}}^2. \]

(3.14)

This is used to determine the heat generation within the beds.

### 3.5 Effective Permittivity

When metallic catalyst particles are attached to a ceramic support, the overall electric properties are altered. Several mixture formulae are available to account for the addition of the catalyst. We would like to be able to determine the permittivity of the mixture so that equation (3.14) can be used to compute the heat generation per unit volume. In particular, we use the Rayleigh mixture formula [6] to compute the effective permittivity.

For small spherical inclusions within a ceramic support, the permittivity is estimated by [6]

\[ \epsilon_1 = \epsilon' - j \frac{\sigma_2}{\omega}, \]

(3.15)

and for small conducting spheres, the permittivity is estimated with

\[ \epsilon_2 = \epsilon_0 - j \frac{\sigma_2}{\omega}, \]

(3.16)
where $\sigma_2$ is the size-dependent conductivity discussed in the first chapter. The effective permittivity of the support/catalyst mixture, where the support is a continuous medium with dispersed spherical catalysts is given by

$$
\epsilon_m = \frac{\epsilon_1(2\epsilon_1 + \epsilon_2) + 2\Phi\epsilon_1(\epsilon_2 - \epsilon_1)}{2\epsilon_1 + \epsilon_2 - \Phi(\epsilon_2 - \epsilon_1)},
$$

(3.17)

where $\Phi$ is the volume fraction of catalyst within the support/catalyst system.

### 3.6 Maxwell-Wagner Effect

Real materials contain impurities which need to be accounted for when calculating the electric field within the materials. The presence of conducting impurities within a dielectric material is explained by the Maxwell-Wagner effect. When an external electric field is applied to the material, the charge distribution around the material is non-uniform. The time in which the charge density decays to 1/e of its original value is called the time constant and is given by:

$$
\tau = \frac{\epsilon'}{\sigma}.
$$

(3.18)

For a perfectly conducting sphere, the charge time constant approaches 0 and so a surface charge is produced almost immediately. In a semiconducting sphere immersed within a dielectric and irradiated by an external step electric field, an initial electric field exists inside the sphere and is given by:

$$
E_2 = \frac{3\epsilon_1}{2\epsilon_1 + \epsilon_2} E_0,
$$

(3.19)

where $E_0$ is the applied electric field. The surface charge around the sphere is initially zero because the charge has not had sufficient time to respond to the external field. As time progresses, a surface charge arises due to free charges within the semiconductor. The charge keeps moving until the internal electric field is zero. Thus steady-state is reached. In general, the internal field is a function of the electric properties of the semiconductor, as well as the spherical dimensions and the frequency of the applied electric field.
Chapter 4

Packed Beds

4.1 Porous Media

A permeable solid, or porous medium, is a material which consists of a solid matrix with an interconnected void. Many important industrial applications such as chemical reactors, groundwater flow, and gas flow in reservoirs require an understanding of heat and fluid flow within a permeable solid. The permeability is a measure of the flow conductance of a solid matrix which accounts for hydrodynamic characteristics such as the interstitial surface area and fluid particle path, and has the units $m^2$. A more precise definition is given in the section below.

Porous media can be natural or artificial. The flow through a porous medium can be viewed as flow through conduits, or pores. The pore distribution within a natural porous solid is highly irregular. An analysis of flow phenomena is complicated due to geometrical considerations. Thermo-fluid quantities are highly irregular near the pore region. However, experimental quantities are measured over surfaces which coincide with a sufficiently large number of pores. Hence, more regular changes with respect to space and time are observed in the thermo-fluid quantities and a theoretical analysis based on plain media becomes possible.

In a porous medium, the pore sizes may vary from molecular size to the order of centimeters and the system dimensions are usually much larger than that of the

---

1Most of the discussion in this chapter is based on Ref. [40].
pores. In the case where the system dimensions are comparable to those of the pores, it is common to perform the analysis for a small number of pores.

The voids in a porous medium can be interconnected, dead end, or isolated. Dead end voids are those in which the void is connected to only one other pore. The porosity, $\phi$, is defined as the fraction of the total volume of the porous medium which is occupied by the voids. Flow phenomena may only occur within an interconnected void system. The volume fraction of the interconnected pores is called the effective porosity. In a porous solid, the difference between the effective porosity and the porosity can be significant. In a loose medium such as packed beds, the porosity and the effective porosity are the same. The pore length scale is an important parameter in characterizing a porous matrix. Since pore geometries are highly irregular, defining the pore length is a complicated task. The distributed linear scale for each void is typically used in defining the pore length. Here, the linear scale is the diameter of a sphere that occupies the cross section at an arbitrary location along the pore. The average pore diameter is then determined from a statistical average of the distribution of length scales. The nonuniformities around the pore boundaries have a significant influence on the transfer rates at the boundaries and require local porosity distributions. The pore velocity, $u_p$, is the average velocity in a conduit.

Dybbs and Edwards[41] define a Reynolds number which is based on the average pore velocity, $\bar{u}_p$ and an average pore length scale, $\bar{d}$,

$$Re_d = \frac{\rho \bar{u}_p \bar{d}}{\mu},$$

(4.1)

where $\rho$ is the density of the fluid and $\mu$ is the dynamic fluid viscosity. They defined four flow regimes based on this Reynolds number:

- $Re_d \leq 1$, creep flow regime:

  In this regime, the viscous effects are dominant, and the flow is influenced by the pore geometry. Channeling is found to occur at the wall because the particle packing is much more loose in that region of the bed. The velocities adjacent to the walls may be nearly twice that found in the rest of the bed. The effects
due channeling propagate up to two particle diameters from the wall. The flow is fully developed at about three particle diameters from the entrance region.

- $1 \leq Re_d \leq 150$, inertial flow regime:
  
  When $1 \leq Re_d \leq 10$, both viscous and inertial forces are important. This is the most difficult problem to solve. For flows where $10 \leq Re_d$, the boundary layer thickness decreases compared to flows with $Re_d < 10$, due to increasing dominance of the inertial effects. The pressure drop becomes dependent on the lateral and longitudinal pore dimensions as the flow develops in each pore.

- $150 \leq Re_d \leq 300$, unsteady laminar flow regime:
  
  In this regime, oscillations become apparent. The observed frequencies are on the order of 1 Hz while the amplitudes are approximately one-tenth of a particle diameter. The flow remains laminar with a wake instability causing the flow to become unsteady.

- $300 < Re_d$, unsteady turbulent flow regime:
  
  A turbulent dispersion of injected dye occurs in this regime. The normalized pressure drop becomes constant with increasing $Re_d$.

The flow development through pores in the inertial flow regime is significant. As the diameter-to-length ratio approaches unity, the average pressure drop becomes much larger than that in fully developed flows. In the following sections a development of the drag force exerted by the gas on the porous system is presented. The expression for the drag force is used in the Navier-Stokes equations to describe the velocity profile of the gas.

### 4.2 Darcy’s Law

In 1856, Henri Darcy devised an experiment to relate the pressure drop in a pipe to the filter velocity, $u_D$. In his experiment, Darcy partially filled a pipe with randomly and loosely packed uniform-size particles. The flow within the pipe was steady and
one-dimensional and the filter velocity was determined by dividing the mass flow rate by the product of the fluid density and the cross-sectional area of the voids of the porous particle system. The filter velocity and the pore velocity are related by

\[ u_D = \phi u_p. \] (4.2)

Darcy found the relation

\[ \nabla P = -\frac{\mu}{K} u_D, \] (4.3)

where \( K \) is the permeability matrix, \( \nabla P \) is the pressure drop in the flow direction, \( u_D \) is the velocity of the fluid. It can be seen that the permeability is the ratio of the shear stress to the pressure drop for a system which obeys equation (4.3). For an anisotropic medium equation (4.3) becomes

\[ u_D = -\mu^{-1} K \cdot \nabla P, \] (4.4)

where \( K \) is a symmetric second-order tensor

\[
K = \begin{pmatrix}
K_{11} & K_{12} & K_{13} \\
K_{21} & K_{22} & K_{23} \\
K_{31} & K_{32} & K_{33}
\end{pmatrix}.
\] (4.5)

The permeability for simple porous structures such as packed spheres can be expressed in terms of the porosity and the particle diameter using the hydraulic radius model or the Carman-Kozeny theory. This is a semiheuristic model of flow through a porous medium which implements the concept of the hydraulic radius and tortuosity, \( \tau \), defined as the ratio of the distance to the displacement traveled by a fluid particle between two points.

The specific surface area of a porous matrix is defined by

\[ A_0 = \frac{A_{fs}}{V_s}, \] (4.6)

where \( A_{fs} \) is the interfacial area between the solid and fluid phases, and \( V_s \) is the volume of the solid. The hydraulic diameter is defined by

\[ D_h = \frac{4 \times \text{void volume}}{\text{surface area}} = \frac{4\phi}{A_0(1 - \phi)}. \] (4.7)
The tortuosity is used to account for a correction of the pressure gradient,
\[ \nabla p_{\text{mod}} = \frac{\nabla p}{\tau}, \tag{4.8} \]
and the pore velocity,
\[ \mathbf{u}_D = \mathbf{u}_p \frac{\phi}{\tau} = -\frac{K}{\mu} \nabla p_{\text{mod}}. \tag{4.9} \]

The filter velocity is now determined by modifying the Hagen-Poiseulle equation [40],
\[ u_p = -\frac{d^2}{32 \mu} \frac{dp}{dx}, \tag{4.10} \]
for flow along straight tubes of diameter \( d \). The modification of equation (4.9) involves the application of the tortuosity and the addition of a shape parameter \( k_0 \), and becomes
\[ u_p = -\frac{D^2}{16k_0\mu} \nabla p_{\text{mod}}, \tag{4.11} \]
where \( k_0=2 \) for a circular shape and 2-2.5 for rectangular, elliptical, and annular shapes. Combining equations (4.8), (4.9), and (4.11), we get,
\[ K = \frac{\phi^3}{k_K (1 - \phi)^2 A_0^2}, \tag{4.12} \]
where \( k_K \) is called the Kozeny constant. For a bed of uniformly-sized spherical particles of diameter \( d \), we have,
\[ K = \frac{\phi^3}{36k_K (1 - \phi)^2 d^2}, \tag{4.13} \]
where \( A_0 = 6/d \) and \( d \) is the diameter of the spherical particle with the same \( A_0 \). Taking the Kozeny constant to be 5 approximates the permeability in packed beds reasonably well and equation (4.13) becomes [42]
\[ K = \frac{\phi^3}{180(1 - \phi)^2 d^2}. \tag{4.14} \]

The Darcy equation deviates from experimental results for liquid flows at high velocities and gas flows at very low and high velocities because it exhibits the characteristics of Stokes flow. At high velocities, the inertial effects dominate the viscous
effects. The existence of viscous and inertial asymptotes has been observed by MacDonald et al.
[43]. Ergun [44], extended the hydraulic radius theory in order to account for the inertial effects in high-velocity flows. He developed a correlation based on the particle Reynolds number,

\[ Re_d = \frac{\rho u_D d}{\mu}, \]

which was later modified by Macdonald et al. as,

\[ -\frac{dp}{dx} \frac{\phi^3}{\rho u_D^2} \frac{d}{1 - \phi} = \frac{180(1 - \phi)}{Re_d} + 1.8, \]

(4.16)

for smooth surfaces, and

\[ -\frac{dp}{dx} \frac{\phi^3}{\rho u_D^2} \frac{d}{1 - \phi} = \frac{180(1 - \phi)}{Re_d} + 4, \]

(4.17)

for rough surfaces. Multiplying both sides of equation (4.16) by \(\rho u_D^2 / d\) gives

\[ -\frac{dp}{dx} = \frac{\mu}{K} u_D + 1.8 \frac{1 - \phi}{\phi^3 d} \rho u_D^2. \]

(4.18)

This equation has been extended heuristically to multi-dimensional flows and becomes,

\[ -\nabla p = \frac{\mu}{K} u_D + 1.8 \frac{1 - \phi}{\phi^3 d} \rho |u_D| u_D. \]

(4.19)

Equation (4.19) has not been verified experimentally and when simulating multi-dimensional flows, the coefficient of the second term on the right may need to be adjusted. A relatively large perpendicular velocity component causes a decrease in the coefficient.

4.3 The Semiheuristic Momentum Equations

As mentioned earlier, geometric considerations introduce a level of complexity which is currently difficult to overcome. As a result, it is very difficult to derive a momentum equation which would be of practical use. One possibility is to find extentions of Darcy’s law to account for: 1) flow development, 2) boundary generated vorticity,
and 3) the high Reynolds number effect. In the first extension, the inertial and viscous effects were added with the assumption of steady flow, given as \[40\]

\[
\frac{\rho_0}{\phi^2} (\mathbf{u}_D \cdot \nabla \mathbf{u}_D) = -\frac{\mu}{K} \mathbf{u}_D - \nabla p + \rho g + \frac{\mu}{\phi} \nabla^2 \mathbf{u}_D. \tag{4.20}
\]

There is no rigorous reasoning for the multiplication of the viscous term by $1/\phi$, and the inertial term by $1/\phi^2$. It is believed that since the pore velocities should be greater than the average values, then the viscous and inertial forces should be evaluated at the pore level. This is achieved with a multiplication of the velocity by the factor $1/\phi$. To account for high Reynolds number flows and gravitational effects, equation (4.20) was extended to,

\[
\frac{\rho_0}{\phi^2} \left( \frac{\partial u_{Di}}{\partial t} + u_{Di} \cdot \nabla u_{Di} \right) = -\frac{\mu}{K} u_{Di} - \frac{\partial p}{\partial x_i} + \rho g + \frac{\mu}{\phi} \nabla^2 u_{Di} - \frac{C_E}{K^{1/2} \rho} |u_{Di}| u_{Di}, \tag{4.21}
\]

where $C_E$ is the Ergun constant which represents the deviation from Stokes flow. A typical value for $C_E$ is 0.55.

### 4.4 Packed Bed Model

A reduced form of equation (4.20) has been applied to packed beds by Cheng and Zhu\[45\], Vortmeyer and Schuster\[46\], and more recently Thomas and Faucher\[29\]. In their model, Thomas and Faucher also accounted for the heat transfer through the bed container. In the current model, the equations derived based on the work of Anderson and Jackson \[22\] are implemented. The following assumptions are made:

1) the analysis is performed using the method of volume-averaging,
2) the flow is assumed to be 2-d, steady, and fully developed,
3) only the z-component of the gas velocity is relevant,
4) the thermal model is 2-d, symmetric, and transient,
5) the porosity in the z-direction is constant,
6) heat generated by chemical reactions is small relative to that generated by the microwaves,
7) the electric field is assumed to be uniform, and
8) radiation heat transfer is neglected.

A more accurate model of the electric field could be obtained by solving Maxwell’s equations via the finite element method, however this is beyond the scope of the current work. The transients are important in the thermal model because the dielectric properties can vary significantly with temperature. Thus, in order to predict the steady-state of the bed correctly, the thermal transients must be included [36]. The bed container is neglected because it requires a lot of computational effort and does not provide any additional information. The equation governing the fluid flow in the bed is given by

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \phi \mu \frac{\partial u_{Dz}}{\partial r} \right) = \frac{\partial P}{\partial z} + \frac{b}{d_p} \frac{1 - \phi}{\phi} \rho u_{Dz}^2 + \frac{\mu}{K} u_{Dz}, \tag{4.22}
\]

where \( b = 1.75 \) is recommended [45] instead of 1.8 as presented in equation (4.18). Equation (4.14) is then substituted for \( K \) with a recommended value of 150 in the denominator rather than 180. The boundary conditions are

\[
u_{Dz}(0) = 0, \tag{4.23}
\]

and

\[
\left. \frac{\partial u_{Dz}}{\partial r} \right|_{0} = 0. \tag{4.24}
\]

The equations governing the temperature distribution in the bed are given by [29]

\[
(1 - \phi) \rho C_{ps} \frac{\partial T_s}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r (1 - \phi) k_s \frac{\partial T_s}{\partial r} \right) + (1 - \phi) \frac{\partial}{\partial z} \left( k_s \frac{\partial T_s}{\partial z} \right) + h_v (T_f - T_s) + (1 - \phi) \dot{q}, \tag{4.25}
\]

and

\[
\phi \rho C_{pf} \frac{\partial T_f}{\partial t} + \phi \rho C_{pf} u_{Dz} \frac{\partial T_f}{\partial z} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \phi k_f \frac{\partial T_f}{\partial r} \right) + \phi \frac{\partial}{\partial z} \left( k_f \frac{\partial T_f}{\partial z} \right) + h_v (T_s - T_f), \tag{4.26}
\]

where \( T_s \) is the solid temperature, \( T_f \) is the gas temperature, and \( h_v \) is the volumetric heat transfer coefficient which is obtained from the correlation [10]

\[
Nu = 2 + 1.2 R e_d ^{\frac{1}{2}} P r ^{\frac{1}{2}}. \tag{4.27}
\]
The boundary conditions for the solid phase are

$$\frac{\partial T_s}{\partial r} \bigg|_0 = 0, \quad - \phi_s k_s \frac{\partial T_s}{\partial r} \bigg|_R = U(T_s - T_\infty) \bigg|_R,$$

(4.28)

and

$$\frac{\partial T_s}{\partial z} \bigg|_0 = \frac{\partial T_s}{\partial z} \bigg|_H = 0,$$

(4.29)

where $R$ is the radius of the bed, $H$ is the bed height, and $U$ is the overall heat transfer coefficient given by [47]

$$U = \frac{1}{R_{tot} A}$$

(4.30)

where

$$R_{tot} = \frac{\ln(r_o/r_i)}{k_g A} + \frac{1}{h A}$$

(4.31)

In the above equation, $k_g$ is the conductivity of the container, $r_i$ is the radius of the bed, $r_o$ is the radius of the bed plus the thickness of the container, and $h$ is the heat transfer coefficient given by,

$$h = 0.29 \left( \frac{\Delta T}{L} \right).$$

(4.32)

For the gas phase,

$$\frac{\partial T_f}{\partial r} \bigg|_0 = 0, \quad - \phi_f k_f \frac{\partial T_f}{\partial r} \bigg|_R = U(T_f - T_\infty) \bigg|_R,$$

(4.33)

$$T_f(0) = T_m,$$

(4.34)

and

$$\frac{\partial T_f}{\partial z} \bigg|_H = 0.$$

(4.35)

The radial porosity distribution is given by the equation [45],

$$\epsilon = \phi_0 \left( 1 + C_1 \exp \left[ - \frac{N_1 (R - r)}{d_p} \right] \right),$$

(4.36)

where $\phi_0$ is the porosity at the center of the bed.
The proposed model was solved using the upwind finite-difference scheme following the procedure proposed by Patankar [48]. Equations (4.22) and (4.23) are solved iteratively. The $u_D^2$ term is approximated by $u_g u_D$ where $u_g$ is the guessed value for $u_D$. The discretized form of the momentum equation for a general node is

$$
- (\mu r \phi_f) \left( \frac{u_E - u_P}{\Delta r} \right) + (\mu r \phi_f) \left( \frac{u_P - u_W}{\Delta r} \right) + f_2 \left( \frac{r_e^2 - r_w^2}{2} \right) u_g u_P
$$

$$
+ f_1 \left( \frac{r_e^2 - r_w^2}{2} \right) u_P = - \frac{\partial P}{\partial z} \left( \frac{r_e^2 - r_w^2}{2} \right),
$$

where $\partial P/\partial z$ is constant because the flow is assumed to be fully developed. The subscripts E, W, N, and S represent the location of the immediate grid points which are located east, west, north, and south of the main grid point P respectively. The lower case subscripts e, w, n, and s represent the east, west, north, and south control volume faces located half-way between the grid points P and E, W, N, and S respectively. The superscripts 0, and 1 stand for the current and subsequent time steps respectively. The equation for the nodal velocities is obtained by rearranging equation (4.30)

$$
\left[ \frac{(\mu r \phi_f)_e}{\Delta r} + \frac{(\mu r \phi_f)_w}{\Delta r} + f_2 u_g \left( \frac{r_e^2 - r_w^2}{2} \right) + f_1 \left( \frac{r_e^2 - r_w^2}{2} \right) \right] u_P
$$

$$
- \left[ \frac{(\mu r \phi_f)_e}{\Delta r} \right] u_E - \left[ \frac{(\mu r \phi_f)_w}{\Delta r} \right] u_W = - \frac{\partial P}{\partial z} \left( \frac{r_e^2 - r_w^2}{2} \right),
$$

where the functions $f_1$, and $f_2$ are given by

$$
f_1 = \frac{150 \mu_f (1 - \phi)^2}{d_p^2 \phi^3},
$$

and

$$
f_2 = \frac{1.75 \rho_f (1 - \phi)}{d_p \phi^3}.
$$

The discretized form of the energy equation with the upwind scheme for a general
node is

\[
(\rho C p \phi) \Delta z \left( \frac{r_e^2 - r_w^2}{2} \right) (T_{P_i}^1 - T_{P_i}^0) = (r k_i \phi_i) e \Delta z \left( \frac{T_{E_i}^1 - T_{P_i}^1}{\Delta r} \right) - (r k_i \phi_i) w \Delta z \left( \frac{T_{P_i}^1 - T_{W_i}^1}{\Delta r} \right) + (k_i \phi_i) n \Delta z \left( \frac{T_{P_i}^1 - T_{S_i}^1}{\Delta r} \right) - (k_i \phi_i) s \Delta z \left( \frac{T_{P_i}^1 - T_{P_j}^1}{\Delta r} \right) + \phi_i \dot{q}_i
\]

where the subscripts i and j represent either the solid or fluid phase and j is not i. In the above equation, \( u_{Dz,s} \) and \( \dot{q}_f \) are zero. Rearranging equation (4.34) in terms of the nodal temperatures gives

\[
[a_t + a_E + a_W + a_N + a_S + a_h] T_{P_i}^1 = a_E T_{E_i}^1 + a_W T_{W_i}^1 - a_N T_{N_i}^1 + a_S T_{S_i}^1 + a_h T_{P_j}^1 = a_i T_{P_i}^0 + \epsilon_i \dot{q}_i
\]

where

\[
a_t = \frac{(\rho C p \phi) i}{\Delta t} \Delta z \left( \frac{r_e^2 - r_w^2}{2} \right),
\]

\[
a_E = \frac{(r k_i \phi_i) e}{\Delta r} \Delta z,
\]

\[
a_W = \frac{(r k_i \phi_i) w}{\Delta r} \Delta z,
\]

\[
a_N = \frac{(k_i \phi_i) n}{\Delta z} \left( \frac{r_e^2 - r_w^2}{2} \right),
\]

\[
a_S = \frac{(k_i \phi_i) s}{\Delta z} \left( \frac{r_e^2 - r_w^2}{2} \right) + (\phi_i \rho_i C p_i u_{Dz,i}) n \left( \frac{r_e^2 - r_w^2}{2} \right),
\]

\[
a_h = h_v \left( \frac{r_e^2 - r_w^2}{2} \right) \Delta z.
\]
Chapter 5

Results for the Packed Bed

In this study, air flow through a packed bed consisting of gamma alumina particles is examined. The effects of the particle diameter and inlet velocity on the bed temperature and the temperature difference between both phases are analyzed. In the first study, these effects are observed for particle diameters of 0.5, 1, 2, and 3 mm. The gas enters the bed at 10 cm/s and at 300.15 K. The radius and height of the bed are 1 cm and 2.54 cm respectively as shown in Figure 1 of chapter 1. These dimensions were chosen as typical of experimental arrangements reported in the literature. For computational purposes, the bed was subdivided into 30 radial cells and 20 axial cells with a time step of 100 seconds. This was determined after computing the percent error of the velocity and temperature profiles using the 30 by 20 grid relative to those using a 40 by 40 grid. The largest errors occurred for the 0.5 mm diameter case which were 3 and 4.2 percent for the velocity and temperature profiles respectively. The computations were performed with a uniform electric field of 5 kV/m in all cases.

