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3-D Turbulent Particle Dispersion Submodel Development

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Project Manager: James Hickerson

from the Department of Chemical Engineering
University of Utah
Salt Lake City, UT 84112

Graduate Students: S. Jain & S. Kumar

Phillip J. Smith

principal investigator

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1.0 Abstract

The lack of a mathematical description of the interactions of fluid turbulence with other physico-chemical processes is a major obstacle in modeling many industrial processes. Turbulent two-phase flow is a phenomenon that is of significant practical importance to coal combustion as well as other disciplines. The interactions of fluid turbulence with the particulate phase have yet to be accurately and efficiently modeled for these industrial applications.

On 15 April 1991 work was initiated to cover four major tasks toward the development of a computational submodel for turbulent particle dispersion that would be applicable to coal combustion simulations. Those four tasks are:

1. A critical evaluation of the 2-D Lagrangian particle dispersion submodel,
2. Development of 3-D submodels for turbulent particle dispersion,
3. Evaluation of the 3-D submodels for turbulent particle dispersion,
4. Exploration of extensions of the Lagrangian dispersion theory to other applications including chemistry-turbulence interactions.

Work on task 1 had been essentially completed during the first quarter of this project. The framework of a 3-D model had been initiated as per task 2. This report summarizes work accomplished during the second quarter of this project which involves the development of solution algorithms for the theory described in our last quarterly report. The algorithms described in this report involve not only the solution procedures for two turbulence dispersion submodels (one for dilute phases and one for dense phases), but how those submodels can be coupled with the fluid-dynamics, heat transfer and reaction chemistry submodels. Specifically, it describes the procedures for incorporation of particle dispersion submodels into the existing framework of a coal combustion model developed by the principal investigator under separate funding.

2.0 Overview of Project

Many practical combustion processes which use solid particles, liquid droplets, or slurries as fuels introduce these fuels into turbulent environments. Examples include spray combustion, pulverized coal and coal slurry combustion, fluidized beds, sorbent injection, and hazardous waste incineration. The interactions of the condensed phases with turbulent environment have not been well described. Such a description is complicated by the difficulty of describing turbulence in general, even in the absence of particles or droplets. But the complications in describing the dispersion and reaction of the condensed phases in turbulent environments do not stem entirely or even primarily from the uncertainties in the description of the turbulence. Theoretical descriptions of the turbulent dispersion of particles and droplets are not well established, even when the characteristics of the turbulence are known.

Several reviews of turbulent particle dispersion document the progress in this area of research to date. Faeth [1983] provides a review of mixing and transport in turbulent spray environments. Other discussions of some of the aspects of turbulent dispersion of particles are developed by Kuo [1986], Hinze [1975], Goldschmidt and coworkers [1972], Fletcher [1980], Lumley [1978], Chigier [1976], Lilly [1973], Crowe [1982], and Smith and Baxter [1986]. In terms of an analytical and comprehensive description of turbulent dispersion, Shuen and coworkers [1983] have shown modifications of a model originally proposed by Gosman and Ioannides [1981] which yields reasonably good predictions in a variety of flows and could be viewed as the most rigorous technique currently available. The approach, called a stochastic separated flow (SSF) model, is essentially a Monte-Carlo simulation of the particle flow field. Several thousand trajectories are typically used to compute the overall particle or droplet behavior. The success of this approach is also strongly dependent on a rather arbitrary choice of methods of evaluating its parameters. Other approaches, which are both less computationally intensive and less rigorous, are discussed by Smith and Baxter [1986] and Fletcher [1980]. The success of these models also depends on the accuracy of modeled terms. A truly fundamental description of turbulent dispersion cast in a computationally efficient form has not yet been documented in the literature.

2.1 3-D Modeling

The emphasis of current research by the principal investigator and funded by other agencies in this area is the development of a three-dimensional predictive computer program to simulate the combustion process in industrial pulverized coal-fired furnaces. Among the difficulties inherent to this development is the disparity of scales in industrial configurations and the subsequent resolution of nodal properties in areas of large numerical gradients, both of which are issues for turbulent particle dispersion. In order for computer simulations to be economically feasible, the code must incorporate the most efficient applicable numerical technique. The computer model is based on an extension of previous research performed in the development of two-dimensional combustion codes, for example, Smoot and Smith [1985].

Figure 1 Three-dimensional computational mesh using 114,240 (84x34x40) grid points. The first view shows a slice off the near side to illustrate the computational domain and the walls (note the 12 burners and the refined mesh through them).

Several furnace configurations have been successfully solved with the 3-D model. These have included wall-fired and corner-fired furnaces. For illustrative purposes, a sample calculation is shown in Figure 1 and Figure 2. The sample is that of a wall-fired utility boiler burning natural gas fuel. The grid spacing used in this case is illustrated in

Figure 1. Grid points (computational nodes) are located at each intersection of any two lines. For simplicity, only the outside faces of the computational domain are shown, but the grid spacing is continued throughout the domain.

The predicted flow and temperature fields for this boiler are illustrated in with several planes cutting the three-dimensional computation.

Figure 2 Flow and Temperature field for computation of Figure 1. Notice the velocity vectors at the outlet plane and the streakline showing a particle path for a particle entering the bottom burner.

2.2 Work Statements

The work to be accomplished under this contract over a two year period is to develop a new three-dimensional particle dispersion submodel, incorporated into a 3-D coal combustion model, and evaluate it. The tasks for the accomplishment of this work are as follows:

2.2.1 Task 1: Critical Evaluation of 2-D Lagrangian Particle Dispersion Model

The work accomplished to date on two dimensional geometries will be critically evaluated by comparison of predictions to a wide set of experimental conditions. The

experimental data will be selected based on the best available information for particle dispersion. Specific emphasis will be placed on data that are similar to pulverized coal combustion applications. But, evaluation will also explore wider ranges of applicability for example, dense-phase (fluidized bed) applications, liquid phase dispersion, etc. depending on data availability.

- Duration: 0.75 years
- Deliverables: A detailed report and technical papers summarizing model evaluation including applicability and limitations.

2.2.2 Task 2: Development of 3-D Submodel for Turbulent Particle Dispersion

The two-dimensional submodel theory and computer coding will be extended to include Cartesian, and if possible polar-cylindrical three-dimensional geometries. The submodel will be incorporated into an existing 3-D comprehensive coal combustion model and rendered applicable to practical, industrial furnaces. This will include the incorporation of appropriate boundary conditions to handle multiple inlets and arbitrary flow intrusions. The submodel will be developed for reacting coal systems with poly-dispersed size distributions.

- Duration: 1 year
- Deliverables: 1) The implementation of a 3-D comprehensive combustion model with the new 3-