Figures 5.1-5.4 show the time evolution of the radial and axial temperature profiles of the gas and solids for the 3 mm particles. Note that time increases towards the left. The points for the radial profiles are located midway along the bed height and the points for the axial profiles are located midway between the center and the wall of the bed. It can be seen that the radial and axial temperatures increase in time. The smaller particles produce the greatest temperatures because their arrangement yields the smallest interstices, thus creating more solid contact. Equation (4.29)
captures this effect by yielding smaller porosity values within the bed for smaller particle diameters.

Figures 5.5-5.8 show the steady-state temperature profiles for the gas and solid for the 3 mm particles. The steady-state temperature profiles reveal that radial temperature gradients are relatively small and are greater at the inlet of the bed. The small temperature gradient can be attributed to the uniform electric field assumption. The temperature gradients are greater at the inlet because the gas velocity is higher towards the wall and the gas is cooler at the inlet of the bed. As the gas propagates through the bed it absorbs heat from the hotter particles and its temperature increases with bed height.

Figures 5.9-5.12 display the temperature difference between the gas and solid and the gas velocity profiles for the particle diameters discussed above. The gas velocity is larger in a small region close to the wall than in the rest of the bed because the larger porosity in that region produces channeling of the gas. Also, the gas velocity decreases with increasing particle diameter because the smaller interstices resulting from the smaller particles cause larger pressure drops at the same inlet velocity. The temperature difference between the solid and gas increases with increasing particle diameter because the larger interstices do not allow the gas to remove heat as efficiently from the solids as the smaller interstices. Since the porosity is larger near the wall, the temperature difference between the solid and gas remains larger for a greater distance along the bed height. The variation of the temperature difference with particle diameter is shown in figure 13 for two locations in the bed. The locations of the points were selected in low and high velocity regions close to the bed inlet, that is near the bed center and wall respectively. The node near the wall shows a larger temperature difference than the one near the bed center because the porosity near the wall is higher and hence the fluid offers more resistance to heating.

In the next study, we examine the effects of inlet velocity on the parameters discussed above. From the above study, we see that a temperature difference occurs throughout more of the bed when the 3 mm particles are used and hence the effects of the inlet gas velocity are investigated for these particles. From the above study,
we have data for an inlet velocity of 0.1 m/s. Additional data for inlet velocities of 0.05, 0.2, and 0.4 m/s was also obtained.

The time evolution of the radial and axial temperature profiles for the gas and 3 mm solid particles at the inlet velocities mentioned above are similar to those in figure 1 and will not be shown. Again all temperatures increase with time as expected for the same reasons discussed above. The temperatures are highest for the smallest inlet gas velocity (0.05 m/s) because the gas does not remove heat as efficiently from the solids as it does at higher gas velocities. Hence, the temperatures decrease with increasing inlet gas velocity. The steady-state temperature distributions are similar to those in figures 5.5-5.8.

Figures 5.14-5.16 exhibit the temperature difference and the gas velocity profiles for the 3 mm particles at the inlet gas velocities discussed above. The gas velocity distributions are similar to those in the previous study and the gas velocity in the bed is directly proportional to the inlet gas velocity. The temperature difference between the solid and gas decreases at the bed inlet with increasing inlet velocity because heat is removed more efficiently from the solids. However, since fluid at a higher velocity does not reside in the container for as long as a lower velocity fluid, the temperature difference penetrates further into the bed for the higher velocity fluid. Figure 5.17 shows the variation of the temperature difference with inlet gas velocity for the two points from the previous study. It can be seen that the temperature difference decreases with increasing inlet gas velocity.

In our final study, we investigate the effects of the electric field on the temperature difference in the bed. For this study, we assume a bed composed of 3 mm particles with an inlet gas velocity of 0.4 m/s because the previous study revealed that the temperature difference penetrates further into the bed for these values. We already analyzed the case for an electric field of 5 kV/m. We now investigate the cases for electric fields of 10, 15, and 20 kV/m.

Figures 5.18-5.20 show the temperature difference and velocity profiles for the electric fields above. It is seen from these figures that an increase in the magnitude of the electric field induces an increase in the temperature difference. This
occurs because the heat generated in the solid is directly proportional to square of the magnitude of the electric field. Figure 5.21 shows the variation of the temperature difference with the electric field for the same two points as in the previous studies. The temperature difference increases with an increase in electric field as expected.
Figure 5.1: Temporal radial and axial temperature profiles for gas and 0.5 mm solid particles.
Figure 5.2: Temporal radial and axial temperature profiles for gas and 1 mm solid particles.
Figure 5.3: Temporal radial and axial temperature profiles for gas and 2 mm solid particles.
Figure 5.4: Temporal radial and axial temperature profiles for gas and 3 mm solid particles.
Figure 5.5: Steady-state temperature profiles for gas and 0.5 mm solid particles.
Figure 5.6: Steady-state temperature profiles for gas and 1 mm solid particles.
Figure 5.7: Steady-state temperature profiles for gas and 2 mm solid particles.
Figure 5.8: Steady-state temperature profiles for gas and 3 mm solid particles.
Figure 5.9: Temperature difference and gas velocity profile for 0.5 mm solid particles.
Figure 5.10: Temperature difference and gas velocity profile for 1 mm solid particles.
Figure 5.11: Temperature difference and gas velocity profile for 2 mm solid particles.
Figure 5.12: Temperature difference and gas velocity profile for 3 mm solid particles.
Figure 5.13: Effect of particle diameter on the temperature difference between the gas and solid.
Figure 5.14: Temperature difference and gas velocity profile at an inlet velocity of 0.05 m/s.
Figure 5.15: Temperature difference and gas velocity profile at an inlet velocity of 0.2 m/s.
Figure 5.16: Temperature difference and gas velocity profile at an inlet velocity of 0.4 m/s.
Figure 5.17: Effect of inlet gas velocity on the temperature difference between the gas and solid.
Figure 5.18: Temperature difference and gas velocity profile for an electric field of 10 kV/m.
Figure 5.19: Temperature difference and gas velocity profile for an electric field of 15 kV/m.
Figure 5.20: Temperature difference and gas velocity profile for an electric field of 20 kV/m.
Figure 5.21: Effect of electric field on the temperature difference between the gas and solid.
Chapter 6

Fluidized Beds

6.1 Fluidization

Fluidization is the process by which a group of particles is suspended by a fluid flowing through a confined region. This occurs when the drag force exerted by the fluid on the particles exceeds the total weight of the particles. Some areas in which fluidized beds are utilized include solids drying, chemical reactors and combustors.

The main components of a fluidized bed excluding the external equipment are the gas distributor which is placed at the bottom of the bed and the surrounding container. The purpose of the distributor is to control the distribution of the inlet gas. The distributor design is important in producing high quality fluidization. Some common distributors include ceramic or sintered metal porous plate distributors and perforated plate distributors. A ceramic or sintered metal porous plate distributor is most commonly used in small-scale studies because of its ability to deliver the gas uniformly across the bed inlet. Although the gas distribution is not perfectly uniform at the inlet, it is sufficiently close. These distributors have several disadvantages: 1) high pumping power is required due to large pressure-drops, 2) high cost for materials, 3) clogging caused by corrosion or fine particles. However, compacted wire plates or sandwiched beds of small particles are used despite the disadvantages. Perforated plate distributors are frequently used in industry because they are cost-efficient and

\[1\] Most of the discussion in this section is based on Ref. [49].
easy to fabricate. These distributors are not used in a high-temperature or a highly reactive environment with large loads because they tend to undergo severe deflections which can produce undesirable results.

Fluidization occurs in several states. When the fluid is passed through the bed at flow rates that cannot induce a drag force sufficient to overcome the weight of the bed, the fluid percolates through the voids and the bed remains fixed. If the flow rate is increased to the point at which the drag force just balances the total weight of the particles, the pressure drop in any portion of the bed equals the weight of the fluid and particles in that region. The inlet gas velocity which causes this to occur is called the minimum fluidization velocity, \( u_{mf} \), and a bed in this state is said to be at minimum fluidization and has a uniform particle distribution. Such beds are called homogeneous. When the flow rate is increased beyond minimum fluidization, instabilities are accompanied by bubbling and channeling of gas. Such beds are referred to as bubbling or heterogeneous fluidized beds. The volume in these beds does not differ by much compared with the volume at minimum fluidization. The size of the bubbles increase with the height of the bed. For sufficiently deep beds, the bubble may become as large as the length of the bed. This phenomenon is known as slugging. When slugging occurs in beds of fine particles, the particles flow downward by the wall around the rising bubble. For beds made up of coarse particles, the particles above the bubble are displaced upwards in a manner which is similar to a piston-cylinder configuration. The particles then fall down and the slug vanishes. Another slug is formed at about this time and an oscillatory pattern occurs. When the terminal velocity of the particles is exceeded by the gas, the particles propagate in turbulent clusters due to entrainment and the size and shape of the gas voids varies. A bed in this state is called a turbulent fluidized bed. A further increase in gas flow rates results in the exiting of the solid particles from the bed. Eventually the solids concentration is very low and the bed is said to be a dilute- or lean-phase fluidized bed. A fluidized bed is said to be dense if there is a distinct upper surface. Within a dense bed, the solids concentration is at least 25 percent. The primary focus of this work is on dense and homogeneous gas-solid fluidized beds. The homogeneous fluidization state will
be discussed in more detail in the next section.

The quality of the fluidization process depends strongly on the particle size and the gas to solid density ratio. Other factors which may influence the quality of fluidization include vessel geometry, distributor type, and type of solids used. Beds consisting of fine particles need to be agitated to maintain quality fluidization because the particles tend to clump together when they become moist. This is accomplished either with a mechanical stirrer or by using the kinetic energy of high flow rate gas jets to agitate the solids. Fine particle beds can be large and deep because these beds can be fluidized in a broad range of gas flow rates. Beds consisting of large particles tend to fluidize poorly because of bumping and slugging. Even though the fluidization quality can be improved with the addition of fine particles, large particle beds fluidize in a narrow range of gas flow rates. Hence shallower beds must be implemented. In general, gas solid fluidized beds tend to fluidize heterogeneously. However, it is possible to avoid heterogeneity by using low-density particles in a dense gas.

Geldart [50] determined the fluidization properties of various particles through numerous experiments and classified them according to their density and diameter. He determined four groups of particles which are described from smallest to largest particle as follows:

- **Group C:**
  These particles are typically less than 50 microns and are very difficult to fluidize because the interparticle adhesive forces are stronger than those produced by the drag force. These particles will tend to rise as a plug of solids in small-diameter beds and will not fluidize in larger diameter beds. A common approach which is implemented in order to fluidize these particles in larger diameter beds is to inject them into a bed which consists of the same but larger particles. Some examples of group C particles are face powder, flour, and starch.

- **Group A:**
  The size of these particles is typically between 50 and 200 microns and their
density ranges between 700 and 1400 kg/m$^3$. One of the most important attributes of these particles is that they can fluidize homogeneously at sufficiently low gas flow rates. When the minimum fluidization state is attained in the bed, these particle beds expand considerably from their initial state. This expansion continues at a lower rate until the minimum bubbling velocity, $u_{mb}$, is reached. In the bubbling state, the bubbles rise more rapidly than the rest of the gas and appear to split and coalesce. The bubbles typically reach a maximum size of approximately 10 cm.

- **Group B:**
  
  The size of these particles is typically between 40 and 500 microns and their density ranges between 1400 and 4000 kg/m$^3$. These particles do not undergo homogeneous fluidization. Bubbles begin to form at minimum fluidization. At higher velocities, small bubbles form at the distributor and will grow and coalesce as they propagate through the bed. The size of the bubble is proportional to the relative gas velocity, $u_g - u_{mf}$, and is independent of the particle size.

- **Group D:**
  
  These are spoutable particles which fluidize poorly in deep beds. If the gas distribution is uneven, these particles will agitate and produce large bubbles or spout. The bubbles coalesce rapidly and become large. They rise more slowly than the rest of the gas. Most applications do not implement such large particles, but in some instances such as in the processing of agricultural products this is unavoidable. Particles belonging to this group require a much greater gas supply than is required for the particular application. This is usually solved by implementing a spouting bed. The 3.3mm alumina catalyst pellets manufactured by the Engelhard Corporation are examples of this type of particle.

**Fluidization States**

In this section, the homogeneous, bubbling, and slugging fluidization states are discussed in more detail. The turbulent and dilute fluidization states occur more fre-
quently in circulating fluidized beds (CFB) and hence will not be discussed.

As previously stated, the homogeneous state is one in which the particle concentration is nearly uniform. Such a state can only be achieved by group A particles because of their density and diameter. The minimum fluidization velocity is typically predicted by the following equation [51]:

\[
\frac{1.75}{\phi_{mf}^3 \Phi_s} \left( \frac{d_p u_{mf} \rho_g}{\mu} \right)^2 + \frac{150(1 - \phi_{mf})}{\phi_{mf}^2 \Phi_s^2} \left( \frac{d_p u_{mf} \rho_g}{\mu} \right) = \frac{d_p^3 \rho_g (\rho_s - \rho_g) g}{\mu^2},
\]

(6.1)

where \(\phi_{mf}\) is the porosity at the minimum fluidization state, and \(\Phi_s\) is the sphericity, which is defined as the ratio of the external surface area of a sphere having the same volume as the particle considered to the external surface area of this particle. The minimum bubbling velocity for group A particles is predicted by [51]

\[
u_{mb} = 33d_p \left( \frac{\rho_g}{\mu} \right).
\]

(6.2)

The two-phase theory tries to simplify fluidization by breaking it up into two phases. This results in an emulsion state where at a superficial gas velocity \(u_e\) and the voidage \(\phi_e\) remain at \(u_{mf}\) and \(\phi_{mf}\) respectively. Abrahamson and Geldart found that \(u_e\) and \(\phi_e\) change with the inlet gas flow rate \(u_0\). For small solids such as those in group A, they found that these changes could be reasonably represented by

\[
\left( \frac{\phi_e}{\phi_{mf}} \right)^3 \left( \frac{1 - \phi_{mf}}{1 - \phi_e} \right) = \left( \frac{u_e}{u_{mf}} \right)^{0.7},
\]

(6.3)

In the following section, the expression for the interphase drag force is developed according to [52]. This expression is similar to that in chapter 4 with the velocity of the solid particles accounted for and it is used in the two-phase Navier-Stokes equation model [9] to predict the velocity profiles for the gas and solid phase.

The Drag Force in a Fluidized Bed

An expression for the drag force in a fluidized bed is derived based on a static analysis. The drag force is obtained for a packed bed and is extended to an expression for the drag force of the homogeneous state in a fluidized bed.\(^2\)

\(^2\)The discussion in the next two sections is based mainly on ref. [52].
Consider a control volume which consists of a uniform bed of particles of unit cross-sectional area and vertical length L. The power which is dissipated by a fluid flowing through such a control volume is given by

$$\delta E = U \Delta P,$$  \hspace{1cm} (6.4)

where U is the volumetric flux and $\Delta P$ is the induced pressure drop. The fluid velocity in the control volume is $U/\epsilon$ and the energy dissipation rate for a single stationary particle under the influence of a drag force $f_d$ is $U f_d/\phi$. The total number of particles in the bed is $6(1 - \phi)L/\pi d_p^3$ and the total rate of energy loss is given by

$$\delta E = \frac{6(1 - \phi)L U f_d}{\pi d_p^3 \phi}.$$ \hspace{1cm} (6.5)

Substituting equation (6.4) into (6.5) yields

$$f_d = \frac{\pi d_p^3 \phi}{6L(1 - \phi)} \Delta P.$$ \hspace{1cm} (6.6)

The equation for the pressure drop in a packed bed is given by [52]

$$\Delta P = 60 \mu_f L U \frac{(1 - \phi)^2}{d_p^2 \phi^4}, \text{ for viscous flow}$$ \hspace{1cm} (6.7)

or

$$\Delta P = 1.17 \rho_f L U^2 \frac{(1 - \phi)^2}{d_p \phi^4}, \text{ for inertial flow.}$$ \hspace{1cm} (6.8)

Substituting equation (6.7) into equation (6.6) yields

$$f_d = 3\pi d_p \mu_f U \frac{3.33(1 - \phi)}{\phi^3}.$$ \hspace{1cm} (6.9)

The term $3.33(1 - \phi)/\phi^3$ is called the ‘voidage function’. As $\phi \to 1$, the voidage function becomes zero which is not correct. To remedy this, a 1 is added to the voidage function expression and the correct limit is attained:

$$f_d = 3\pi d_p \mu_f U \left(\frac{3.33(1 - \phi)}{\phi^3} + 1\right).$$ \hspace{1cm} (6.10)

Repeating the same analysis for the inertial flow regime yields

$$f_d = 0.055\pi \rho_f d_p^2 U^2 \left(\frac{3.55(1 - \phi)}{\phi^3} + 1\right).$$ \hspace{1cm} (6.11)
The voidage functions in equations (6.10) and (6.11) are numerically similar to $\phi^{-3.8}$ and so the equations become

\[ f_d = 3\pi d_p \mu_f U \phi^{-3.8}, \]  

(6.12)

for the viscous flow regime,

\[ f_d = 0.055\pi \rho_f d_p^2 U^2 \phi^{-3.8}, \]  

(6.13)

for the inertial flow regime. These expressions can now be extended to the simple case of a single particle suspension. The effective weight of a particle is defined as the net effect of gravity and buoyancy, and is expressed as

\[ w_e = \frac{\pi d_p^3}{6} (\rho_p - \rho_f) g \phi. \]  

(6.14)

The effective weight of the particle can also be interpreted as the drag force which is required to suspend a single, unhindered particle and hence for viscous flow we have

\[ w_e = 3\pi d_p \mu_f u_t, \]  

(6.15)

where $u_t$ is terminal velocity of the particle. Equations (6.12), (6.14), and (6.15) give the drag force for a single particle in the viscous flow regime

\[ f_d = \frac{\pi d_p^3}{6} (\rho_p - \rho_f) g \frac{U}{u_t} \phi^{-3.8}. \]  

(6.16)

The drag force for all flow regimes is given by

\[ f_d = \frac{\pi d_p^3}{6} (\rho_p - \rho_f) g \left( \frac{U}{u_t} \right)^{4.8} \phi^{-3.8}, \]  

(6.17)

where $n$ is determined from the Archimedes number, $Ar = gd_p^3 \rho_f (\rho_p - \rho_f)/\mu_f^2$ by

\[ \frac{4.8 - n}{n - 2.4} = 0.043 Ar^{0.57}. \]  

(6.18)

The drag force in a fluidized bed can now be obtained by extension of the drag coefficient relation experienced by a solitary, unhindered particle subjected to a steady fluid velocity $U_0$

\[ f_d = C_D \frac{r \rho_f U_0^2}{2} \frac{\pi d_p^2}{4}, \]  

(6.19)
where the drag coefficient \( C_D \) is given by

\[
C_D = \left( 0.63 + \frac{4.8}{Re^{0.5}} \right)^2, \quad Re = \frac{\rho_f u_0 d_p}{\mu_f}.
\]  

(6.20)

Combining equations (6.18), (6.19), and (6.20) yields

\[
f_d = \frac{\pi d_p^3}{6} (\rho_p - \rho_f) g \left( \frac{U_0}{u_t} \right)^{4.8} \frac{\rho_f}{\mu_f} \phi^{-3.8}.
\]  

(6.21)

In general, the drag force must be expressed in terms of relative velocities in multiple dimensions, and so equation (6.21) in terms of the drag coefficient becomes

\[
f_d = \frac{\pi d_p^3}{6} C_D \left( \frac{3 \rho_f (u_f - u_p) |u_f - u_p|}{4d_p} \right) \phi^{-1.8}.
\]  

(6.22)

In the following section, we discuss the criterion for the transition from the homogeneous fluidization state to the bubbling state. This criterion provides an allowable range of inlet velocities which will yield a uniform bed distribution.

**Stability Criterion for Fluidized Beds**

The stability criterion is used to establish the homogeneous, transition, and the heterogeneous states in a fluidized bed based on the particle density and diameter. When a fluid flux, \( U \), is applied to a bed which is initially fixed at a void fraction, \( \epsilon_1 \), and the minimum fluidization velocity is only slightly surpassed, the bed first propagates upwards in a piston-like manner. Two interfaces are then established at the top and bottom of the bed. If the top interface is subjected to a small perturbation which displaces a particle into the clear fluid region above, the particle experiences a reduced drag force. This results in a net downward force which returns the particle back to its position. This implies that the top interface is stable, a phenomenon which is also observed experimentally. If the bottom interface is subjected to a small disturbance, the displaced particle also experiences a net downward force. This time the particle is driven further downward and adjacent particles follow as a result of the increase in void fraction in the region abdicated by the original particle. The particles above will fall continuously in this manner causing the particle piston to break down. The bottom interface is thus unstable. The falling particles are stopped at the bottom by
the distributor causing a growing zone of stationary particles at the bottom of the bed. As the particles are falling down from the particle piston, they form a new zone where the void fraction becomes $\epsilon_2$ while the particles above are traveling upwards at $\epsilon_1$. Hence a traveling interface between the $\epsilon_1$ and $\epsilon_2$ zones is created. This interface travels faster than the top surface of the bed. When this interface catches up with the top surface, the rearrangement process is complete. The velocity of this interface is given by $dL/dt$ where $L$ is the distance from the bottom of the bed to the interface. By performing a mass balance on the two zones, one obtains a relationship between the interface velocity and the inlet fluxes,

\[
\frac{dL}{dt} = (1 - \phi_1) \frac{U_2 - U_1}{\phi_2 - \phi_1},
\]  

where $U_1$ is the initial inlet flux, and $U_2$ is the new inlet flux. Equation (6.23) describes the propagation of a finite discontinuity, or shock, separating the two equilibrium states. The formulation of equation (6.23) is based strictly on mass balances and hence assumes that the particles immediately switch from one equilibrium zone to the other one as the shock wave passes over them. No inertial effects are accounted for as the particles would have to slow down before reaching the new equilibrium state. For this condition to hold, the inertial response time for the particles must be negligibly small.

The kinematic wave velocity, $u_K$, is the limiting value of $dL/dt$ as the amplitude of the imposed fluid flux change $\Delta U = U_2 - U_1$ goes to zero. Hence, we have

\[
u_K = (1 - \phi) \frac{dU}{dt}.
\]  

The solids flux has been related to the terminal velocity and void fraction by Lewis et al.\cite{53}

\[
U = u_t \phi^n,
\]  

where $n$ is determined from equation (6.18). Substituting equation (6.25) into (6.24) gives

\[
u_K = nu_t(1 - \phi)\phi^{n-1}.
\]
The dynamic wave speed, $u_D$, is a measure of the speed at which inertial effects propagate through the system. When a piston in a cylinder moves forward, it exerts a force on the gas immediately ahead and induces a pressure wave which travels at sonic speed $u_D$. Under adiabatic conditions,

$$u_D = \sqrt{\frac{\partial p}{\partial \rho_f}} \quad (6.27)$$

The particle phase in a homogeneously fluidized bed can be thought of as a compressible gas with the distributor being analogous to the piston. An idealized experiment is devised in which the particles are assumed to be arranged in perfectly horizontal layers. The distributor is displaced upwards and the particles in the immediate vicinity are similarly displaced and come in contact with the above adjacent layer. The decrease in local void fraction results in a net force on this adjacent layer causing it to accelerate upwards restoring local equilibrium below it, but exerting a net force on the layer immediately above. This occurs throughout the bed inducing a propagating compression wave analogous to the compressible fluid case. The pressure impulse is $\delta p \equiv \delta(N_Lf)$, where $N_L$ is the number of particles in a layer of unit area and $f$ is the net force experienced by each of the particles as a result of the local void fraction change brought about by the displacement of the distributor. A formula similar to equation (6.34) is applied to determine $u_D$ for the wave traveling through the fluidized bed. Instead of $\rho_f$, we use $\rho_{pp} = (1 - \phi)\rho_p$. This is the ’compressible density’ for which the differential form is given by

$$\delta \rho_{pp} \equiv \delta[(1 - \phi)\rho_p]. \quad (6.28)$$

Hence, $u_D$ for the solid phase is given by

$$u_D = \sqrt{\frac{\delta p}{\delta \rho_{pp}}} = \sqrt{\frac{\delta(N_Lf)}{\delta((1 - \phi)\rho_p)}}. \quad (6.29)$$

The concentration wave can be assumed to be the consequence of an imposed perturbation in void fraction, and so equation (6.29) may be expressed by

$$\sqrt{\frac{\partial(N_Lf)/\partial \phi}{\partial(1 - \phi)\rho_p/\partial \phi}} = \sqrt{-\frac{1}{\rho_p} \frac{\partial(N_Lf)}{\partial \phi}}. \quad (6.30)$$
$N_L$ is estimated assuming that the void fraction on the horizontal planes that bisect the particle layers is representative of the average void fraction in the bed

$$N_L = 4(1 - \phi)/\pi d_p^2. \quad (6.31)$$

The net primary force acting on a fluidized particle in equilibrium is the sum of the drag and effective weight. Hence, from equations (6.14), (6.22), (6.25), and (6.30) we get

$$\frac{\partial (N_L f)}{\partial \phi} = N_L \pi d_p^3/6 (\rho_p - \rho_f) g \left[-3.8 \left(\frac{U}{u_t}\right)^{4.8} \phi^{-4.8} - 1\right] + f \frac{\partial N_L}{\partial \phi}. \quad (6.32)$$

Evaluating the above equation for a void fraction perturbation about the equilibrium condition ($f=0, U = u_t \phi^n$), with $N_L$ given by equation (6.31) and substituting in equation (6.30) gives

$$u_D = \sqrt{3.2gd_p(1 - \phi)(\rho_p - \rho_f)/\rho_p}. \quad (6.33)$$

Using equations (6.26) and (6.33) we arrive at the stability criterion. If $u_D - u_K > 0$, the system is homogeneous; if $u_D - u_K = 0$, the system has reached the stability limit; and if $u_D - u_K < 0$ the system is bubbling.

**Heat Transfer Mechanisms in a Fluidized Bed**

The main heat transfer mechanisms in a microwave-heated fluidized bed are the heat generated by microwaves within the solid particles, the gas flow around the pellets transporting heat from the bottom to the top of the bed, and solids mixing. It is very difficult to separate the latter two heat transfer mechanisms due to the nature of the fluidization problem, hence they are both accounted for in the convective heat transfer coefficient between the gas and solids. There is considerable controversy among the fluidization researchers as to the correct way to determine the heat transfer coefficient. Some researchers think that the thermal conductivity is not an important contribution to the Nusselt number while others think that accounting for the thermal conductivity is the correct way to determine the Nusselt number and that the Nusselt number
should be above 2. None of the points of view on this matter can be disregarded due to the complexity of the problem.

For Reynolds number which is less than 100, Kothari [54] found that the Nusselt number is a function of only the Reynolds number

\[ \text{Nu}_{\text{bed}} = 0.03 R_{p}^{1.3}, \] (6.34)

where \( R_{p} \) is given by

\[ R_{p} = \frac{d_{p} u \rho_{g}}{\mu}. \] (6.35)

The applicability of equation (6.34) has not been proven for particle diameters less than 230µm. However, due to the lack of available data, it is recommended that the above correlation be applied for such particles. It also fails in instances where the solid concentration is too low. In the situation for which the solid concentration is too low and \( 100 \leq R_{p} \), the Ranz correlation is recommended

\[ \text{Nu} = 2 + (0.6 \rightarrow 1.8) R_{p}^{0.5} Pr^{0.33}, \] (6.36)

where 0.6 \( \rightarrow \) 1.8 means that the constant coefficient ranges from 0.6 to 1.8 which are the single sphere and the packed bed limits, respectively. The difference between equations (6.34) and (6.36) are very drastic for Reynolds numbers below 100. Kunii and Levenspiel [49] claim that this is due to formation of clouded bubbles which greatly reduce the contact between the solid and the gas. Gunn [55] derived an expression for gas-solid systems in which the voidage varies between 0.35 and 1:

\[ \text{Nu} = (7 - 10 \phi + 5 \phi^{2})(1 + 0.7 R_{p}^{0.2} Pr^{0.33}) + (1.33 - 2.4 \phi + 1.2 \phi^{2}) R_{p}^{0.7} Pr^{0.33}. \] (6.37)

This correlation predicts results which are similar to the Ranz formula, but has the disadvantage of requiring the knowledge of the overall voidage as function of gas velocity.

Walton et. al [56] found that for coal particles whose size ranges from 0.3 to 0.8mm and for Reynolds numbers ranging from 6 to 50, the Nusselt number is given
by

\[ Nu = 0.0028 Re_p^{1.7} \left( \frac{d_p}{D} \right), \]  

(6.38)

where D is the hydraulic bed diameter. For particle sizes ranging from 0.83 to 8.9mm and for Reynolds numbers ranging from 30 to 120, Siriomiatnikov et al [57] derived the relation

\[ Nu = 0.0097 Re_p F e^{0.53} \left( \frac{L_{fb}}{d_p} \right)^{-0.45}, \]  

(6.39)

and for Reynolds numbers ranging from 120 to 2500 the relation

\[ Nu = 0.015 Re_p^{0.805} F e^{0.53} \left( \frac{L_{fb}}{d_p} \right)^{-0.45}, \]  

(6.40)

where Fe is the Federov number and is given by

\[ Fe = 1.1 A_r^{0.33}. \]  

(6.41)

A more sophisticated model has been developed by Kunii and Levenspiel for fine-particle bubbling beds from mass transfer considerations. The heat transfer coefficient, \( h_{bc} \), at the bubble-cloud interface is given by

\[ h_{bc} = 0.975 \rho_g C_{pg} \left( \frac{k_g}{\rho_g C_{pg}} \right)^{0.5} \left( \frac{g}{d_b} \right)^{0.25}. \]  

(6.42)

Based on a unit volume of bubble phase, the overall heat transfer coefficient across the bubble-cloud boundary is

\[ H_{bc} = \frac{v C_{pg} + h_{bc} S_{bc}}{V_b} = 4.5 \left( \frac{u_{mf} \rho_g C_{pg}}{d_b} \right) + 5.85 \left( \frac{k_g \rho_g C_{pg}}{d_b^{1.25}} \right)^{0.5} g^{0.25}, \]  

(6.43)

where \( v \) is the volumetric flow of gas from bubble to cloud, and \( S_{bc} \) is the surface area of the bubble cloud. Since \( H_{bc} \) does not account for the heat transfer from the particles within the bubble to the bed of solids, the overall convective heat transfer coefficient is given by

\[ H_{tot} = \gamma_b \frac{6 Nu k_g}{\Phi_s d_p^2} \eta_b + H_{bc}, \]  

(6.44)
where $\gamma_b$ is the volume of solid dispersed within the bubble. From the definition of the heat transfer coefficient

$$\delta H_{tot} = \frac{6}{\Phi_s d_p} (1 - \epsilon) h_{bed}$$

(6.45)

we get the bed Nusselt number by substituting equation (6.43) and (6.44) into equation (6.45)

$$Nu_{bed} = \frac{h_{bed} d_p}{k_g} = \frac{\delta}{1 - \phi} \left[ \gamma_b N u_{h} + \Phi_s d_p^2 \frac{H_{bc}}{6 k_g} \right],$$

(6.46)

where $\delta$ is the bubble fraction in a fluidized bed and is given by

$$\delta = \left( \frac{1 - \phi}{1 - \phi_{mf}} \right) \left( \frac{u_0 - u_{mf}}{u_{br}} \right),$$

(6.47)

where $u_{br}$ is the velocity at which the bubble rises. The heat transfer adsorption efficiency, $\eta_h$ is given by

$$\eta_h = \frac{1}{1 + \alpha \frac{p_s C_p}{p_s C_p}}.$$  

(6.48)

For fine particles, $\alpha \approx 20-1000$, and so $\eta_h \approx 0.98-0.91$. The problem with the above formulation is that it relies on many intermediate relationships that may yield incorrect results. Knowledge of the spacing between grid holes, the bubble size and rise velocity are required to implement this correlation.

**Thermo-Fluid Model of the Fluidized Bed**

Fluidized beds are categorized as multiphase flow problems. As mentioned in chapter two, there are currently five approaches to model multiphase flow problems. The best overall balance between computational time and accuracy seems to be achieved by implementing the volume-averaging or Eulerian-Granular approach. Assumptions 1, 6, and 8 of the packed bed model hold for the fluidized bed as well. In addition we assume

1) temperature dependence of the fluid properties is neglected,
2) the bed is 2-d and rectangular,
3) the velocity and volume fraction profile is assumed to be the time-averaged values over a specified time interval,
4) only homogeneous fluidization is considered,
5) only the expanded bed region is considered in the analysis, i.e., the outflowing gas is not analyzed,
6) compressibility and viscous heating effects are neglected, and
7) the electric field can vary linearly in the flow direction.

The fluid mechanics portion of the analysis was performed with FLUENT 6.1 [9]. FLUENT is a commercial CFD software package which provides capabilities for solving multiphase fluid flow problems. The multiphase fluid flow problem is very complicated and involved and would be difficult to solve otherwise. FLUENT simplifies this by merely requiring the user to provide the solid and fluid properties as well as the boundary conditions. The boundary conditions for the fluidized bed considered in this work are as follows: 1) the gas and solid velocities as well as the void fraction are specified at the bed inlet. The solid velocities are set to zero and the void fraction is 1. The inlet gas velocity is also specified; 2) The no-slip condition was implemented at the walls for both phases; 3) The pressure is specified at the bed outlet. For all cases, atmospheric pressure was assumed.

The detailed equations which are solved by FLUENT will not be discussed here. For details, see reference [58]. To solve the multiphase Navier-Stokes equations, the viscosity and pressure for the solid phase must be quantified. This is accomplished in FLUENT by implementing a kinetic theory approach in which the solid particles are treated as gas molecules and the granular temperature of the solid phase is computed. The granular temperature is a measure of the solid phase chaos within the bed and the solids pressure and viscosity are functions of this quantity. The granular temperature equation is a differential equation which is derived from the Boltzmann equation. FLUENT requires the user to specify the granular temperature at the inlet. FLUENT’s default value for the granular temperature at the inlet is $10^{-4}$ and is retained for all cases.

The system of equations and constitutive relations required to ultimately solve
the multiphase fluid flow problem is computationally intensive. It could easily take several weeks to fully analyze one case. The reason that this occurs is because the fluidized bed requires a transient analysis with time steps no greater than $10^{-3}$. In some cases [7], time steps as small as $10^{-4}$ or even $10^{-5}$ are necessary. For this reason, an approximation must be made in order to decrease the computational time. In several discussions with the fluidization group in the chemical engineering department at The Illinois Institute of Technology (IIT), it is known that fluidized beds reach an oscillating “steady state” after approximately 10-15 seconds. The group at IIT has done extensive research in fluidization technology since the early 60’s. Today, most of the research in this area is carried out by students under the guidance of professors Dimitri Gidaspow and Hamid Arastoopour. Professors Gidaspow and Arastoopour have authored many articles in the area of fluidization. To get a list of many of their publications, see reference [7].

Hence, all relevant quantities such as solid and gas velocities and void fractions are time-averaged over a specific time interval. The time intervals for specific cases are discussed in the next chapter. The resulting time-averaged quantities are then implemented in a thermal model. The required computational effort is greatly reduced because the heat transfer analysis must be performed on minute time scales whereas the fluid mechanics codes are designed for second time scales.

A FORTRAN code was developed for the purpose of computing the temperature distribution in the bed. The time-averaged values from the fluid mechanics analysis were used as inputs for the heat transfer code. The equations governing the temperature distribution in the bed are given by

$$\phi_s \rho_s C_{ps} \frac{\partial T_s}{\partial t} + C_{ps} \frac{\partial}{\partial x}(\phi_s \rho_s u_s T_s) + C_{ps} \frac{\partial}{\partial y}(\phi_s \rho_s v_s T_s)$$

$$= \frac{\partial}{\partial x} \left( \phi_s k_s \frac{\partial T_s}{\partial x} \right) + \frac{\partial}{\partial y} \left( \phi_s k_s \frac{\partial T_s}{\partial y} \right) + h_v(T_f - T_s) + \phi_s \dot{q}, \quad (6.49)$$

and

$$\phi_f \rho_f C_{pf} \frac{\partial T_f}{\partial t} + C_{pf} \frac{\partial}{\partial x}(\phi_f \rho_f u_f T_f) + C_{pf} \frac{\partial}{\partial y}(\phi_f \rho_f v_f T_f)$$

$$= \frac{\partial}{\partial x} \left( \phi_f k_f \frac{\partial T_f}{\partial x} \right) + \frac{\partial}{\partial y} \left( \phi_f k_f \frac{\partial T_f}{\partial y} \right) + h_v(T_s - T_f), \quad (6.50)$$
where \( T_s \) is the solid temperature, \( T_f \) is the gas temperature, and \( h_v \) is the volumetric heat transfer coefficient which is obtained from equation (6.34). The boundary conditions for the solid phase are

\[
-\phi_s k_s \frac{\partial T_s}{\partial x} \bigg|_0 = U(T_s - T_{\infty})|_0, \quad -\phi_s k_s \frac{\partial T_s}{\partial x} \bigg|_L = U(T_s - T_{\infty})|_L, \tag{6.51}
\]

and

\[
\frac{\partial T_s}{\partial y} \bigg|_0 = \frac{\partial T_s}{\partial y} \bigg|_H = 0, \tag{6.52}
\]

where \( L \) is the length of the bed, \( H \) is the bed height, \( U \) is given by equation (4.30), and \( R_t \) is given by,

\[
R_{tot} = \frac{L}{k_g A} + \frac{1}{h A}, \tag{6.53}
\]

where \( h \) is defined by equation (4.32). For the gas phase,

\[
-\phi_f k_f \frac{\partial T_f}{\partial x} \bigg|_0 = U(T_f - T_{\infty})|_0, \quad -\phi_f k_f \frac{\partial T_f}{\partial x} \bigg|_L = U(T_f - T_{\infty})|_L, \tag{6.54}
\]

\[
T_f(0) = T_{in}, \tag{6.55}
\]

and

\[
\frac{\partial T_f}{\partial y} \bigg|_H = 0. \tag{6.56}
\]

The solution procedure for the energy equations is similar to that described in chapter 4. The approach is described in chapter 5 of [48]. A brief outline is given for the solid phase. The gas phase is similar. Equation (6.49) can be rewritten in the form

\[
\rho_s \phi_s \frac{\partial T_s}{\partial t} + \frac{\partial J_{sx}}{\partial x} + \frac{\partial J_{sy}}{\partial y} - \frac{h_v}{C_p s} (T_f - T_s) = S_s, \tag{6.57}
\]

where,

\[
J_{sx} = \phi_s \rho_s u_s T_s - \Gamma_s \frac{\partial T_s}{\partial x}, \tag{6.58}
\]
\[ J_{sy} = \phi_s \rho_s v_s T_s - \Gamma_s \frac{\partial T_s}{\partial y} , \]  
\[ (6.59) \]

\[ \Gamma_s = \frac{\phi_s k_s}{C_p} , \]  
\[ (6.60) \]

\[ S_s = \frac{\phi_s}{C_p} \dot{q}_s . \]  
\[ (6.61) \]

Let \( \vec{F} = \phi_s \rho_s \vec{V}_s \), \( D_s = \rho \phi_s / \delta x \), and \( \vec{P} = \vec{F} / D_s \), where \( \vec{V} \) is the velocity vector. The discretized forms of these, with e, w, n, and s notation as in chapter 4, become

\[ F_{se} = (\rho_s \phi_s u_s)_e \Delta y, \quad D_{se} = \frac{\Gamma_e \Delta y}{\Delta x}, \quad P_{se} = \frac{F_{se}}{D_{se}} , \]  
\[ (6.62) \]

\[ F_{sw} = (\rho_s \phi_s u_s)_e \Delta y, \quad D_{sw} = \frac{\Gamma_w \Delta y}{\Delta x}, \quad P_{sw} = \frac{F_{sw}}{D_{sw}} , \]  
\[ (6.63) \]

\[ F_{sn} = (\rho_s \phi_s v_s)_e \Delta x, \quad D_{sn} = \frac{\Gamma_n \Delta x}{\Delta y}, \quad P_{sn} = \frac{F_{sn}}{D_{sn}} , \]  
\[ (6.64) \]

\[ F_{ss} = (\rho_s \phi_s v_s)_e \Delta x, \quad D_{ss} = \frac{\Gamma_s \Delta x}{\Delta y}, \quad P_{ss} = \frac{F_{ss}}{D_{ss}} . \]  
\[ (6.65) \]

The discretized form of equation (6.49) is

\[ a_{Ps} T^1_{Ps} - a_{Es} T^1_{Es} - a_{Ws} T^1_{Ws} - a_{Ns} T^1_{Ns} - a_{Ss} T^1_{Ss} - a_{Pf} T^1_{Pf} = b, \]  
\[ (6.66) \]

where

\[ a_{Es} = D_{se} A(|P_{se}|) + \max[-F_{se}, 0] , \]  
\[ (6.67) \]

\[ a_{Ws} = D_{sw} A(|P_{sw}|) + \max[-F_{sw}, 0] , \]  
\[ (6.68) \]

\[ a_{Ns} = D_{sn} A(|P_{sn}|) + \max[-F_{sn}, 0] , \]  
\[ (6.69) \]

\[ a_{Ss} = D_{ss} A(|P_{ss}|) + \max[-F_{ss}, 0] , \]  
\[ (6.70) \]
\[ a_{Pf} = \frac{h_{Pv}}{C_P p_s} \Delta x \Delta y, \quad (6.71) \]

\[ a_{Ps}^0 = \frac{\rho_s \phi_{Ps}}{\Delta t} \Delta x \Delta y, \quad (6.72) \]

\[ a_{Ps} = a_{Es} + a_{Ws} + a_{Ns} + a_{Ss} + a_{Pf} + a_{Ps}^0, \text{ and} \quad (6.73) \]

\[ b = \frac{\phi_{Ps}}{C_P p_s} q_{Ps}^0 \Delta x \Delta y + a_{Ps}^0 T_p^0, \quad (6.74) \]

where \( A(|P_{sc}|), A(|P_{sw}|), A(|P_{sn}|), \) and \( A(|P_{ss}|) \) are determined by the numerical scheme to be implemented. The possible choices in [48] are the central difference, upwind, hybrid, and power law schemes. The upwind scheme was chosen in all analyses. For more details on these schemes, see [48].
Chapter 7

Results for the Fluidized Bed

In this study, air flow through a fluidized bed consisting of gamma alumina particles heated by microwaves is examined. The effects of the particle diameter and inlet velocity on the bed temperature and the temperature difference between the phases are analyzed. These effects are observed for particle diameters of 100, 125, and 150 \( \mu \text{m} \). The nominal minimum fluidization velocities of these particles as predicted by equation (6.1) are 33, 51, and 73 mm/s respectively. The simulations were performed at 6 times the nominal minimum fluidization velocity for each particle diameter and at 4 times the nominal minimum fluidization velocity for the 150 micron particles. The hypothetical container has a length of 40 cm and a height of 60 cm as shown in figure 2 of chapter 1. Initially, the container is filled to 1/4 of its height with solid particles. For the hydrodynamic portion of the computation, the bed was subdivided into a 50 by 50 grid with a time step of \( 5 \times 10^{-4} \) seconds. The grid size and time step were determined by the parameter \( F = \Delta t/(\Delta x)^2 \) [59]. The value for \( F \) was chosen comparable with those in reference [7]. Typical values for \( F \) in reference [7] were about 2.5, and the value of \( F \) for the current grid is 7.8. Also, the y-direction is chosen as the flow direction. As mentioned in the previous chapter, the hydrodynamic analysis is decoupled from the thermal analysis. This allows the flexibility of choosing a different time step for the thermal analysis. Also, the x and y components of velocity for both phases as well as the solid volume fraction were time-averaged over an interval of 90-100 seconds for the 6 times minimum fluidization cases and 120-130 seconds for
the 4 times minimum fluidization case. The expanded bed height ranged from 21.6 to 26.4 cm after the application of the time-averaging for all cases. This resulted in a grid which ranged from 50 cells in the x-direction by 18 to 21 cells in the y-direction for the thermal analysis. A time step of 10 seconds was chosen for the thermal analysis after a comparison of the results between a 10 and 0.1 seconds time step yielded a 1.2 percent error for the 150 micron particles at 6 times nominal minimum fluidization. The air enters the bed at 300.15 K. In the following figures, the standard 2-dimensional, right-hand coordinate system is assumed, i.e., +x points towards the right of the page and +y points up and is the flow direction. The color scale in the contour plots does not vary with time, but the magnitude associated with this scale varies with time.

Figures 7.1-7.3 display the time evolution of the solid x and y-components of velocity for the 100 micron particles at 6 times the nominal minimum fluidization velocity at 10 second intervals. It can be seen that the flow achieves a steady pattern after 40 seconds.

Figures 7.3-7.6 display similar behaviour for 150 micron particles at 6 times nominal minimum fluidization. For this case, it can be seen that a steady pattern is achieved after 50 seconds. The solid particles appear to fall in the center and next to the walls of the bed in both cases. The solids appear to rise in the region right next to the center and next to the falling region near the walls. The 150 micron particles rise closer to the wall than do the 100 micron particles. It can be seen from the figures that the velocity profiles are slightly asymmetrical even though the boundary conditions are identical at the walls and the initial condition is a uniform packed bed. It is believed by FLUENT’s [9] multiphase flow staff that this could be caused by perturbations in the void fraction which occur after the third or fourth significant figure. These perturbations induce asymmetries in the void fraction which in turn induce asymmetries in the drag force because the drag force is inversely proportional to the cube of the void fraction. Such anomalies have also been encountered by previous authors [52, 60-62]. While it is believed [9] that the asymmetries represent actual physical phenomena, the reasons for such asymmetries
have not been determined and are still under investigation.

Figures 7.7-7.10 display the time-averaged distributions of the x and y-components of velocity for the gas and solid phase as well as the solid volume fraction for the four cases mentioned above. These figures reveal that the y-component of velocity is dominant throughout and that the solid volume fraction is constant throughout most of the bed. An interesting observation is that for the 100 micron particles the solids flow in the same direction relative to the gas while the solids flow in the opposite direction relative to the gas towards the center of the bed in the remaining cases. Also, it can be seen that the y-component of velocity is nearly symmetrical while the x-component is asymmetrical in the current cases.

Figures 7.11-7.14 display the time evolution of the x and y-components of solid velocity as well as the solid volume fraction over the time-averaging interval for a point located in the middle of the bed for each case. The time evolution was plotted for nine points in the bed for each case, but due to the similarity of the plots it is sufficient to display the plots for the point located at the center of the bed. It can be seen that that the quantities in question show very small fluctuations and hence time-averaging is a reasonable approximation.

Figures 7.15-7.22 display the time evolution of the temperature, the steady-state temperature profiles, and the temperature difference between the gas and solid phases for the cases mentioned above. Just as for the packed bed, the points for the horizontal profiles are located at half of the bed height and the points for the vertical profiles are located halfway between the center and the wall of the bed. As expected, the temperature increases with time along the horizontal and vertical directions. The steady-state profiles reveal that the temperature increases towards the center of the bed near the inlet and towards the right away from the inlet for the 100 micron particles and decreases towards the center near the inlet for the remaining cases at 6 times the nominal minimum fluidization velocity. The variation in temperature in the x-direction is more pronounced at the inlet than away from the inlet. This behaviour near the inlet could be due to a combination of the fact that the solid is heated at the inlet while the gas maintains a constant temperature there and the
y-component of velocity of the solid phase having the same direction as the gas phase throughout the bed. This does not allow the gas to remove as much energy from the solid as would be possible if the solids were either stationary or moving in the opposite direction because of the lower relative velocity between the gas and solid phases. The nonmonotonicity in the vertical direction, and the off-center maximum temperature in the x-direction can be attributed to the distribution of the x and y-velocity components of the gas and solid phases. At certain points in the bed, the x-component of velocity may be as much as 30 times smaller than its neighbors and hence less energy enters than exits a control volume surrounding such points. The y-component of velocity is nonmonotonic in the horizontal and vertical directions and hence more heat is removed in some regions than in others. The asymmetrical distribution of the x-component of velocity, shown in figure 7.9, could be a large contributing factor in the asymmetrical temperature profile in the 150 micron case at 4 times the nominal minimum fluidization velocity.

All computations discussed so far have been performed with a uniform electric field of 3 kV/m. In order to induce a greater temperature difference between the solid and gas throughout the bed, the rate of heat generation must be increased as the distance away from the inlet increases. One way to do this is to assume a nonuniform electric field in the y-direction. Hence, a computation was performed for the 150 micron particle case at 4 times the nominal minimum fluidization velocity where the electric field is assumed to vary linearly in the flow direction. The electric field is described by the equation \( E = ay + E_0 \), where \( E \) is the electric field, \( a \) is a constant whose value is taken to be \( 10^5 \text{V/m}^2 \), \( y \) is the location at which the electric field is determined, and \( E_0 \) is the electric field at the inlet, taken to be 2 kV/m. Figure 23 shows the steady-state temperature, and the temperature difference between the gas and solid phase. Qualitatively, the steady-state plots are similar to those in figure 20 with higher temperatures. Once again, the maximum temperature is off-center for both phases. The temperature difference between the gas and solid reach 300 K on the right boundary and is asymmetrical at the inlet.

In general, problems which involve flow reversal have many things occurring
simultaneously. The flow downstream is influenced by the flow upstream and vice versa. This makes it very difficult to explain the physics in these types of problems.
Figure 7.1: Time evolution of the solid volume fraction, and the x, and y-components of solid velocity for the 100 micron particles at 6 the times nominal minimum fluidization. Note that the scale is relative.
Figure 7.2: Time evolution of the solid volume fraction, and the x, and y-components of solid velocity for the 100 micron particles at 6 times the nominal minimum fluidization. Note that the scale is relative.
Figure 7.3: Time evolution of the solid volume fraction, and the x, and y-components of solid velocity for the 100 micron particles at 6 times nominal minimum fluidization. Note that the scale is relative.
Figure 7.4: Time evolution of the solid volume fraction, and the x, and y-components of solid velocity for the 150 micron particles at 6 times nominal minimum fluidization. Note that the scale is relative.
Figure 7.5: Time evolution of the solid volume fraction, and the x, and y-components of solid velocity for the 150 micron particles at 6 times nominal minimum fluidization. Note that the scale is relative.
Figure 7.6: Time evolution of the solid volume fraction, and the x, and y-components of solid velocity for the 150 micron particles at 6 times nominal minimum fluidization. Note that the scale is relative.
Figure 7.7: Time-averaged x and y-components of velocity as well as the solid volume fraction for 100 micron particles at 6 time minimum fluidization.
Figure 7.8: Time-averaged x and y-components of velocity as well as the solid volume fraction for 125 micron particles at 6 time minimum fluidization.
Figure 7.9: Time-averaged x and y-components of velocity as well as the solid volume fraction for 150 micron particles at 4 time minimum fluidization.
Figure 7.10: Time-averaged x and y-components of velocity as well as the solid volume fraction for 150 micron particles at 6 time minimum fluidization.
Figure 7.11: Time evolution of $x$ and $y$-components of velocity as well as the solid volume fraction for a node at the center of the bed over the 10 seconds time-averaging period for the 100 micron particles at 6 times the nominal minimum fluidization.
Figure 7.12: Time evolution of x and y-components of velocity as well as the solid volume fraction for a node at the center of the bed over the 10 seconds time-averaging period for the 125 micron particles at 6 times the nominal minimum fluidization.
Figure 7.13: Time evolution of x and y-components of velocity as well as the solid volume fraction for a node at the center of the bed over the 10 seconds time-averaging period for the 150 micron particles at 4 times the nominal minimum fluidization.
Figure 7.14: Time evolution of x and y-components of velocity as well as the solid volume fraction for a node at the center of the bed over the 10 seconds time-averaging period for the 150 micron particles at 6 times the nominal minimum fluidization.
Figure 7.15: Time evolution of the temperature for the 100 micron particles at 6 times minimum fluidization.
Figure 7.16: Steady-state temperature profiles for the 100 micron particles at 6 times minimum fluidization.
Figure 7.17: Time evolution of the temperature for the 125 micron particles at 6 times minimum fluidization.
Figure 7.18: Steady-state temperature profiles for the 125 micron particles at 6 times minimum fluidization.
Figure 7.19: Time evolution of the temperature for the 150 micron particles at 4 times minimum fluidization.
Figure 7.20: Steady-state temperature profiles for the 150 micron particles at 4 times minimum fluidization.
Figure 7.21: Time evolution of the temperature for the 150 micron particles at 6 times minimum fluidization.
Figure 7.22: Steady-state temperature profiles for the 150 micron particles at 6 times minimum fluidization.
Chapter 8

Conclusions and Future Work

8.1 Conclusions

From the preceding studies of the packed bed, we can conclude that the spatial temperature variations in the solid phase are negligible, i.e. the solids can be heated uniformly. This could be attributed to a combination of a uniform electric field along with the small conductive resistance induced by the size of the packed bed. Perhaps a lumped capacitance approach could be used to model the solid phase under these conditions. It is possible to produce a temperature difference of more than 5 degrees between the solid and the gas in about 15-25 percent of the packed bed. As expected, the electric field has greater influence on the temperature difference than the inlet gas velocity and particle diameter. An increase in particle diameter increases the temperature difference by a greater factor at nodes near the center than near the wall while an increase in the electric field increases the temperature difference by a greater factor at nodes near the wall than near the center. The inlet gas velocity effects the temperature difference at both nodes similarly. We also see that larger particles at higher inlet gas velocities and higher uniform electric fields produce the greatest temperature difference that penetrates the furthest into the packed bed. From the thermal perspective, a small packed bed is an efficient reactor.

From the preceding studies of the fluidized bed, we can conclude that homogeneous fluidization can be achieved for the particle diameters considered in this study
even though the stability criterion discussed in chapter 6 and the Geldart classification chart predict that bubbling should occur for such particles. In the current study we are dealing with a two-dimensional bed containing very low-density particles, but Geldart’s data was obtained using three-dimensional cylindrical fluidized beds and the stability criterion was derived assuming a one-dimensional idealized bed configuration. Equation (6.1) predicts the same minimum fluidization velocity for all beds, but it has been demonstrated experimentally by Saxena et. al [63] that the minimum fluidization velocity is higher in two-dimensional beds than in three-dimensional beds. This is qualitatively consistent with current results. The 150 micron particles at 4 times the nominal minimum fluidization velocity exhibit a behaviour which is typical of beds at minimum fluidization in which the bed expands and the solid particles are nearly stationary. The range of inlet velocities for which the bed maintains a homogeneous state is very narrow for gas-solid systems. When the inlet velocity is increased to 8 times the nominal minimum fluidization velocity, homogeneity breaks down.

The steady-state temperature profiles are asymmetric and nonmonotonic for the gas and solid phases due to the erratic distribution of velocity. It is very difficult to produce a temperature difference with similar penetrations in a fluidized bed under a uniform electric field because the heat transfer coefficient between solid and gaseous phases is very large. The temperature difference is fairly sizable at the inlet because the gas temperature is fixed while the solid is heated continuously. At the bed boundaries, the gas looses energy at faster rate than the solid because the gas has a much lower thermal capacitance than the solid hence inducing a temperature difference between the two phases. The temperature difference between the gas and solid is very small within the bed even with a non-uniform electric field. A non-uniform electric field in the flow direction cannot overcome the effects of the large heat transfer coefficient between the gas and solid and the much lower thermal capacitance of the gas relative to the solid. Also, to achieve a sizable temperature difference around the bed perimeter, the current bed must be heated to temperatures of about 1500 K. Hence, from the thermal point of view the packed bed is a more efficient reactor than
8.2 Future Work

Based on the conducted study, it is recommended that:

• A more detailed model of the electric field needs to be implemented. A simplified electric field model will not capture any potential “hot zones” that a model based on Maxwell’s equations can capture.

• A mass transfer model needs to be implemented to observe the temperature effects on the concentration gradients and vice versa. This will allow for observation of product yields in a particular reaction.

• A new correlation for the gas-solid heat transfer coefficient accounting for microwave heating needs to be determined. The current correlation was obtained under conventional heating conditions.

• Extend the current model to account for bubbling and to investigate three-dimensional fluidized beds. This can be achieved as computational capabilities are enhanced.

• Investigate the effects of the electric field on the hydrodynamics. The electric field may influence the motion of the solids because of attraction/repulsion forces which may develop between closely interacting particles.

• Nonthermal effects such as mixing (fluidized beds), contact area, and gas residence time need to be incorporated into the models for predicting the efficiency of reactions. Mixing is very difficult to incorporate into any model, but a possible indicator of the extent of mixing, such as the granular temperature, can be used to accomplish this.

• Ultimately, an optimization of the conditions which will yield the best reaction rates needs to be performed, i.e. the optimal particle diameter, electric field, and inlet gas velocity, should be determined.
• To develop a molecular dynamics or a quantum mechanical model of an individual catalyst particle to demonstrate selective heating.
Bibliography


[9] FLUENT Incorporated, 10 Cavendish Court, Centerra Park Lebanon, New Hampshire 03766.


Appendix A

Packed Bed Program

c This program will determine the temperature and velocity profiles and
the temperature difference between the solid and gas in a small
cylindrical packed bed.
c
The following is a definition of the input variables.
c
initer = number of inner iterations.
c ncr = number of cells in the radial direction.
c ncz = number of cells in the axial direction.
c nnf = total number of nodes for a single phase.
c nnt = total number of nodes for both phases.
c nn2 = total number of nodes in the computation including the fluids.
c ntime = number of time steps.
c job = parameter set to zero to solve Ax = b in the matrix solver.
c kg = conductivity of glass (W/m\cdot K).
c hn = heat transfer coefficient between container and surroundings
   (W/m^2\cdot K).
c rb = radius of the bed (m).
c ro = radius of the bed plus that of the container (m).
c rc = radius of the waveguide (m).
area = cross-sectional area of the bed (m).

h = height of the bed (m).

dr = length of a control volume in the computational grid (m).

dz = height of a control volume in the computational grid (m).

dt = time step (s).

epsi = volume fraction of the bed at the center.

dpt = particle diameter of the metallic catalyst particle (m).

pf = volume fraction of metallic catalyst particle in the ceramic support.

rhoal = density of alumina (kg/m^3).

rhopt = density of platinum (kg/m^3).

vin = inlet gas velocity (m/s).

vflow = inlet volume flow rate of the gas (m^3/s).

dp = particle diameter (m).

rhos = density of the ceramic support/metallic catalyst mixture (kg/m^3).

tmpin = inlet gas temperature (K).

frequ = microwave frequency (Hz).

eps0 = permittivity of free space (f/m).

mu0 = permeability of free space (h/m).

c0 = speed of light (m/s).

ef0 = electric field within the bed (V/m).

dpdz = pressure drop across the bed (N/m^3).

tol = tolerance in the mass flow iterations.

tol1 = tolerance in velocity iterations.

bc = constant for bessel function J0.

flag = determines whether the support will be alpha or gamma-alumina:

    if set to 1, then alpha alumina is used; otherwise gamma alumina is used.

flag1 = controls electric field: if set to 1, the electric field is
uniform; if set to 2, the electric field varies linearly in the flow direction; otherwise, the electric field is described by a radial bessel function.

flag2 = determines the inlet boundary condition for the solid phase: if set to 1, the solid is insulated; otherwise the solid is set to the inlet temperature of the gas.

use msimsl
implicit real*8(a-h,o-y)
real*8 kg,mu0,z
integer ncr,ncz,nnf,nnt,ntime,flag,flag2,flag1,nn,lda,ipvt,nout
integer job,flag3
c
parameter(initer=4)
parameter(ncr=30)
parameter(ncz=20)
parameter(nnf=2*(ncz+ncr)+ncr*ncz)
parameter(nnt=2*nnf)
parameter(nn2=nnt+ncr+2)
parameter(nn=nn2)
parameter(lda=nn)
c
dimension tprev(nnt),z(nn),ipvt(nn),temp(nnt),a(lda,nn),rhs(nn2)
dimension taves(ncz),efelds(ncz),efs(nnf),tavesf(ncr)
dimension vguess(ncr+1)
c
common/param/flag,flag2,flag3
common/dielectric/pi,frequ,eps0,c0,mu0,ef0
common/solgas/rhos,dp,pf,dpt,vf,tmpin,kg,epsi,rb,ro,hn
common/delta/h,dt,dr,dz
open(1, file='\pabed\radiuspb')
open(2, file='\pabed\heightpb')
open(3, file='\pabed\timepb')
open(4, file='\pabed\tfrpb500')
open(5, file='\pabed\tsrpb500')
open(6, file='\pabed\tfzpb500')
open(7, file='\pabed\tszpb500')
open(8, file='\pabed\velpb500')
open(9, file='\pabed\tfbedss500')
open(10, file='\pabed\tsbedss500')
open(11, file='\pabed\tdiff500')

c
    ntime=21
    pi=dacos(-1.d0)
    job=0
    kg=1.4d0
    hn=2.d0
    rb=1.d-2
    ro=1.1d-2
    rc=6.d-1
    area=pi*rb**2/2.d0
    h=2.5d-2
    dr=rb/dble(ncr)
    dz=h/dble(ncz)
    dt=1.d2
    epsi=4.d-1
    dpt=4.d-8
    pf=.01d0
    rhoal=700.d0
    rhopt=21450.d0
    vin=1.d-1
    vflow=vin*area
dp=5.d-4

vf=(pf/rhopt)/((pf/rhopt)+(1.d0-pf)/rhoal)

rhos=pf*rhopt+(1.d0-pf)*rhoal

tmpin=300.15d0

frequ=.915d9

eps0=8.854d-12

mu0=4.d-7*pi

c0=3.d8

ef0=5.d3

flag=2

flag1=1

flag2=1

c flag3=2

efelds(ncz)=ef0

dpdz=-1.5d2

tol=1.d-6

tol1=1.d-4

bc=2.4049d0

c
do i=1,nnt

    tprev(i)=tmpin

    temp(i)=tmpin

    rhs(i)=0.d0

enddo

c
do i=1,ncr+1

    rhs(nnt+i)=vin

    vguess(i)=vin

    if(i .lt. ncr+1) then
        tavesf(i)=tmpin
    endif

endo
do i2=1,ntime
  k=nnf+ncz+2
  l=nnt-2*ncz
  do i=1,ncz
    sum=0.d0
    do j=k,l,ncz+2
      sum=sum+temp(j)
    enddo
    taves(i)=sum/dble(ncr)
    k=k+1
    l=l+1
  enddo
if(flag1 .eq. 1) then
  call efields(taves,efelds,eppm,ncz)
  write(*,*) eppm
  do i=1,nnf-2*(ncz+ncr)
    efs(i)=ef0
  enddo
elseif(flag1 .eq. 2) then
  call efields(taves,efelds,eppm,ncz)
  k=ncz+2
  l=nnf-2*ncz
  do i=1,ncz
    do j=k,l,ncz+2
      efs(j)=efelds(i)
    enddo
  enddo
  k=k+1
  l=l+1
else
k = ncz + 2
l = k + ncz - 1
p = 1.d0

do i = 1, ncr
    r = p * dr
    do j = k, l
        efs(j) = ef0 * dsj0(bc * r / rc)
        call umach(2, nout)
    enddo
    k = k + ncz + 2
    l = l + ncz + 2
    p = p + 1.d0
enddo
endif

do k = 1, nnt
    temp(k) = tprev(k)
enddo

5 do j2 = 1, initer
    call assemble(tprev, a, rhs, temp, efs, eppm, lda, nn, ncr,  
    ncz, nnf, nnt, nn2, vguess, tavesf, dpdz)
    if((i2.eq.1) .and. (j2.eq.1)) then
        do j3 = 1, lda
            do j4 = 1, nn
                write(1, *) j3, j4, a(j3, j4), rhs(j3)
            enddo
        enddo
    endif
    call dgeco(a, lda, nn, ipvt, rcond, z)
    write(*, *) 'the condition # is', 1.d0 / rcond, i2
call dgesl(a,lda,nn,ipvt,rhs,job)
c     if ((i2.eq.ntime) .and. (j2.eq.3)) then
c          do j3=1,nnt
          write(*,*) j3, rhs(j3)
          enddo
c     endif
c
do l=1,nnt
   temp(l)=rhs(l)
endo
do i3=1,lda
   do j3=1,nn
      a(i3,j3)=0.d0
   enddo
endo
do l=1,nnt
   temp(l)=rhs(l)
endo
c
   k=ncz+2
   l=2*ncz+1
do i=1,ncr
   sum=0.d0
   do j=k,l
      sum=sum+temp(j)
   enddo
tavesf(i)=sum/dble(ncz)
k=k+ncz+2
l=l+ncz+2
endo
c
   p=0.d0
   rhs1=0.d0
   do j2=nnt+2,nnt+ncr+1
rhs1=rhs1+\pi*((p+1.d0)**2-p**2)*dr**2*rhs(j2)/2.d0
p=p+1.d0
enddo
c write(*,*) rhs1, vflow
c
if((dabs(vflow-rhs1).gt.tol).and.((vflow-rhs1).gt.0.d0))then
dpdz=dpdz+dpdz/2.d0
goto 5
elseif((dabs(vflow-rhs1).gt.tol).and.((vflow-rhs1).lt.0.d0))then
dpdz=dpdz-dpdz/2.d0
goto 5
endif
c
tdiff=0.d0
do j2=1,ncr+1
if(dabs(rhs(nnt+j2)-vguess(j2)) .gt. vdiff) then
  vdiff=dabs(rhs(nnt+j2)-vguess(j2))
endif
dendo
if(vdiff .gt. tol1) then
do j2=1,ncr+1
  vguess(j2)=rhs(nnt+j2)
dendo
goto 5
endif
c
c if(mod(i2,10) .eq. 1) then
  write(4,11) rhs(int(ncz/2)),(rhs(l),l=int(ncz/2)+ncz+1,(ncr-1)*
1 (ncz+2)+int(ncz/2)+ncz+1,ncz+2),rhs((ncr-1)*
1 (ncz+2)+int(ncz/2)+2*(nc+1))
write(5,11) rhs(nnf+int(ncz/2)),(rhs(l),l=nnf+int(ncz/2)+ncz+1,
1 nnf+(ncr-1)*(ncz+2)+int(ncz/2)+ncz+1,ncz+2),rhs(nnf+
1  
\((ncr-1)*(ncz+2)+\text{int}(ncz/2)+2*(ncz+1))\)

\text{write}(6,15) \((\text{rhs}(1), l=\text{int}(ncr/2)*(ncz+2)+ncz+1, \text{int}(ncr/2)*(ncz+2)+2*(ncz+1))\)

1

\text{write}(7,15) \((\text{rhs}(1), l=\text{nnf}+\text{int}(ncr/2)*(ncz+2)+ncz+1, \text{nnf}+\text{int}(ncr/2)*(ncz+2)+2*(ncz+1))\)

\text{c}

11  \text{format}(1x,32(f6.2,3x))

15  \text{format}(1x,22(f6.2,3x))

16  \text{format}(f7.1,2x,f7.1,2x,f7.1,2x,f7.1,2x,f7.1,2x,f7.1,2x,f7.1)

\text{c}

\text{endif}

\text{if}(i2 .eq. 1) \text{then}

\text{do} \ l=1,ncr+2

\text{if}(l .eq. 1) \text{then}

\text{write}(1,17) 0.d0

\text{elseif}(l .eq. ncr+2) \text{then}

\text{write}(1,17) 1.d0

\text{else}

\text{write}(1,17) (dble(l)-1.5d0)*dr/rb

\text{endif}

\text{enddo}

\text{h}=2.5d-2

\text{do} \ l=1,ncz+2

\text{if}(l .eq. 1) \text{then}

\text{write}(2,17) 0.d0

\text{elseif}(l .eq. ncr+2) \text{then}

\text{write}(2,17) 1.d0

\text{else}

\text{write}(2,17) (dble(l)-1.5d0)*dz/h

\text{endif}

\text{enddo}

17  \text{format}(f6.4)

\text{endif}

120
if(mod(i2,10) .eq. 1) then
    write(3,18) dble(i2)*dt
18 format(f7.1)
endif

if(i2 .lt. ntime) then
    do l=1,nnt
        tprev(l)=rhs(l)
    enddo
endif
enddo

k=0
    do l=1,ncz+2
        if(l .eq. 1) then
            write(9,20) (rhs(m), m=ncz+1,nnf-2*ncz-1,ncz+2)
        elseif(l .eq. ncz+2) then
            write(9,20) (rhs(m), m=2*(ncz+1),nnf-ncz,ncz+2)
        else
            k=k+1
            write(9,19) rhs(k),(rhs(m), m=ncz+1+k,nnf-2*ncz-1+k,ncz+2),
            rhs(nnf-ncz+k)
        endif
    enddo
enddo

k=0
    do l=1,ncz+2
        if(l .eq. 1) then
            write(10,20) (rhs(m), m=nnf+ncz+1,2*nnf-2*ncz-1,ncz+2)
        elseif(l .eq. ncz+2) then
            write(10,20) (rhs(m), m=nnf+2*(ncz+1),2*nnf-ncz,ncz+2)
        else
            k=k+1
            write(10,19) rhs(k),(rhs(m), m=nnf+ncz+1+k,2*nnf-2*ncz-1+k,ncz+2),
            rhs(2*nnf-ncz+k)
        endif
    enddo
enddo
else
k=k+1
write(10,19) rhs(nnf+k),(rhs(m), m=nnf+ncz+1+k, 2*nnf-2*ncz-1+k, 
ncz+2), rhs(2*nnf-ncz+k)
endif
endo
c
k=0
do l=1,ncz+2
if(l .eq. 1) then
write(11,22) (rhs(m+nnf)-rhs(m), m=ncz+1,nnf-2*ncz-1,ncz+2)
elseif(l .eq. ncz+2) then
write(11,22) (rhs(m+nnf)-rhs(m), m=2*(ncz+1),nnf-ncz,ncz+2)
else
k=k+1
write(11,21) rhs(k+nnf)-rhs(k),(rhs(m+nnf)-rhs(m), m=ncz+1+k, 
nnf-2*ncz-1+k,ncz+2), rhs(2*nnf-ncz+k)-rhs(nnf-ncz+k)
endif
enddo
c
write(8,23) (rhs(l),l=nnt+1,nn2)
c
19 format(1x,32(f6.2,3x))
20 format(1x,30(f6.2,3x))
21 format(1x,32(f9.4,3x))
22 format(1x,30(f9.4,3x))
23 format(1x,32(f6.4,3x))
write(*,*) 'the pressure drop is', dpdz
c
close(1)
close(2)
close(3)
subroutine assemble(tprev,a,rhs,temp,efs,eppm,lda,nn,ncr,ncz,nnf,nnt,nn2,vguess,tavesf,dpdz)
implicit real*8(a-h,o-y)
real*8 kg,mug,mu0,nu
integer flag,flag2,flag3,e,s,w,n,nn,lda,ncr,ncz,nnf,nnt,nn2

dimension a(lda,nn),temp(nnt),tprev(nnt),rhs(nn2),tavesf(ncr)
dimension efs(nnf),vguess(ncr+1)

c
common/param/flag,flag2,flag3
common/dielectric/pi,frequ,eps0,c0,mu0,ef0
common/solgas/rhos,dp,pf,dpt,vf,tmpin,kg,eps1,rb,ro,hn
common/delta/h,dt,dr,dz

c gas boundary nodes

do i=1,ncz
  tp=temp(i)
a(i,i)=1.d0
a(i,i+ncz+1)=-1.d0
rhs(i)=0.d0
k=nnf-ncz+i
tp=temp(k)
rtot=rb*dlog(ro/rb)/kg+rb/(hn*ro)
a(k,k)=1.d0/rtot+eps(rb)*cgas(tp)/dr
\[ a(k,k-ncz-1) = -\text{eps}(rb) \times \text{cgas}(tp)/\text{dr} \]

\[ \text{rhs}(k) = \text{tmpin}/\text{rtot} \]

\[ \text{c gas inlet temperature boundary} \]

\[ \text{do } i=ncz+1,\text{nnf}-2*ncz-1,ncz+2 \]
\[ a(i,i) = 1.d0 \]
\[ \text{rhs}(i) = \text{tmpin} \]

\[ \text{endo} \]

\[ \text{c gas boundary nodes} \]

\[ \text{do } i=2*(ncz+1),\text{nnf}-ncz,ncz+2 \]
\[ a(i,i) = 1.d0 \]
\[ a(i,i-1) = -1.d0 \]
\[ \text{rhs}(i) = 0.d0 \]

\[ \text{endo} \]

\[ \text{c gas eqns. for a typical node} \]

\[ j=ncz+2 \]
\[ m=2*ncz+1 \]
\[ p=0.d0 \]

\[ \text{do } i=1,\text{ncr} \]

\[ \text{do } i1=j,m \]
\[ n=i1+1 \]
\[ s=i1-1 \]
\[ w=i1-ncz-2 \]
\[ e=i1+ncz+2 \]
\[ j1=i1+\text{nnf} \]
\[ \text{drw}=\text{dr} \]
\[ \text{dre}=\text{dr} \]
\[ \text{dzs}=\text{dz} \]
\[ \text{dzn}=\text{dz} \]

\[ \text{if}(i .eq. 1) \text{ then} \]
\[ w=i1-ncz-1 \]
\[ \text{drw} = \text{dr}/2.d0 \]
elseif(i .eq. ncr) then
    e=i1+ncz+1
    dre=dr/2.d0
endif
if(i1 .eq. j) then
    dzs=dz/2.d0
elseif(i1 .eq. m) then
    dzn=dz/2.d0
endif

    tp=temp(i1)
    te=temp(e)
    tw=temp(w)
    tn=temp(n)
    ts=temp(s)
    tm=temp(j1)
    ce=(cgas(tp)+cgas(te))/2.d0
    cw=(cgas(tp)+cgas(tw))/2.d0
    cn=(cgas(tp)+cgas(tn))/2.d0
    cs=(cgas(tp)+cgas(ts))/2.d0
    cpg=cpgas(tp)
    ta=tavesf(i)
    rhog=rhof(ta)
    mug=viscf(ta)
    re=dp*rhog*rhs(nnt+i+1)/mug
        pr=cpg*mug/cgas(tp)
        nu=2.d0+1.2d0*re**(0.5d0)*pr**(1.d0/3.d0)
        h1=nu*cgas(tp)/dp
    r=(p+5.d-1)*dr
        aa=6.d0*(1.d0-eps(r))/dp
        h1=h1*aa
    r=(p+1.d0)*dr
    a(i1,e)=-eps(r)*ce*(p+1.d0)*dr*dz/dre
r=p*dr
a(i1,w)=-eps(r)*cw*p*dr*dz/drw
r=(p+5.d-1)*dr
a(i1,n)=-cn*eps(r)/dzn*((p+1.d0)**2-p**2)/2.d0*dr**2
a(i1,s)=(-rhog*cpg*eps(r)*rhs(nnt+i+1)*((p+1.d0)**2-p**2)/2.d0*
      1   dr**2-cs*eps(r)/dzs*((p+1.d0)**2-p**2)/2.d0*dr**2)
a(i1,j1)=-h1*dz*((p+1.d0)**2-p**2)/2.d0*dr**2
a(i1,i1)=rhog*cpg*eps(r)*dz*((p+1.d0)**2-p**2)/2.d0*dr**2/dt-
      1   a(i1,e)-a(i1,w)-a(i1,s)-a(i1,j1)-a(i1,n)
rhs(i1)=eps(r)*rhog*cpg*eps(r)*dz*((p+1.d0)**2-p**2)/2.d0*dr**2/dt*
      1   tprev(i1)
enddo
j=j+ncz+2
m=m+ncz+2
p=p+1.d0
enddo
c solid boundary nodes
do i=nnf+1,nnf+ncz
tp=temp(i)
a(i,i)=1.d0
a(i,i+ncz+1)=-1.d0
rhs(i)=0.d0
k=nnt-ncz+i-nnf
tp=temp(k)
rtot=rb*dlog(ro/rb)/kg+rb/(hn*ro)
a(k,k)=1.d0/rtot+(1.d0-eps(rb))*cons(tp,pf)/dr
a(k,k-ncz-1)=-(1.d0-eps(rb))*cons(tp,pf)/dr
rhs(k)=tmpin/rtot
enddo
c
if(flag2 .eq. 1) then
c insulated boundary
do i=nnf+ncz+1,nnt-2*ncz-1,ncz+2
  c if(flag3 .eq. 2) then
  a(i,i)=1.d0
  a(i,i+1)=-1.d0
  rhs(i)=0.d0
  c else
  c r=0.d0
  c tp=temp(i)
  c tm=temp(i-nnf)
  c h2=2.d0*cgas(tm)/dp
  c a(i,i)=h2*dr-(1.d0-eps(r))*cons(tp,pf)
  c a(i,i+1)=(1.d0-eps(r))*cons(tp,pf)
  c rhs(i)=h2*dr*tm
  c endif
  enddo
else
  c temperature boundary
  do i=nnf+ncz+1,nnt-2*ncz-1,ncz+2
    a(i,i)=1.d0
    rhs(i)=tmpin
  enddo
endif
endc
else
  c solid boundary nodes
  do i=nnf+2*(ncz+1),nnt-ncz,ncz+2
    if(flag3 .eq. 2) then
      a(i,i)=1.d0
      a(i,i-1)=-1.d0
      rhs(i)=0.d0
    else
      r=rb
      tp=temp(i)
      tm=temp(i-nnf)
      c .
  enddo
h2=2.d0*cgas(tm)/dp
a(i,i)=h2*dr-(1.d0-eps(r))*cons(tp,pf)
a(i,i-1)=(1.d0-eps(r))*cons(tp,pf)
rhs(i)=h2*dr*tm
endif
enddo

c solid eqns. for a typical node
p=0.d0
    j=nnf+ncz+2
m=j+ncz-1
do i=1,ncr
    do i1=j,m
        n=i1+1
        s=i1-1
        w=i1-ncz-2
        e=i1+ncz+2
        j1=i1-nnf
        drw=dr
dre=dr
dzn=dz
        dzs=dz
if(i .eq. 1) then
        w=i1-ncz-1
        drw=dr/2.d0
elseif(i .eq. ncr) then
        e=i1+ncz+1
        dre=dr/2.d0
endif
if(i1 .eq. j) then
        dzs=dz/2.d0
elseif(i1 .eq. m) then
        dzn=dz/2.d0
endif

tp=temp(i1)
te=temp(e)
    tw=temp(w)
tn=temp(n)
ts=temp(s)
tm=temp(j1)
cps=cpspt(tp,pf)
ce=(cons(tp,pf)+cons(te,pf))/2.d0
cw=(cons(tp,pf)+cons(tw,pf))/2.d0
cn=(cons(tp,pf)+cons(tn,pf))/2.d0
cs=(cons(tp,pf)+cons(ts,pf))/2.d0
ta=tavesf(i)
rhog=rhof(ta)
mug=viscf(ta)
    re=dp*rhog*rhs(nnt+i+1)/mug
        pr=cpgas(tm)*mug/cgas(tm)
        nu=2.d0+1.2d0*re**((0.5d0)*pr**(1.d0/3.d0)
        h1=nu*cgas(tm)/dp
r=(p+5.d-1)*dr
    aa=6.d0*(1.d0-eps(r))/dp
    h1=h1*aa
qgen=dabs(2.d0*pi*frequ*efs(j1)**2*eppm*eps0)
r=(p+1.d0)*dr
a(i1,e)=-(1.d0-eps(r))*ce*(p+1.d0)*dr*dz/dre
r=p*dr
a(i1,w)=-(1.d0-eps(r))*cw*p*dr*dz/drw
r=(p+5.d-1)*dr
a(i1,n)=-(1.d0-eps(r))*cn*((p+1.d0)**2-p**2)/2.d0*dr**2/dzn
a(i1,s)=-(1.d0-eps(r))*cs*((p+1.d0)**2-p**2)/2.d0*dr**2/dzs
a(i1,j1)=-h1*((p+1.d0)**2-p**2)/2.d0*dr**2*dz
a(i1,i1)=rhos*cps*(1.d0-eps(r))*((p+1.d0)**2-p**2)/2.d0*dr**2*
\[ \frac{dz}{dt} = a(i1,e) - a(i1,w) - a(i1,n) - a(i1,s) - a(i1,j1) \]

\[ \text{rhs}(i1) = (1.0 - \varepsilon(r)) \times ((p+1.0)^2 - p^2) / 2.0 \times dr^2 \times dz \times \left( \rho_0 \times c_\text{ps} / dt \times t_{\text{prev}(i1)} + q_{\text{gen}} \right) \]

\enddo

\]

\[
\]

\]
r=(p+1.d0)*dr
a(i,i+1)=-r*eps(r)*mug/dre
r=p*dr
a(i,i-1)=-r*eps(r)*mug/drw
r=(p+5.d-1)*dr
vol=((p+1.d0)**2-p**2)/2.d0*dr**2
f1=1.5d2*mug*(1.d0-eps(r))**2/(dp**2*eps(r)**3)
f2=1.75d0*rhog*(1.d0-eps(r))/(dp*eps(r)**3)
a(i,i)=-a(i,i+1)-a(i,i-1)+(f1+f2*vguess(i-nnt))*vol
rhs(i)=-dpdz*vol
p=p+1.d0
enddo

c
return
end

c
function eps(r)
implicit double precision(a-h,o-y)
real*8 kg,n,mu0
integer flag,flag2,flag3

c
common/param/flag,flag2,flag3
common/dielectric/pi,frequ,eps0,c0,mu0,ef0
common/solgas/rhos,dp,pf,dpt,vf,tmpin,kg,eps,rb,ro,hn
common/delta/h,dt,dr,dz

c
c=1.d0
n=2.d0
eps=epsi*(1.d0+c*dexp(-n*(rb-r)/dp))
c eps=epsi
Appendix B

Fluidized Bed Program

c This program will determine the temperature and velocity profiles and
the temperature difference between the solid and gas in a 2-d fluidized
bed.
c
The following is a definition of the input variables.
c
initer = number of inner iterations.
c
ncx = number of cells in the x-direction.
c
ncy = number of cells in the flow, or y-direction in the expanded bed
region.
c
ncyp = total number of cells in the y-direction.
c
nnf = total number of nodes for a single phase.
c
nnt = total number of nodes for both phases.
c
ntime = number of time steps.
c
job = parameter set to zero to solve Ax = b in the matrix solver.
c
kg = conductivity of glass (W/m\(\cdot\)K).
c
hn = heat transfer coefficient between container and surroundings
\((W/m^{2}\cdot K)\).
c
len = length of the bed (m).
c
lout = thickness of the bed container (m).
h = height of the bed (m).
dx = length of a control volume in the computational grid (m).
dy = height of a control volume in the computational grid (m).
dt = time step (s).
dpt = particle diameter of the metallic catalyst particle (m).
pf = volume fraction of metallic catalyst particle in the ceramic support.
rhoal = density of alumina (kg/m³).
rhopt = density of platinum (kg/m³).
vin = inlet gas velocity (m/s).
vflow = inlet volume flow rate of the gas (m³/s).
dp = particle diameter (m).
rhos = density of the ceramic support/metallic catalyst mixture (kg/m³).
tin = inlet gas temperature (K).
frequ = microwave frequency (Hz).
eps0 = permitivity of free space (f/m).
mu0 = permeability of free space (h/m).
c0 = speed of light (m/s).
ef0 = electric field within the bed (V/m).
rhog = density of the gas (kg/m³).
mug = dynamic viscosity of the gas (N·s/m²).
eps = solid volume fraction array.
vxa = gas x-velocity array.
vxs = solid x-velocity array.
vya = gas y-velocity array.
vys = solid y-velocity array.

flag = determines whether the support will be alpha or gamma-alumina:
    if set to 1, then alpha alumina is used; otherwise gamma alumina is used.
flag1 = controls the numerical scheme: if set to 1, the central difference scheme is implemented; if set to 2, the upwind scheme is implemented; if set to 3, the hybrid scheme is implemented; and if set to 4, the power law is implemented.

flag2 = determines the inlet boundary condition for the solid phase: if set to 1, the solid is insulated; otherwise the solid is set to the inlet temperature of the gas.

flag3 = controls electric field: if set to 1, the electric field varies linearly in the flow direction; otherwise, the electric field is uniform.

implicit real*8(a-h,o-y)
real*8 k1,kg,mug,mu0,z,len,lout
integer ncx,ncy,nnf,nnt,ntime,flag,flag1,flag2,flag3,nn,lda,ipvt
integer job,nill,initer,flag4,flag5

parameter(initer=4)
parameter(ncx=50)
parameter(ncy=21)
parameter(nill=(ncx+1)*(ncy+1))
parameter(nnf=2*(ncy+ncx)+ncx*ncy)
parameter(nnt=2*nnf)
parameter(nn=nnt)
parameter(lda=nn)

dimension tprev(nnt),z(nn),ipvt(nn),temp(nnt),a(lda,nn),rhs(nnt)
dimension taves(ncy),efelds(ncy),efs(nnf),vya(nill),vxa(nill)
dimension vys(nill),vxs(nill),eps(nill),epf(nill)

c
common/param/flag,flag1,flag2,flag4,flag5
common/dielectric/pi,freq,eps0,c0,mu0,ef0
common/solgas/rhog,mug,vin,rhos,dp,pf,dpt,vf,tin,qflux
common/delta/dt,dx,dy,h,lout,hn,kg

c
open(1,file='c:\fbed\eps_100_.033')
open(2,file='c:\fbed\yair_100_.033')
open(3,file='c:\fbed\xair_100_.033')
open(4,file='c:\fbed\ysol_100_.033')
open(5,file='c:\fbed\xsol_100_.033')
c
c open(1,file='c:\fbed\eps_125_.051')
c open(2,file='c:\fbed\yair_125_.051')
c open(3,file='c:\fbed\xair_125_.051')
c open(4,file='c:\fbed\ysol_125_.051')
c open(5,file='c:\fbed\xsol_125_.051')
c
c open(1,file='c:\fbed\eps_150_.049')
c open(2,file='c:\fbed\yair_150_.049')
c open(3,file='c:\fbed\xair_150_.049')
c open(4,file='c:\fbed\ysol_150_.049')
c open(5,file='c:\fbed\xsol_150_.049')
c
c open(1,file='c:\fbed\eps_150_.073')
c open(2,file='c:\fbed\yair_150_.073')
c open(3,file='c:\fbed\xair_150_.073')
c open(4,file='c:\fbed\ysol_150_.073')
c open(5,file='c:\fbed\xsol_150_.073')
c
c open(6,file='c:\fbed\length')
 open(7,file='c:\fbed\height')
 open(8,file='c:\fbed\time')
c
135
open(9,file='c:\fbed\txf_100_33')
open(10,file='c:\fbed\tsx_100_33')
open(11,file='c:\fbed\tfy_100_33')
open(12,file='c:\fbed\tsy_100_33')
open(14,file='c:\fbed\xvela_100_33')
open(15,file='c:\fbed\xvels_100_33')
open(16,file='c:\fbed\yvela_100_33')
open(17,file='c:\fbed\yvels_100_33')
open(18,file='c:\fbed\epsilon_100_33')
c
c open(9,file='c:\fbed\txf_125_51')
c open(10,file='c:\fbed\tsx_125_51')
c open(11,file='c:\fbed\tfy_125_51')
c open(12,file='c:\fbed\tsy_125_51')
c open(14,file='c:\fbed\xvela_125_51')
c open(15,file='c:\fbed\xvels_125_51')
c open(16,file='c:\fbed\yvela_125_51')
c open(17,file='c:\fbed\yvels_125_51')
c open(18,file='c:\fbed\epsilon_125_51')
c
c open(9,file='c:\fbed\txf_150_495')
c open(10,file='c:\fbed\tsx_150_495')
c open(11,file='c:\fbed\tfy_150_495')
c open(12,file='c:\fbed\tsy_150_495')
c open(14,file='c:\fbed\xvela_150_49')
c open(15,file='c:\fbed\xvels_150_49')
c open(16,file='c:\fbed\yvela_150_49')
c open(17,file='c:\fbed\yvels_150_49')
c open(18,file='c:\fbed\epsilon_150_49')
c
c open(9,file='c:\fbed\txf_150_73')
c open(10,file='c:\fbed\tsx_150_73')
c open(11, file='c:\fbed\tfy_150_73')
c open(12, file='c:\fbed\tsy_150_73')
c open(14, file='c:\fbed\xvela_150_73')
c open(15, file='c:\fbed\xvels_150_73')
c open(16, file='c:\fbed\yvela_150_73')
c open(17, file='c:\fbed\yvels_150_73')
c open(18, file='c:\fbed\epsilon_150_73')
c
open(19, file='c:\fbed\tgas_100_33')
open(20, file='c:\fbed\tsol_100_33')
open(21, file='c:\fbed\tdiff_100_33')
c
   ntime=600
   pi=dacos(-1.d0)
   job=0
   hn=2.d0
   kg=1.4d0
   k1=1.d5
   qflux=0.d0
   ncy=50
   vin=3.3d-2
       dp=1.d-4
   len=4.d-1
   lout=4.d-2
   h=6.d-1
   dx=len/dble(ncx)
   dy=h/dble(ncy)
   dt=1.d1
   dpt=4.d-8
   pf=.01d0
   rhoal=7.d2
   rho=21450.d0
rhog=1.2d0
mug=1.8e-5
    vf=(pf/rhopt)/((pf/rhopt)+(1.d0-pf)/rhoal)
rhos=pf*rhopt+(1.d0-pf)*rhoal
tin=300.15d0
freq=.915d9
eps0=8.854d-12
mu0=4.d-7*pi
c0=3.d8
ef0=3.d3
flag=2
flag1=2
flag2=1
flag3=2
flag4=2
flag5=2
c efields(ncy)=ef0
tol=1.d-4
c
    do i=1,nnt
        tprev(i)=tin
        temp(i)=tin
    enddo
c
do i=1,nill
    read(1,*) eps(i)
    epf(i)=1.d0-eps(i)
    read(2,*) vya(i)
    read(3,*) vxa(i)
    read(4,*) vys(i)
    read(5,*) vxs(i)
enddo
do i2=1,ntime
  k=nnf+ncx+2
  l=k+ncx-1
  do i=1,ncy
    sum=0.d0
    do j=k,l
      sum=sum+temp(j)
    enddo
    taves(i)=sum/dble(ncx)
    k=k+ncx+2
    l=l+ncx+2
  enddo

  call efields(k1,taves,efelds,eppm,ncy)

  do k=1,nnt
    temp(k)=tprev(k)
  enddo

k=ncx+2
l=k+ncx-1
do i=1,ncy
  do j=k,l
    if(flag3 .eq. 1) then
      efs(j)=efelds(i)
    else
      efs(j)=ef0
    endif
  enddo
k=k+ncx+2
l=l+ncx+2
enddo
c5 do j2=1,initer
c    call assemble(tprev,a,rhs,vya,vxa,vys,vxs,eps,temp,efs,eppm,
                    lda,nn,ncx,ncy,nnf,nnt,nill,epf)
c    if(i2.eq.ntime) then
do j3=1,lda
do j4=1,nn
    write(*,*) j3, j4, a(j3,j4), rhs(j3)
endo
do j3=1,nnt
    write(*,*) i2, j3, rhs(j3)
endo
doi2,nnt
    write(*,*) i2, j3, rhs(j3)
endo
dendif
c    call dgeco(a,lda,nn,ipvt,rcond,z)
c    write(*,*) 'the condition # is', 1.d0/rcond, i2
c    if(1.d0/rcond .gt. 1.d3) then
    write(*,*) 1.d0/rcond, 'is too large at the time-step', i2
    goto 30
endif
c    call dgesl(a,lda,nn,ipvt,rhs,job)
c    if(i2.gt.2000) then
do j3=1,nnt
    write(6,*) i2, j3, rhs(j3)
endo
dendif
cdo l=1,nnt
    temp(l)=rhs(l)
dendo
do i3=1,lda
  do j3=1,nn
    a(i3,j3)=0.d0
  enddo
enddo

c
if(mod(i2,tint).eq.1) then
  write(8,18) dble(i2)*dt
  write(9,11) (rhs(l),l=int(ncy/2)*(ncx+2)-1,int(ncy/2)*(ncx+2)+1(ncx))
  write(10,11) (rhs(l),l=nnf+int(ncy/2)*(ncx+2)-1,nnf+int(ncy/2)*1(ncx+2)+ncx)
  write(11,15) rhs(int(ncx/2)),(rhs(l),l=ncx+1+int(ncx/2),ncx+1+int(ncx/2)+(ncy-1)*(ncx+2),ncx+2),rhs(2*(ncx+1)+int(ncx/2)+(ncy-1)*(ncx+2))
  write(12,15) rhs(nnf+int(ncx/2)),(rhs(l),l=nnf+ncx+1+int(ncx/2),nnf+ncx+1+int(ncx/2)+(ncy-1)*(ncx+2),ncx+2),rhs(nnf+2*(ncx+1)+int(ncx/2)+(ncy-1)*(ncx+2))
  endif

if(i2 .eq. 1) then
  do l=1,ncx+2
    if(l .eq. 1) then
      write(6,17) 0.d0
    elseif(l .eq. ncx+2) then
      write(6,17) 1.d0
    else
      write(6,17) (dble(l)-1.5d0)*dx/len
    endif
  enddo
endif
enddo
h=6.d-1
   do l=1,ncy+2
if(l .eq. 1) then
     write(7,17) 0.d0
elseif(l .eq. ncy+2) then
     write(7,17) 1.d0
else
     write(7,17) (dble(l)-1.5d0)*dy/h
endif
   enddo
17   format(f6.4)
do l=1,ntime
   write(8,18) dble(l)*dt
enddo
18   format(f6.1)
   endif

c
   if(i2 .lt. ntime) then
      do l=1,nnt
         tprev(l)=rhs(l)
      enddo
   endif
enddo

c
k=1
l=ncx+1
do i=1,ncy+1
   write(14,19) (vxa(m), m=k,l)
   write(15,19) (vxs(m), m=k,l)
   write(16,20) (vya(m), m=k,l)
   write(17,20) (vys(m), m=k,l)
write(18,21) (eps(m), m=k,l)
k=k+ncx+1
l=l+ncx+1
enddo

19 format(1x,51(f9.6,3x))
20 format(1x,51(f9.6,3x))
21 format(1x,51(f8.6,3x))
c
k=0
do l=1,ncy+2
if(l .eq. 1) then
write(19,23) (rhs(m), m=1,ncx)
write(20,23) (rhs(m+nnf), m=1,ncx)
write(21,25) (rhs(m+nnf)-rhs(m), m=1,ncx)
elseif(l .eq. ncy+2) then
write(19,23) (rhs(m), m=nnf-ncx+1,nnf)
write(20,23) (rhs(m+nnf), m=nnf-ncx+1,nnf)
write(21,25) (rhs(m+nnf)-rhs(m), m=nnf-ncx+1,nnf)
else
write(19,22) (rhs(m),m=ncx+1+k,2*(ncx+1)+k)
write(20,22) (rhs(m+nnf),m=ncx+1+k,2*(ncx+1)+k)
write(21,24) (rhs(m+nnf)-rhs(m), m=ncx+1+k,2*(ncx+1)+k)
endif
if(l .gt. 1) then
k=k+ncx+2
endif
enddo
c
22 format(1x,52(f7.2,3x))
23 format(1x,50(f7.2,3x))
24 format(1x,52(f9.4,3x))
25 format(1x,50(f9.4,3x))
c
  close(1)
close(2)
close(3)
close(4)
close(5)
close(6)
close(7)
close(8)
close(9)
close(10)
close(11)
close(12)
close(14)
close(15)
close(16)
close(17)
close(18)
close(19)
close(20)
close(21)
  30 end
c
subroutine assemble(tprev,a,rhs,vya,vxa,vys,vxs,eps,temp,efs,
  eppm,lda,nn,ncx,ncy,nnf,nnt,nill,epf)
implicit real*8(a-h,o-y)
real*8 kg,mug,mu0,nu,lout
integer flag,flag1,flag2,flag4,flag5,e,s,w,n,nn,lda,ncx,ncy
integer nnf,nnt,nill
c
dimension a(lda,nn),temp(nnt),tprev(nnt),rhs(nnt),eps(nill)
dimension vya(nill),vxa(nill),vys(nill),vxs(nill),efs(nnf)
dimension epf(nill)
c
common/param/flag,flag1,flag2,flag4,flag5
common/dielectric/pi,freq,eps0,c0,mu0,ef0
common/solgas/rhog,mug,vin,rhos,dp,pf,dpt,vf,tin,qflux
common/delta/dt,dx,dy,h,lout,hn,kg
c gas boundary nodes
k=1
do i=ncx+1,nnf-2*ncx-1,ncx+2
  eps1=(epf(i+k)+epf(i-ncx-1+k))/2.d0
  tp=temp(i)
  rtot=lout/kg+1.d0/hn
  a(i,i)=1.d0/rtot+eps1*cgas(tp)/dx
  a(i,i+1)=-eps1*cgas(tp)/dx
  rhs(i)=tin/rtot
  k=k+1
enddo
c
c
  k=0
do i=2*(ncx+1),nnf-ncx,ncx+2
  eps1=(epf(i+k)+epf(i-ncx-1+k))/2.d0
  tp=temp(i)
  rtot=lout/kg+1.d0/hn
  a(i,i)=1.d0/rtot+eps1*cgas(tp)/dx
  a(i,i-1)=-eps1*cgas(tp)/dx
  rhs(i)=tin/rtot
  k=k+1
    enddo
c
do i=nnf-ncx+1,nnf
  a(i,i)=1.d0
  a(i,i-ncx-1)=-1.d0
rhs(i) = 0.d0
enddo

C gas inlet temperature boundary
    do i=1,ncx
        a(i,i) = 1.d0
        rhs(i) = tin
    enddo

C gas eqns. for a typical node
    nt = 0
    nt1 = ncx + 1
    j = ncx + 2
    m = 2 * ncx + 1
    do i = 1,ncy
        do i1 = j, m
            n = i1 + ncx + 2
            s = i1 - ncx - 2
            w = i1 - 1
            e = i1 + 1
            j1 = i1 + nnf
            fee = .5d0
            few = .5d0
            fen = .5d0
            fes = .5d0
            ee = (epf(i1-nt1+1) + epf(i1-nt1))/2.d0
            ew = (epf(i1-nt1) + epf(i1-nt))/2.d0
            en = (epf(i1-nt) + epf(i1-nt+1))/2.d0
            es = (epf(i1-nt1) + epf(i1-nt1+1))/2.d0
            epfi1 = (epf(i1-nt1+1) + epf(i1-nt+1) + epf(i1-nt1) + epf(i1-nt))/4.d0
            epfe = (epf(i1+1-nt1+1) + epf(i1-nt+1) + epf(i1+1-nt1) + epf(i1+1-nt1))/4.d0
            1 epf(i1+1-nt))/4.d0
            epfw = (epf(i1-1-nt1+1) + epf(i1-1-nt1) + epf(i1-1-nt1)+
                1 epf(i1-1-nt))/4.d0
\text{epfn}=(\text{epf}(i1+ncx+2-(nt1+1)+1)+\text{epf}(i1+ncx+2-(nt+1)+1)+
1 \quad \text{epf}(i1+ncx+2-(nt1+1))+\text{epf}(i1+ncx+2-(nt+1)))/4.d0
\text{epfs}=(\text{epf}(i1-ncx-2-(nt1-1)+1)+\text{epf}(i1-ncx-2-(nt-1)+1)+
1 \quad \text{epf}(i1-ncx-2-(nt1-1))+\text{epf}(i1-ncx-2-(nt-1)))/4.d0
\text{if}(i \text{ .eq. 1}) \text{ then}
\quad s=i1-ncx-1
\quad fes=0.d0
\quad epfs=es
\text{elseif}(i \text{ .eq. ncy}) \text{ then}
\quad n=i1+ncx+1
\quad fen=0.d0
\quad epfn=en
\text{endif}
\text{if}(i1 \text{ .eq. j}) \text{ then}
\quad dfw=0.d0
\quad epfw=ew
\text{elseif}(i1 \text{ .eq. m}) \text{ then}
\quad dfe=0.d0
\quad epfe=ee
\text{endif}
\text{tp}=\text{temp}(i1)
\quad \text{te}=\text{temp}(e)
\quad \text{tw}=\text{temp}(w)
\text{tn}=\text{temp}(n)
\text{ts}=\text{temp}(s)
\text{tm}=\text{temp}(j1)
\text{cpg}=\text{cpgas}(tp)
\text{ue}=(\text{vxa}(i1-nt1+1)+\text{vxa}(i1-nt+1))/2.d0
\text{uw}=(\text{vxa}(i1-nt1)+\text{vxa}(i1-nt))/2.d0
\text{vn}=(\text{vya}(i1-nt)+\text{vya}(i1-nt+1))/2.d0
\text{vs}=(\text{vya}(i1-nt1)+\text{vya}(i1-nt1+1))/2.d0
\text{cee}=1.d0/((1.d0-fee)/(\text{epfi1*cgas}(tp))+fee/(\text{epfe*cgas}(te)))
cwe = 1.d0/((1.d0-few)/(epfi1*cgas(tp)) + few/(epfw*cgas(tw)))
cne = 1.d0/((1.d0-fen)/(epfi1*cgas(tp)) + fen/(epfn*cgas(tn)))
cse = 1.d0/((1.d0-fes)/(epfi1*cgas(tp)) + fes/(epfs*cgas(ts)))
fe = rhog*ee*ue*dy
fw = rhog*ew*uw*dy
fn = rhog*en*vn*dx
fs = rhog*es*vs*dx
de = cee/cpg*dy/dx
dw = cwe/cpg*dy/dx
dn = cne/cpg*dx/dy
ds = cse/cpg*dx/dy
pe = fe/de
pw = fw/dw
pn = fn/dn
ps = fs/ds

vvi1 = (vya(i1-nt1+1) + vya(i1-nt+1) + vya(i1-nt1) + vya(i1-nt))/4.d0
vvj1 = (vys(i1-nt1+1) + vys(i1-nt+1) + vys(i1-nt1) + vys(i1-nt))/4.d0
vui1 = (vxa(i1-nt1+1) + vxa(i1-nt+1) + vxa(i1-nt1) + vxa(i1-nt))/4.d0
vuj1 = (vxs(i1-nt1+1) + vxs(i1-nt1+1) + vxs(i1-nt1) + vxs(i1-nt))/4.d0
vmag = dsqrt((vvi1-vvj1)**2 + (vui1-vuj1)**2)
c
re = (1.d0-epfi1)*dp*rhog*vmag/mug

re = dp*rhog*vin/mug
nu = 3.d-2*re**(1.3d0)
c
pr = cpg*mug/cgas(tp)
c
nu = 2.d0+1.2d0*re**(1.3d0)

h1 = nu*cgas(tp)/dp
aa = 6.d0*(1.d0-epfi1)/dp
h1 = h1*aa

a(i1,e) = -(de*ap(pe,flag1) + dmax1(-fe,0.d0))
a(i1,w) = -(dw*ap(pw,flag1) + dmax1(fw,0.d0))
a(i1,n) = -(dn*ap(pn,flag1) + dmax1(-fn,0.d0))
a(i1,s) = -(ds*ap(ps,flag1) + dmax1(fs,0.d0))
a(i1,j1)=-h1*dx*dy/cpg
a(i1,i1)=rhog*epfi1*dx*dy/dt-a(i1,e)-a(i1,w)-a(i1,n)-
a(i1,s)-a(i1,j1)

rhs(i1)=epfi1*rhog*dx*dy/dt*tprev(i1)

j=j+ncx+2
m=m+ncx+2
nt=nt+1
nt1=nt1+1

enddo

c solid boundary nodes

k=1

do i=nnf+ncx+1,2*nnf-2*ncx-1,ncx+2
eps1=1.d0-(epf(i-nnf+k)+epf(i-nnf-ncx-1+k))/2.d0

tp=temp(i)

rtot=lout/kg+1.d0/hn

a(i,i)=1.d0/rtot+eps1*cons(tp,pf)/dx

a(i,i+1)=-eps1*cons(tp,pf)/dx

rhs(i)=tin/rtot

k=k+1

enddo

c

k=0

do i=nnf+2*(ncx+1),2*nnf-ncx,ncx+2

eps1=1.d0-(epf(i-nnf+k)+epf(i-nnf-ncx-1+k))/2.d0

tp=temp(i)

rtot=lout/kg+1.d0/hn

a(i,i)=1.d0/rtot+eps1*cons(tp,pf)/dx

a(i,i-1)=-eps1*cons(tp,pf)/dx

rhs(i)=tin/rtot

k=k+1

enddo
c
nt=1
   do i=2*nnf-ncx+1,2*nnf
   c if(flag4 .eq. 2) then
      a(i,i)=1.d0
      a(i,i-ncx-1)=-1.d0
      rhs(i)=0.d0
   c else
   c      tp=temp(i)
   c      tm=temp(i-nnf)
   c      h2=2.d0*cgas(tm)/dp
   c      epsi1=(eps(ncy*(ncx+1)+nt+1)+eps(ncy*(ncx+1)+nt))/2.d0
      a(i,i)=h2*dx+epsi1*cons(tp,pf)
      a(i,i-ncx-1)=-epsi1*cons(tp,pf)
      rhs(i)=h2*dx*tm
   c nt=nt+1
   c endif
   enddo

   if(flag2 .eq. 1) then
   c heat flux boundary
      do i=nnf+1,nnf+ncx
      c if(flag5 .eq. 2) then
         a(i,i)=1.d0
         a(i,i+ncx+1)=-1.d0
         rhs(i)=0.d0
      c else
      c         tp=temp(i)
      c         tm=tin
      c         h2=2.d0*cgas(tm)/dp
      c         epsi1=(eps(i-nnf)+eps(i+1-nnf))/2.d0
         a(i,i)=h2*dx+epsi1*cons(tp,pf)
      c endif
      enddo
c a(i,i+ncx+1)=-epsi1*cons(tp,pf)
c rhs(i)=h2*dx*tm
c endif
   enddo
else
   c temperature boundary
   do i=nnf+1,nnf+ncx
      a(i,i)=1.d0
      rhs(i)=tin
   enddo
endif

c solid eqns. for a typical node
   nt=0
   nt1=ncx+1
   j=nnf+ncx+2
   m=j+ncx-1
   do i=1,ncy
      do i1=j,m
         n=i1+ncx+2
         s=i1-ncx-2
         w=i1-1
         e=i1+1
         j1=i1-nnf
         fee=.5d0
         few=.5d0
         fen=.5d0
         fes=.5d0
         ee=(eps(j1-nt1+1)+eps(j1-nt+1))/2.d0
         ew=(eps(j1-nt1)+eps(j1-nt))/2.d0
         en=(eps(j1-nt)+eps(j1-nt+1))/2.d0
         es=(eps(j1-nt1)+eps(j1-nt1+1))/2.d0
         epsi1=(eps(j1-nt1+1)+eps(j1-nt1)+eps(j1-nt1+1)+eps(j1-nt))/4.d0
\begin{verbatim}
epse=(eps(j1+1-nt1+1)+eps(j1+1-nt1)+eps(j1+1-nt))/4.d0
epsw=(eps(j1-1-nt1+1)+eps(j1-1-nt1)+eps(j1-1-nt))/4.d0
epsn=(eps(j1+ncx+2-(nt1+1)+1)+eps(j1+ncx+2-(nt1+1))+
    eps(j1+ncx+2-(nt1+1))+eps(j1+ncx+2-(nt1+1)))/4.d0
epss=(eps(j1-ncx-2-(nt1-1)+1)+eps(j1-ncx-2-(nt1-1))+
    eps(j1-ncx-2-(nt1-1))+eps(j1-ncx-2-(nt1-1)))/4.d0
if(i .eq. 1) then
    s=i1-ncx-1
    fes=0.d0
    epss=es
elseif(i .eq. ncy) then
    n=i1+ncx+1
    fen=0.d0
    epsn=en
endif
if(i1 .eq. j) then
    few=0.d0
    epsw=ew
elseif(i1 .eq. m) then
    fee=0.d0
    epse=ee
endif
tp=temp(i1)
te=temp(e)
    tw=temp(w)	nn=temp(n)
    ts=temp(s)
    tm=temp(j1)
cps=cpspt(tp,pf)
ue=(vxs(j1-nt1+1)+vxs(j1-nt1+1))/2.d0
\end{verbatim}
uw=(vxs(j1-nt1)+vxs(j1-nt))/2.d0
vn=(vys(j1-nt)+vys(j1-nt+1))/2.d0
vs=(vys(j1-nt1)+vys(j1-nt1+1))/2.d0
cee=1.d0/((1.d0-fee)/(epsi1*cons(tp,pf))+fee/(epse*cons(te,pf)))
cwe=1.d0/((1.d0-few)/(epsi1*cons(tp,pf))+few/(epsw*cons(tw,pf)))
cne=1.d0/((1.d0-fen)/(epsi1*cons(tp,pf))+fen/(epsn*cons(tn,pf)))
cse=1.d0/((1.d0-fes)/(epsi1*cons(tp,pf))+fes/(epss*cons(ts,pf)))
fe=rhos*ee*ue*dy
fw=rhos*ew*uw*dy
fn=rhos*en*vn*dx
fs=rhos*es*vs*dx
de=cee/cps*dy/dx
dw=cwe/cps*dy/dx
dn=cne/cps*dx/dy
ds=cse/cps*dx/dy
pe=fe/de
pw=fw/dw
pn=fn/dn
ps=fs/ds
vvi1=(vya(j1-nt1+1)+vya(j1-nt+1)+vya(j1-nt1)+vya(j1-nt))/4.d0
vvj1=(vys(j1-nt1+1)+vys(j1-nt+1)+vys(j1-nt1)+vys(j1-nt))/4.d0
vu1=(vxa(j1-nt1+1)+vxa(j1-nt+1)+vxa(j1-nt1)+vxa(j1-nt))/4.d0
vuj1=(vxs(j1-nt1+1)+vxs(j1-nt+1)+vxs(j1-nt1)+vxs(j1-nt))/4.d0
vmag=dsqrt((vvi1-vvj1)**2+(vu1-vuj1)**2)
c re=epsi1*dp*rhog*vmag/mug
re=dp*rhog*vin/mug
nu=3.d-2*re**(1.3d0)
c pr=cpg*mug/cgas(tp)
c nu=2.d0+1.2d0*re**(0.5d0)*pr**(1.d0/3.d0)
h1=nu*cgas(tm)/dp
aa=6.d0*epsi1/dp
h1=h1*aa
qgen = dabs(2.d0*pi*freq*efs(j1)**2*eppm*eps0)
a(i1,e) = -(de*ap(pe,flag1)+dmax1(-fe,0.d0))
a(i1,w) = -(dw*ap(pw,flag1)+dmax1(fw,0.d0))
a(i1,n) = -(dn*ap(pn,flag1)+dmax1(-fn,0.d0))
a(i1,s) = -(ds*ap(ps,flag1)+dmax1(fs,0.d0))
a(i1,j1) = -h1*dx*dy/cps
    a(i1,i1) = rhos*epsi1*dx*dy/dt - a(i1,e) - a(i1,w) - a(i1,n) - a(i1,s) - 1
    rhs(i1) = epsi1*rhos*dx*dy/dt*tprev(i1) + epsi1*qgen*dx*dy/cps
enddo
j = j + ncx + 2
m = m + ncx + 2
nt = nt + 1
nt1 = nt1 + 1
enddo
return
end

function ap(p,flag1)
  implicit real*8(a-h,o-y)
  integer flag1
  c
  if(flag1 .eq. 1) then
    c central difference
    ap = 1.d0 - dabs(p)/2.d0
  elseif(flag1 .eq. 2) then
    c upwind
    ap = 1.d0
  elseif(flag1 .eq. 3) then
    c hybrid
    ap = dmax1(0.d0,1.d0 - 5d-1*dabs(p))
  elseif(flag1 .eq. 4) then

c  power law
    ap = dmax1(0.d0, (1.d0-1d-1*dabs(p))**5)
endif

c
return
end
Appendix C

Subroutines and Functions Used By the Packed and Fluidized Bed Programs

c

function cap1(t1)

c
...heat capacity for alumina

c
implicit double precision(a-h,o-y)
dimension a(6)
data a/-210.672d0,5.1956d0,-7.95646d-03,6.23173d-06,
& -2.40174d-09,3.61348d-13/
  sum=0.0d0
  do 5 i=1,5
    sum=t1*(sum+a(7-i))
  5 continue
cap1=sum+a(1)
return
end

c
function cpt(t)

c
29 June 1995

c
... heat capacity for platinum

c
implicit real*8(a-h,o-y)
real*8 cpt,cpts
dimension tpts(9),cpts(9)
data tpts/2.d+02,3.d+02,4.d+02,6.d+02,8.d+02,1.d+03,1.2d+03
2,1.5d+03,2.d+03/
data cpts/1.25d2,1.33d2,1.36d2,1.41d2,1.46d2,1.52d2,
2 1.57d2,1.65d2,1.79d2/
if(t.ge.tpts(9))then
  a=(cpts(9)-cpts(8))/(tpts(9)-tpts(8))
  b=cpts(9)-a*tpts(9)
  cpt=a*t+b
  return
endif
do 5 i=1,8
  x=tpts(i)
  y=tpts(i+1)
  if(t.eq.x)then
    cpt=cpts(i)
    return
  elseif(t.gt.x.and.t.lt.y)then
    cpt=cpts(i)+(t-x)*(cpts(i+1)-cpts(i))/(y-x)
    return
  endif
5 continue
return
end
*function cal(x1)*

...conductivity for alumina

*implicit double precision(a-h,o-y)*

\[ cal = 0.55d0 \times \left( \frac{6.788d+03}{(x1-125.0d0)} + (3.562d-33) \times x1^{10} \right) \]

*return*

*end*

*function cpspt(t,pf)*

...heat capacity for catalyst pellets

*implicit real*8(a-h,o-y)*

\[ cpspt = (1.d0-pf) \times cap1(t) + pf \times cpt(t) \]

*return*

*end*

*subroutine efields(k1,taves,efelds,eppm,ncy)*

*implicit real*8(a-h,o-y)*

*implicit complex*16(z)*

*real*8 kg,k1,ks1,ks2,ks3,ks4,mu0,mug,lout

*integer flag,ncy,flag1,flag2,flag4,flag5*

*dimension efelds(ncy),taves(ncy)*

*common/param/flag,flag1,flag2,flag4,flag5*

*common/dielectric/pi,freq,eps0,c0,mu0,ef0*
common/solgas/rhog,mug,vin,rhos,dp,pf,dpt,vf,tin,qflux
common/delta/dt,dx,dy,h,lout,hn,kg

do k=ncy,1,-1
  do k=1,ncy
    tp=taves(k+1)
    ef=efelds(k+1)
    if(flag .eq. 1) then
      zep1=dcmplx(epa(tp),-eppa(tp))
    else
      zep1=dcmplx(epag(tp),-eppag(tp))
    endif
    zep2=dcmplx(1.d0,-eppt(tp,dpt))
    zepm=((2.d0*vf+1.d0)*zep1*zep2+2.d0*zep1**2*(1.d0-vf))/
      1 ((2.d0+vf)*zep1+(1.d0-vf)*zep2)
    eppm=dimag(zepm)
    epm=dreal(zepm)
    tandm=eppm/epm
    efelds(k)=ef0+k1*(dble(k)-.5d0)*dy
    beta=freq*dsqrt(epm)/c0*dsqrt(.5d0*(dsqrt(1.d0+tandm**2)-1.d0))
    ks1=fes(beta,ef)
    ks2=fes(beta,ef+.5d0*dy*ks1)
    ks3=fes(beta,ef+.5d0*dy*ks2)
    ks4=fes(beta,ef+dy*ks3)
    efelds(k)=efelds(k+1)+dy/6.d0*(ks1+2.d0*ks2+2.d0*ks3+ks4)
  enddo
  c
  return
  end

  c
  function fes(beta,ef)

159
implicit real*8(a-h,o-y)
c
fes=-beta*ef
c
return
dend
c
function epa(tt)
c
... computes dielectric loss for alumina
c    interpolates data of Westphal and Sils, p.26
c
implicit real*8(a-h,o-y)
real*8 kpts
dimension tpts(15),kpts(15)
data tpts/2.5d+01,9.9d+01,1.84d+02,2.81d+02,3.56d+02,4.3d+02
2,5.62d+02,7.05d+02,8.0d+02,9.03d+02,9.73d+02,1.025d+03
3,1.05d+03,1.109d+03,1.132d+03/
data kpts/9.31d0,9.41d0,9.58d0,9.72d0,9.84d0,9.96d0,10.17d0
2,10.42d0,10.63d0,10.86d0,10.98d0,11.17d0,11.22d0,11.38d0,11.41d0/
c
t=tt-2.73d+02
if(t.ge.tpts(15))then
    a=(kpts(15)-kpts(14))/(tpts(15)-tpts(14))
b=kpts(15)-a*tpts(15)
epa=a*t+b
return
endif
do 5 i=1,14
   x=tpts(i)
y=tpts(i+1)
   if(t.eq.x)then

160
epa=kpts(i)
return
elseif(t.gt.x.and.t.lt.y)then
  epa=kpts(i)+(t-x)*(kpts(i+1)-kpts(i))/(y-x)
  return
endif
5 continue
return
end

c
function epag(tt)
c
... computes dielectric loss for gamma alumina

c
  interpolates data of Mitch Jackson 5/97
c
implicit real*8(a-h,o-y)
real*8 kpts
dimension tpts(12),kpts(12)
data tpts/2.9d+01,3.5d+01,1.49d+02,2.62d+02,3.71d+02
2,4.78d+02,5.82d+02,6.84d+02,7.84d+02,8.81d+02,9.76d+02
3,1.068d+03/
data kpts/4.487d0,4.498d0,5.040d0,4.448d0,4.652d0
2,4.917d0,4.647d0,4.441d0,4.313d0,4.196d0,4.046d0
3,3.717d0/
c
t=tt-2.73d+02
if(t.ge.tpts(12))then
  a=(kpts(12)-kpts(11))/(tpts(12)-tpts(11))
  b=kpts(12)-a*tpts(12)
  epag=a*t+b
  return
endif
if(t .le. tpts(1)) then
    epag = kpts(1)
    return
endif

do 5 i = 1, 11
    x = tpts(i)
    y = tpts(i+1)
    if(t .eq. x) then
        epag = kpts(i)
        return
    elseif(t .gt. x .and. t .lt. y) then
        epag = kpts(i) + (t-x) * (kpts(i+1) - kpts(i)) / (y-x)
        return
    endif
5 continue
return
end

c

function eppa(tt)
c
... computes dielectric loss for alumina
interpolates data of Westphal and Sils, p.26
c
implicit real*8(a-h,o-y)
real*8 kpts
dimension tpts(15), kpts(15)
data tpts/2.5d+01, 9.9d+01, 1.84d+02, 2.81d+02, 3.56d+02, 4.3d+02,
2.562d+02, 7.05d+02, 8.0d+02, 9.03d+02, 9.73d+02, 1.025d+03, 1.05d+03,
3.109d+03, 1.132d+03/
data kpts/3.63d-03, 3.95d-03, 5.08d-03, 6.8d-03, 8.86d-03, 1.12d-02,
2.163d-02, 2.24d-02, 2.82d-02, 3.58d-02, 4.39d-02, 5.03d-02, 5.61d-02,
3.683d-02, 1.14d-01/
t=tt-2.73d+02
if(t.ge.tpts(15))then
   a=(kpts(15)-kpts(14))/(tpts(15)-tpts(14))
   b=kpts(15)-a*tpts(15)
   eppa=a*t+b
   return
endif
do 5 i=1,14
   x=tpts(i)
   y=tpts(i+1)
   if(t.eq.x)then
      eppa=kpts(i)
      return
   elseif(t.gt.x.and.t.lt.y)then
      eppa=kpts(i)+(t-x)*(kpts(i+1)-kpts(i))/(y-x)
      return
   endif
5 continue
return
end

function eppag(tt)

... computes dielectric loss for gamma alumina
interpolates data of Mitch Jackson 5/97

implicit real*8(a-h,o-y)
real*8 kpts
dimension tpts(12),kpts(12)
data tpts/2.9d+01,3.5d+01,1.49d+02,2.62d+02,3.71d+02,4.78d+02,5.82d+02,6.84d+02,7.84d+02,8.81d+02,9.76d+02
3,1.068d+03/
data kpts/0.3921d0,0.3893d0,0.2260d0,0.1703d0,0.1523d0
2,0.1541d0,0.1469d0,0.1547d0,0.1454d0,0.1681d0,0.1921d0
3,0.1311d0/
c
t=tt-2.73d+02
if(t.ge.tpts(12))then
  eppag=0.15d0
  return
endif
if(t.le.tpts(1))then
  eppag=kpts(1)
  return
endif
do 5 i=1,11
  x=tpts(i)
  y=tpts(i+1)
  if(t.eq.x)then
    eppag=kpts(i)
    return
  elseif(t.gt.x.and.t.lt.y)then
    eppag=kpts(i)+(t-x)*(kpts(i+1)-kpts(i))/(y-x)
    return
  endif
5 continue
return
end

c
function eppt(t1,dpt)
c
c...13 Oct 95
c
Test using formula (1-59) in Harrington

... computes dielectric loss for platinum

implicit double precision(a-h,o-y)

data eps0,pi,freq/8.854d-12,3.141592653589793d0,.915d+09/

data rho0,alph/10.6d-08,3.927d-03/

data rho0,alph/1.6d-08,3.75d-03/

rho=rho0*(1.d0+alph*(t1-2.93d2))
sig=1.d0/rho

...correct for "quantum dot" effect a la Nimtz, et al

sig=(dpt/5.0d-06)**3*sig

eppt=sig/(2.d0*pi*freq*eps0)

return
end

function cpgas(t)

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... specific heat for air

implicit real*8(a-h,o-y)
real*8 khes
dimension tpts(6), khes(6)
data tpts/2.d+02,3.d+02,4.d+02,6.d+02,8.d+02,1.d+03/
data khes/1.007d3,1.007d3,1.014d3,1.051d3,1.099d3,1.141d3/
if(t.ge.tpts(6))then
  a=(khes(6)-khes(5))/(tpts(6)-tpts(5))
  b=khes(6)-a*tpts(6)
  cpgas=a*t+b
  return
endif
do 5 i=1,5
  x=tpts(i)
  y=tpts(i+1)
  if(t.eq.x)then
    cpgas=khes(i)
    return
  elseif(t.gt.x.and.t.lt.y)then
    cpgas=khes(i)+(t-x)*(khes(i+1)-khes(i))/(y-x)
    return
  endif
5 continue
return
end

function cgas(t)
c

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c

... thermal conductivity for air
c

implicit real*8(a-h,o-y)
real*8 khes
dimension tpts(6), khes(6)
data tpts/2.d+02,3.d+02,4.d+02,6.d+02,8.d+02,1.d+03/
data khes/0.0181d0,0.0263d0,0.0338d0,0.0469d0,0.0573d0,0.0667d0/
if(t.ge.tpts(6))then
   a=(khes(6)-khes(5))/(tpts(6)-tpts(5))
   b=khes(6)-a*tpts(6)
   cgas=a*t+b
   return
endif
do 5 i=1,5
   x=tpts(i)
   y=tpts(i+1)
   if(t.eq.x)then
      cgas=khes(i)
      return
   elseif(t.gt.x.and.t.lt.y)then
      cgas=khes(i)+(t-x)*(khes(i+1)-khes(i))/(y-x)
      return
   endif
5 continue
return
end
c
function conpt(t)
c
29 June 1995
c
... thermal conductivity for platinum
c
implicit real*8(a-h,o-y)
real*8 kpts
dimension tpts(9),kpts(9)
data tpts/2.d+02,3.d+02,4.d+02,6.d+02,8.d+02,1.d+03,1.2d+03
2,1.5d+03,2.d+03/
data kpts/72.6d0,71.6d0,71.8d0,73.2d0,75.6d0,78.7d0,82.6d0,89.5d0,99.4d0/
if(t.ge.tpts(9))then
  a=(kpts(9)-kpts(8))/(tpts(9)-tpts(8))
  b=kpts(9)-a*tpts(9)
  conpt=a*t+b
  return
endif
do 5 i=1,8
  x=tpts(i)
  y=tpts(i+1)
  if(t.eq.x)then
    conpt=kpts(i)
    return
  elseif(t.gt.x.and.t.lt.y)then
    conpt=kpts(i)+(t-x)*(kpts(i+1)-kpts(i))/(y-x)
    return
  endif
5 continue
return
end

c

function cons(t,pf)
implicit real*8(a-h,o-y)
data refr,ext,sig/1.5d0,3.0d+03,5.669d-08/
data rho1,rho2/7.d+02,21.45d+03/
ye1=cal(t)
ye2=conpt(t)
vf=pf*rho1/((1.d0-pf)*rho2+pf*rho1)
yfac=(ye2-ye1)/(2.d0*ye1+ye2)
yem=(1.d0+2.d0*vf*yfac)/(1.d0-vf*yfac)*ye1
cons=yem

c  ks=0.95d0*cal(t)+0.05d0*kpt(t)
cons=cons+(1.6d1/3.d0)*refr**2*sig*t**3/ext
return
end
c

SUBROUTINE DGECO(A,LDA,N,IPVT,RCOND,Z)
  INTEGER LDA,N,IPVT(1)
  DOUBLE PRECISION A(LDA,1),Z(1)
  DOUBLE PRECISION RCOND
  DOUBLE PRECISION DDOT,EK,T,WK,WKM
  DOUBLE PRECISION ANORM,S,DASUM,SM,YNORM
  INTEGER INFO,J,K,KB,KP1,L
  ANORM = 0.0D0
  DO 10 J = 1, N
    ANORM = DMAX1(ANORM,DASUM(N,A(1,J),1))
  10 CONTINUE
  CALL DGEFA(A,LDA,N,IPVT,INFO)
  EK = 1.0D0
  DO 20 J = 1, N
    Z(J) = 0.0D0
  20 CONTINUE
  DO 100 K = 1, N
    IF (Z(K) .NE. 0.0D0) EK = DSIGN(EK,-Z(K))
    IF (DABS(EK-Z(K)) .LE. DABS(A(K,K))) GO TO 30
    S = DABS(A(K,K))/DABS(EK-Z(K))
    CALL DSCAL(N,S,Z,1)
    EK = S*EK
  30 CONTINUE
  WK = EK - Z(K)
  WKM = -EK - Z(K)
  S = DABS(WK)

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SM = DABS(WKM)
IF (A(K,K) .EQ. 0.0D0) GO TO 40
   WK = WK/A(K,K)
   WKM = WKM/A(K,K)
GO TO 50
40 CONTINUE
   WK = 1.0D0
   WKM = 1.0D0
50 CONTINUE
   KP1 = K + 1
   IF (KP1 .GT. N) GO TO 90
   DO 60 J = KP1, N
      SM = SM + DABS(Z(J)+WKM*A(K,J))
      Z(J) = Z(J) + WK*A(K,J)
      S = S + DABS(Z(J))
   60 CONTINUE
   IF (S .GE. SM) GO TO 80
      T = WKM - WK
      WK = WKM
      DO 70 J = KP1, N
         Z(J) = Z(J) + T*A(K,J)
   70 CONTINUE
80 CONTINUE
90 CONTINUE
   Z(K) = WK
100 CONTINUE
   S = 1.0D0/DASUM(N,Z,1)
   CALL DSCAL(N,S,Z,1)
   DO 120 KB = 1, N
      K = N + 1 - KB
      IF (K .LT. N) Z(K) = Z(K) + DDOT(N-K,A(K+1,K),1,Z(K+1),1)
      IF (DABS(Z(K)) .LE. 1.0D0) GO TO 110
120 CONTINUE
S = 1.0D0/DABS(Z(K))
CALL DSCAL(N,S,Z,1)

110 CONTINUE
L = IPVT(K)
T = Z(L)
Z(L) = Z(K)
Z(K) = T

120 CONTINUE
S = 1.0D0/DASUM(N,Z,1)
CALL DSCAL(N,S,Z,1)
YNORM = 1.0D0
DO 140 K = 1, N
  L = IPVT(K)
  T = Z(L)
  Z(L) = Z(K)
  Z(K) = T
  IF (K .LT. N) CALL DAXPY(N-K,T,A(K+1,K),1,Z(K+1),1)
  IF (DABS(Z(K)) .LE. 1.0D0) GO TO 130
    S = 1.0D0/DABS(Z(K))
    CALL DSCAL(N,S,Z,1)
    YNORM = S*YNORM
  130 CONTINUE
140 CONTINUE

140 CONTINUE
S = 1.0D0/DASUM(N,Z,1)
CALL DSCAL(N,S,Z,1)
YNORM = S*YNORM
DO 160 KB = 1, N
  K = N + 1 - KB
  IF (DABS(Z(K)) .LE. DABS(A(K,K))) GO TO 150
    S = DABS(A(K,K))/DABS(Z(K))
    CALL DSCAL(N,S,Z,1)
    YNORM = S*YNORM
  150 CONTINUE

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CONTINUE
IF (A(K,K) .NE. 0.0D0) Z(K) = Z(K)/A(K,K)
IF (A(K,K) .EQ. 0.0D0) Z(K) = 1.0D0
T = -Z(K)
CALL DAXPY(K-1,T,A(1,K),1,Z(1),1)

CONTINUE
S = 1.0D0/DASUM(N,Z,1)
CALL DSCAL(N,S,Z,1)
YNORM = S*YNORM
IF (ANORM .NE. 0.0D0) RCOND = YNORM/ANORM
IF (ANORM .EQ. 0.0D0) RCOND = 0.0D0
RETURN
END

SUBROUTINE DGEFA(A,LDA,N,IPVT,INFO)
INTEGER LDA,N,IPVT(1),INFO
DOUBLE PRECISION A(LDA,1)
DOUBLE PRECISION T
INTEGER IDAMAX,J,K,KP1,L,NM1
INFO = 0
NM1 = N - 1
IF (NM1 .LT. 1) GO TO 70
DO 60 K = 1, NM1
   KP1 = K + 1
   L = IDAMAX(N-K+1,A(K,K),1) + K - 1
   IPVT(K) = L
   IF (A(L,K) .EQ. 0.0D0) GO TO 40
      IF (L .EQ. K) GO TO 10
      T = A(L,K)
      A(L,K) = A(K,K)
      A(K,K) = T
   10 CONTINUE
   T = -1.0D0/A(K,K)

   CONTINUE
   IF (A(K,K) .NE. 0.0D0) Z(K) = Z(K)/A(K,K)
   IF (A(K,K) .EQ. 0.0D0) Z(K) = 1.0D0
   T = -Z(K)
   CALL DAXPY(K-1,T,A(1,K),1,Z(1),1)

   CONTINUE
   S = 1.0D0/DASUM(N,Z,1)
   CALL DSCAL(N,S,Z,1)
   YNORM = S*YNORM
   IF (ANORM .NE. 0.0D0) RCOND = YNORM/ANORM
   IF (ANORM .EQ. 0.0D0) RCOND = 0.0D0
   RETURN
END
CALL DSCAL(N-K,T,A(K+1,K),1)
DO 30 J = KP1, N
   T = A(L,J)
   IF (L .EQ. K) GO TO 20
      A(L,J) = A(K,J)
      A(K,J) = T
20    CONTINUE
      CALL DAXPY(N-K,T,A(K+1,K),1,A(K+1,J),1)
30    CONTINUE
   GO TO 50
40    CONTINUE
   INFO = K
50    CONTINUE
60    CONTINUE
70    CONTINUE
   IPVT(N) = N
   IF (A(N,N) .EQ. 0.0D0) INFO = N
RETURN
END
SUBROUTINE DAXPY(N,DA,DX,INCX,DY,INCY)
DOUBLE PRECISION DX(1),DY(1),DA
INTEGER I,INCX,INCY,IXIY,M,MP1,N
IF(N.LE.0)RETURN
IF (DA .EQ. 0.0D0) RETURN
IF(INCX.EQ.1.AND.INCY.EQ.1)GO TO 20
IX = 1
IY = 1
IF(INCX.LT.0)IX = (-N+1)*INCX + 1
IF(INCY.LT.0)IY = (-N+1)*INCY + 1
DO 10 I = 1,N
   DY(IY) = DY(IY) + DA*DX(IX)
   IX = IX + INCX
IY = IY + INCY

10 CONTINUE
RETURN

20 M = MOD(N,4)
IF( M .EQ. 0 ) GO TO 40
DO 30 I = 1,M
   DY(I) = DY(I) + DA*DX(I)
30 CONTINUE
IF( N .LT. 4 ) RETURN

40 MP1 = M + 1
DO 50 I = MP1,N,4
   DY(I) = DY(I) + DA*DX(I)
   DY(I + 1) = DY(I + 1) + DA*DX(I + 1)
   DY(I + 2) = DY(I + 2) + DA*DX(I + 2)
   DY(I + 3) = DY(I + 3) + DA*DX(I + 3)
50 CONTINUE
RETURN
END

DOUBLE PRECISION FUNCTION DDOT(N,DX,INCX,DY,INCY)
DOUBLE PRECISION DX(1),DY(1),DTEMP
INTEGER I,INCX,INCY,IX,IY,M,MP1,N
DDOT = 0.0D0
DTEMP = 0.0D0
IF(N.LE.0)RETURN
IF(INCX.EQ.1.AND.INCY.EQ.1)GO TO 20
IX = 1
IY = 1
IF(INCX.LT.0)IX = (-N+1)*INCX + 1
IF(INCY.LT.0)IY = (-N+1)*INCY + 1
DO 10 I = 1,N
   DTEMP = DTEMP + DX(IX)*DY(IY)
   IX = IX + INCX
10 CONTINUE
RETURN
IY = IY + INCY
10 CONTINUE
DDOT = DTEMP
RETURN
20 M = MOD(N,5)
   IF( M .EQ. 0 ) GO TO 40
   DO 30 I = 1,M
      DTEMP = DTEMP + DX(I)*DY(I)
   30 CONTINUE
   IF( N .LT. 5 ) GO TO 60
40 MP1 = M + 1
   DO 50 I = MP1,N,5
      DTEMP = DTEMP + DX(I)*DY(I) + DX(I + 1)*DY(I + 1) +
             DX(I + 2)*DY(I + 2) + DX(I + 3)*DY(I + 3) + DX(I + 4)*DY(I + 4)
   50 CONTINUE
60 DDOT = DTEMP
RETURN
END
SUBROUTINE DSCAL(N,DA,DX,INCX)
DOUBLE PRECISION DA,DX(1)
INTEGER I,INCX,M,MP1,N,NINCX
IF(N.LE.0)RETURN
IF(INCX.EQ.1)GO TO 20
NINCX = N*INCX
   DO 10 I = 1,NINCX,INCX
      DX(I) = DA*DX(I)
   10 CONTINUE
RETURN
20 M = MOD(N,5)
   IF( M .EQ. 0 ) GO TO 40
   DO 30 I = 1,M
      DX(I) = DA*DX(I)
   30 CONTINUE
CONTINUE
IF( N .LT. 5 ) RETURN

MP1 = M + 1
DO 50 I = MP1,N,5
  DX(I) = DA*DX(I)
  DX(I + 1) = DA*DX(I + 1)
  DX(I + 2) = DA*DX(I + 2)
  DX(I + 3) = DA*DX(I + 3)
  DX(I + 4) = DA*DX(I + 4)
50 CONTINUE
RETURN
END

DOUBLE PRECISION FUNCTION DASUM(N,DX,INCX)
DOUBLE PRECISION DX(1),DTEMP
INTEGER I,INCX,M,MP1,N,NINCX
DASUM = 0.0D0
DTEMP = 0.0D0
IF(N.LE.0)RETURN
IF(INCX.EQ.1)GO TO 20
NINCX = N*INCX
DO 10 I = 1,NINCX,INCX
  DTEMP = DTEMP + DABS(DX(I))
10 CONTINUE
DASUM = DTEMP
RETURN
20 M = MOD(N,6)
  IF( M .EQ. 0 ) GO TO 40
  DO 30 I = 1,M
    DTEMP = DTEMP + DABS(DX(I))
30 CONTINUE
  IF( N .LT. 6 ) GO TO 60
40 MP1 = M + 1
DO 50 I = MP1,N,6
    DTEMP = DTEMP + DABS(DX(I)) + DABS(DX(I + 1)) + DABS(DX(I + 2))
    * + DABS(DX(I + 3)) + DABS(DX(I + 4)) + DABS(DX(I + 5))
50 CONTINUE
60 DASUM = DTEMP
RETURN
END

INTEGER FUNCTION IDAMAX(N,DX,INCX)
DOUBLE PRECISION DX(1),DMAX
INTEGER I,INCX,IX,N
IDAMAX = 0
IF( N .LT. 1 ) RETURN
IDAMAX = 1
IF(N.EQ.1)RETURN
IF(INCX.EQ.1)GO TO 20
IX = 1
DMAX = DABS(DX(1))
IX = IX + INCX
DO 10 I = 2,N
    IF(DABS(DX(IX)).LE.DMAX) GO TO 30
    IDAMAX = I
    DMAX = DABS(DX(IX))
10 CONTINUE
RETURN
20 DMAX = DABS(DX(1))
DO 30 I = 2,N
    IF(DABS(DX(I)).LE.DMAX) GO TO 30
    IDAMAX = I
    DMAX = DABS(DX(I))
30 CONTINUE
RETURN
SUBROUTINE DGESL(A,LDA,N,IPVT,B,JOB)
INTEGER LDA,N,IPVT(1),JOB
DOUBLE PRECISION A(LDA,1),B(1)
DOUBLE PRECISION DDOT,T
INTEGER K,KB,L,NM1
NM1 = N - 1
IF (JOB .NE. 0) GO TO 50
  IF (NM1 .LT. 1) GO TO 30
  DO 20 K = 1, NM1
    L = IPVT(K)
    T = B(L)
    IF (L .EQ. K) GO TO 10
      B(L) = B(K)
      B(K) = T
  10 CONTINUE
  CALL DAXPY(N-K,T,A(K+1,K),1,B(K+1),1)
  20 CONTINUE
  30 CONTINUE
  DO 40 KB = 1, N
    K = N + 1 - KB
    B(K) = B(K)/A(K,K)
    T = -B(K)
    CALL DAXPY(K-1,T,A(1,K),1,B(1),1)
  40 CONTINUE
GO TO 100
  50 CONTINUE
  DO 60 K = 1, N
    T = DDOT(K-1,A(1,K),1,B(1),1)
    B(K) = (B(K) - T)/A(K,K)
  60 CONTINUE
IF (NM1 .LT. 1) GO TO 90
END
DO 80 KB = 1, NM1
   K = N - KB
   B(K) = B(K) + DDOT(N-K,A(K+1,K),1,B(K+1),1)
   L = IPVT(K)
   IF (L .EQ. K) GO TO 70
      T = B(L)
      B(L) = B(K)
      B(K) = T
70    CONTINUE
80    CONTINUE
90    CONTINUE
100   CONTINUE
RETURN
END

SUBROUTINE LIN(ID,IT,IPVT,U,V,S,E,WORK,A,LDA,N,B)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION A(LDA,1),B(1)
DIMENSION IPVT(1)
DIMENSION U(LDA,1),V(LDA,1),S(1),E(1),WORK(1)
1001 FORMAT(25X,'INFO not equal to zero in LIN')
1002 FORMAT(22X,'Incorrect use of ID and/or IT in LIN')
1003 FORMAT(10X,I3,1X,'SINGULAR VALUE(S) LESS THAN 10-14 OBTAINED')
   IF((ID.NE.1).AND.(ID.NE.2).AND.(IT.NE.1).AND.(IT.NE.2))THEN
      WRITE(2,1002)
   ENDIF
   IF(ID.EQ.2)THEN
      IF(IT.NE.2)THEN
         JOB=11
         CALL DSVDC(A,LDA,N,N,S,E,U,LDA,V,LDA,WORK,JOB,INFO)
         IF(INFO.NE.0)THEN
            WRITE(2,1001)
STOP
ENDIF
INDEX=0
VVV=S(I)
DO 10 I=1,N
   CN=S(I)/VVV
   IF(CN.LT.1.D-14)THEN
      INDEX=INDEX+1
      S(I)=0.D0
      IF(I.EQ.N)WRITE(2,1003)INDEX
      ELSE
         S(I)=1.D0/S(I)
      ENDIF
   10 CONTINUE
   IF(INDEX.GT.5) STOP
ENDIF
DO 20 I=1,N
   WORK(I)=0.D0
20 CONTINUE
DO 40 I=1,N
   DO 30 J=1,N
      WORK(I)=WORK(I)+U(J,I)*B(J)*S(I)
30 CONTINUE
40 CONTINUE
DO 50 I=1,N
   B(I)=0.D0
50 CONTINUE
DO 70 J=1,N
   DO 60 I=1,N
      B(I)=B(I)+V(I,J)*WORK(J)
60 CONTINUE
70 CONTINUE
ELSE
  JOB=0
ENDIF
ENDIF
END

SUBROUTINE DSVDC(X,LDX,N,P,S,E,U,LDU,V,LDV,WORK,JOB,INFO)
INTEGER LDX,N,P,LDU,LDV,JOB,INFO
DOUBLE PRECISION X(LDX,1),S(1),E(1),U(LDU,1),V(LDV,1),WORK(1)
INTEGER I,ITER,J,JOBU,K,KASE,KK,L,LL,LLS,LM1,LP1,LS,LU,M,MAXIT,
* MM,MM1,MP1,NCT,NCTP1,NCU,NRT,NRTP1
DOUBLE PRECISION DDOT,T,R
DOUBLE PRECISION B,C,CS,EL,EMM1,F,G,DNRM2,SCALE,SHIFT,SL,SM,SN,
* SMM1,T1,TEST,ZTEST
LOGICAL WANTU,WANTV
MAXIT = 50
WANTU = .FALSE.
WANTV = .FALSE.
JOBU = MOD(JOB,100)/10
NCU = N
IF (JOBU .GT. 1) NCU = MIN0(N,P)
IF (JOBU .NE. 0) WANTU = .TRUE.
IF (MOD(JOB,10) .NE. 0) WANTV = .TRUE.
INFO = 0
NCT = MINO(N-1,P)
NRT = MAXO(0,MINO(P-2,N))

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LU = MAXO(NCT,NRT)

IF (LU .LT. 1) GO TO 170

DO 160 L = 1, LU

LP1 = L + 1

IF (L .GT. NCT) GO TO 20

S(L) = DNRM2(N-L+1,X(L,L),1)

IF (S(L) .EQ. 0.0D0) GO TO 10

IF (X(L,L) .NE. 0.0D0) S(L) = DSIGN(S(L),X(L,L))

CALL DSCAL(N-L+1,1.0D0/S(L),X(L,L),1)

X(L,L) = 1.0D0 + X(L,L)

10 CONTINUE

S(L) = -S(L)

20 CONTINUE

IF (P .LT. LP1) GO TO 50

DO 40 J = LP1, P

IF (L .GT. NCT) GO TO 30
IF (S(L) .EQ. 0.0D0) GO TO 30

\[ T = -\text{DDOT}(N-L+1,X(L,L),1,X(L,J),1)/X(L,L) \]

CALL DAXPY(N-L+1,T,X(L,L),1,X(L,J),1)

30     CONTINUE

E(J) = X(L,J)

40     CONTINUE

50     CONTINUE

IF (.NOT.WANTU .OR. L .GT. NCT) GO TO 70

DO 60 I = L, N

\[ U(I,L) = X(I,L) \]

60     CONTINUE

70     CONTINUE

IF (L .GT. NRT) GO TO 150

\[ E(L) = \text{DNRM2}(P-L,E(LP1),1) \]

IF (E(L) .EQ. 0.0D0) GO TO 80

IF (E(LP1) .NE. 0.0D0) E(L) = DSIGN(E(L),E(LP1))
CALL DSCAL(P-L, 1.0D0/E(L), E(LP1), 1)

E(LP1) = 1.0D0 + E(LP1)

80 CONTINUE

E(L) = -E(L)

IF (LP1 .GT. N .OR. E(L) .EQ. 0.0D0) GO TO 120

DO 90 I = LP1, N

   WORK(I) = 0.0D0

90 CONTINUE

DO 100 J = LP1, P

   CALL DAXPY(N-L, E(J), X(LP1, J), 1, WORK(LP1), 1)

100 CONTINUE

DO 110 J = LP1, P

   CALL DAXPY(N-L, -E(J)/E(LP1), WORK(LP1), 1, X(LP1, J), 1)

110 CONTINUE

120 CONTINUE
IF (.NOT.WANTV) GO TO 140

DO 130 I = LP1, P

V(I,L) = E(I)

130    CONTINUE

140    CONTINUE

150    CONTINUE

160    CONTINUE

170    CONTINUE

M = MIN0(P,N+1)

NCTP1 = NCT + 1

NRTP1 = NRT + 1

IF (NCT .LT. P) S(NCTP1) = X(NCTP1,NCTP1)

IF (N .LT. M) S(M) = 0.0D0

IF (NRTP1 .LT. M) E(NRTP1) = X(NRTP1,M)

E(M) = 0.0D0

IF (.NOT.WANTU) GO TO 300
IF (NCU .LT. NCTP1) GO TO 200

DO 190 J = NCTP1, NCU

DO 180 I = 1, N

U(I,J) = 0.0D0

180 CONTINUE

U(J,J) = 1.0D0

190 CONTINUE

200 CONTINUE

IF (NCT .LT. 1) GO TO 290

DO 280 LL = 1, NCT

L = NCT - LL + 1

IF (S(L) .EQ. 0.0D0) GO TO 250

LP1 = L + 1

IF (NCU .LT. LP1) GO TO 220

DO 210 J = LP1, NCU

T = -DDOT(N-L+1,U(L,L),1,U(L,J),1)/U(L,L)

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CALL DAXPY(N-L+1,T,U(L,L),1,U(L,J),1)

210 CONTINUE

220 CONTINUE

CALL DSCAL(N-L+1,-1.0D0,U(L,L),1)

U(L,L) = 1.0D0 + U(L,L)

LM1 = L - 1

IF (LM1 .LT. 1) GO TO 240

DO 230 I = 1, LM1

U(I,L) = 0.0D0

230 CONTINUE

240 CONTINUE

GO TO 270

250 CONTINUE

DO 260 I = 1, N

U(I,L) = 0.0D0

260 CONTINUE
U(L,L) = 1.0D0

270 CONTINUE

280 CONTINUE

290 CONTINUE

300 CONTINUE

IF (.NOT.WANTV) GO TO 350

DO 340 LL = 1, P

L = P - LL + 1

LP1 = L + 1

IF (L .GT. NRT) GO TO 320

IF (E(L) .EQ. 0.0D0) GO TO 320

DO 310 J = LP1, P

T = -DDOT(P-L,V(LP1,L),1,V(LP1,J),1)/V(LP1,L)

CALL DAXPY(P-L,T,V(LP1,L),1,V(LP1,J),1)

310 CONTINUE
320 CONTINUE

DO 330 I = 1, P

V(I,L) = 0.0D0

330 CONTINUE

V(L,L) = 1.0D0

340 CONTINUE

350 CONTINUE

MM = M

ITER = 0

360 CONTINUE

IF (M .EQ. 0) GO TO 620

IF (ITER .LT. MAXIT) GO TO 370

INFO = M

GO TO 620

370 CONTINUE

DO 390 LL = 1, M
L = M - LL

IF (L .EQ. 0) GO TO 400

TEST = DABS(S(L)) + DABS(S(L+1))

ZTEST = TEST + DABS(E(L))

IF (ZTEST .NE. TEST) GO TO 380

E(L) = 0.0D0

GO TO 400

380 CONTINUE

390 CONTINUE

400 CONTINUE

IF (L .NE. M - 1) GO TO 410

KASE = 4

GO TO 480

410 CONTINUE

LP1 = L + 1

MP1 = M + 1
DO 430 LLS = LP1, MP1

    LS = M - LLS + LP1

    IF (LS .EQ. L) GO TO 440

    TEST = 0.0D0

    IF (LS .NE. M) TEST = TEST + DABS(E(LS))

    IF (LS .NE. L + 1) TEST = TEST + DABS(E(LS-1))

    ZTEST = TEST + DABS(S(LS))

    IF (ZTEST .NE. TEST) GO TO 420

    S(LS) = 0.0D0

    GO TO 440

420       CONTINUE

430       CONTINUE

440       CONTINUE

    IF (LS .NE. L) GO TO 450

    KASE = 3

    GO TO 470
450 CONTINUE

IF (LS .NE. M) GO TO 460

KASE = 1

GO TO 470

460 CONTINUE

KASE = 2

L = LS

470 CONTINUE

480 CONTINUE

L = L + 1

GO TO (490,520,540,570), KASE

490 CONTINUE

MM1 = M - 1

F = E(M-1)

E(M-1) = 0.0D0

DO 510 KK = L, MM1
K = MM1 - KK + L

T1 = S(K)

CALL DROTG(T1,F,CS,SN)

S(K) = T1

IF (K .EQ. L) GO TO 500

F = -SN*E(K-1)

E(K-1) = CS*E(K-1)

500 CONTINUE

IF (WANTV) CALL DROT(P,V(1,K),1,V(1,M),1,CS,SN)

510 CONTINUE

GO TO 610

520 CONTINUE

F = E(L-1)

E(L-1) = 0.0D0

DO 530 K = L, M

T1 = S(K)

193
CALL DROTG(T1,F,CS,SN)

S(K) = T1

F = -SN*E(K)

E(K) = CS*E(K)

IF (WANTU) CALL DROT(N,U(1,K),1,U(1,L-1),1,CS,SN)

530 CONTINUE

GO TO 610

540 CONTINUE

SCALE = DMAX1(DABS(S(M)),DABS(S(M-1)),DABS(E(M-1)),

* DABS(S(L)),DABS(E(L)))

SM = S(M)/SCALE

SMM1 = S(M-1)/SCALE

EMM1 = E(M-1)/SCALE

SL = S(L)/SCALE

EL = E(L)/SCALE

B = ((SMM1 + SM)*(SMM1 - SM) + EMM1**2)/2.0D0
C = (SM*EMM1)**2

SHIFT = 0.0D0

IF (B .EQ. 0.0D0 .AND. C .EQ. 0.0D0) GO TO 550

SHIFT = DSQRT(B**2+C)

IF (B .LT. 0.0D0) SHIFT = -SHIFT

SHIFT = C/(B + SHIFT)

550 CONTINUE

F = (SL + SM)*(SL - SM) - SHIFT

G = SL*EL

MM1 = M - 1

DO 560 K = L, MM1

CALL DROTG(F,G,CS,SN)

IF (K .NE. L) E(K-1) = F

F = CS*S(K) + SN*E(K)

E(K) = CS*E(K) - SN*S(K)

G = SN*S(K+1)

195
\[ S(K+1) = CS \cdot S(K+1) \]

\[ \text{IF (WANTV) CALL DROT(P,V(1,K),1,V(1,K+1),1,CS,SN)} \]

\[ \text{CALL DROTG(F,G,CS,SN)} \]

\[ S(K) = F \]

\[ F = CS \cdot E(K) + SN \cdot S(K+1) \]

\[ S(K+1) = -SN \cdot E(K) + CS \cdot S(K+1) \]

\[ G = SN \cdot E(K+1) \]

\[ E(K+1) = CS \cdot E(K+1) \]

\[ \text{IF (WANTU .AND. K .LT. N)} \]

\[ * \quad \text{CALL DROT(N,U(1,K),1,U(1,K+1),1,CS,SN)} \]

560 CONTINUE

\[ E(M-1) = F \]

\[ \text{ITER = ITER + 1} \]

GO TO 610

570 CONTINUE

\[ \text{IF (S(L) .GE. 0.0D0) GO TO 580} \]
S(L) = -S(L)

IF (WANTV) CALL DSCAL(P,-1.0D0,V(1,L),1)

580 CONTINUE

590 IF (L .EQ. MM) GO TO 600

IF (S(L) .GE. S(L+1)) GO TO 600

T = S(L)

S(L) = S(L+1)

S(L+1) = T

IF (WANTV .AND. L .LT. P)

* CALL DSWAP(P,V(1,L),1,V(1,L+1),1)

IF (WANTU .AND. L .LT. N)

* CALL DSWAP(N,U(1,L),1,U(1,L+1),1)

L = L + 1

GO TO 590

600 CONTINUE

ITER = 0
M = M - 1

610 CONTINUE

GO TO 360

620 CONTINUE

RETURN

END

c

SUBROUTINE DSWAP (N,DX,INCX,DY,INCY)

DOUBLE PRECISION DX(1),DY(1),DTEMP

INTEGER I,INCX,INCY,IX,IY,M,MP1,N

IF(N.LE.0)RETURN

IF(INCX.EQ.1.AND.INCY.EQ.1)GO TO 20

IX = 1

IY = 1

IF(INCX.LT.0)IX = (-N+1)*INCX + 1

IF(INCY.LT.0)IY = (-N+1)*INCY + 1
DO 10 I = 1,N

DTEMP = DX(IX)

DX(IX) = DY(IY)

DY(IY) = DTEMP

IX = IX + INCX

IY = IY + INCY

10 CONTINUE

RETURN

20 M = MOD(N,3)

IF( M .EQ. 0 ) GO TO 40

DO 30 I = 1,M

DTEMP = DX(I)

DX(I) = DY(I)

DY(I) = DTEMP

30 CONTINUE

IF( N .LT. 3 ) RETURN
40 MP1 = M + 1

DO 50 I = MP1,N,3

DTEMP = DX(I)

DX(I) = DY(I)

DY(I) = DTEMP

DTEMP = DX(I + 1)

DX(I + 1) = DY(I + 1)

DY(I + 1) = DTEMP

DTEMP = DX(I + 2)

DX(I + 2) = DY(I + 2)

DY(I + 2) = DTEMP

50 CONTINUE

RETURN

END

c

SUBROUTINE DROTG(DA,DB,C,S)
DOUBLE PRECISION DA,DB,C,S,ROE,SCALE,R,Z

ROE = DB

IF( DABS(DA) .GT. DABS(DB) ) ROE = DA

SCALE = DABS(DA) + DABS(DB)

IF( SCALE .NE. 0.0D0 ) GO TO 10

    C = 1.0D0

    S = 0.0D0

    R = 0.0D0

    GO TO 20

10   R = SCALE*DSQRT((DA/SCALE)**2 + (DB/SCALE)**2)

    R = DSIGN(1.0D0,ROE)*R

    C = DA/R

    S = DB/R

20   Z = 1.0D0

    IF( DABS(DA) .GT. DABS(DB) ) Z = S

    DA = R


DB = Z

RETURN

END

c

DOUBLE PRECISION FUNCTION DNRM2 ( N, DX, INCX)

INTEGER NEXT

DOUBLE PRECISION DX(1), CUTLO, CUTHI, HITEST, SUM, XMAX,ZERO,ONE

DATA ZERO, ONE /0.0D0, 1.0D0/

DATA CUTLO, CUTHI / 8.232D-11, 1.304D19 /

IF(N .GT. 0) GO TO 10

DNRM2= ZERO

GO TO 300

10 ASSIGN 30 TO NEXT

SUM = ZERO

NN = N * INCX

I = 1
20 GO TO NEXT,(30, 50, 70, 110)

30 IF( DABS(DX(I)) .GT. CUTLO) GO TO 85

    ASSIGN 50 TO NEXT

    XMAX = ZERO

50 IF( DX(I) .EQ. ZERO) GO TO 200

    IF( DABS(DX(I)) .GT. CUTLO) GO TO 85

    ASSIGN 70 TO NEXT

    GO TO 105

100 I = J

    ASSIGN 110 TO NEXT

    SUM = (SUM / DX(I)) / DX(I)

105 XMAX = DABS(DX(I))

    GO TO 115

70 IF( DABS(DX(I)) .GT. CUTLO ) GO TO 75

110 IF( DABS(DX(I)) .LE. XMAX ) GO TO 115

    SUM = ONE + SUM * (XMAX / DX(I))**2

    GO TO 115
XMAX = DABS(DX(I))

GO TO 200

115 SUM = SUM + (DX(I)/XMAX)**2

GO TO 200

75 SUM = (SUM * XMAX) * XMAX

85 Hittest = CUTHI/FLOAT( N )

DO 95 J =I,NN,INCX

IF(DABS(DX(J)) .GE. Hittest) GO TO 100

95 SUM = SUM + DX(J)**2

DNRM2 = DSQRT( SUM )

GO TO 300

200 CONTINUE

I = I + INCX

IF ( I .LE. NN ) GO TO 20

DNRM2 = XMAX * DSQRT(SUM)

300 CONTINUE
SUBROUTINE DROT (N,DX,INCX,DY,INCY,C,S)

C

C APPLIES A PLANE ROTATION.

C JACK DONGARRA, LINPACK, 3/11/78.

C

DOUBLE PRECISION DX(1),DY(1),DTEMP,C,S

INTEGER I,INCX,INCY,IX,IY,N

C

IF(N.LE.0)RETURN

IF(INCX.EQ.1.AND.INCY.EQ.1)GO TO 20

C

C CODE FOR UNEQUAL INCREMENTS OR EQUAL INCREMENTS NOT EQUAL

C TO 1
C

IX = 1

IY = 1

IF(INCX.LT.0) IX = (-N+1)*INCX + 1

IF(INCY.LT.0) IY = (-N+1)*INCY + 1

DO 10 I = 1,N

DTEMP = C*DX(IX) + S*DY(IY)

DY(IY) = C*DY(IY) - S*DX(IX)

DX(IX) = DTEMP

IX = IX + INCX

IY = IY + INCY

10 CONTINUE

RETURN

C

C CODE FOR BOTH INCREMENTS EQUAL TO 1
20 DO 30 I = 1,N

DTEMP = C*DX(I) + S*DY(I)

DY(I) = C*DY(I) - S*DX(I)

DX(I) = DTEMP

30 CONTINUE

RETURN

END
Vita

Max Savransky was born in Ukraine Kiev, on November 16, 1971. In June of 1979, Max and his family arrived in New York City after spending a two weeks in Austria and three months in Italy. In 1987, Max began in Fair Lawn High School in New Jersey, and in June of 1990 he received his high school diploma. In the fall of 1990, Max began his undergraduate studies at The New Jersey Institute of Technology, and in the spring of 1994 he received his Bachelor of Science degree in Mechanical Engineering. In the Fall of 1994, Max began his graduate studies in at The Virginia Polytechnic Institute and State University. He completed his Master of Science degree in Mechanical Engineering in December 1996. He then continued his studies as a doctoral student while also pursuing the Master of Science degree in Mathematics which he completed in May 2003. He completed his Ph.D in Mechanical Engineering in December of 2003.

Permanent Address: 36-03 Stelton Terrace
Fair Lawn, NJ 07410

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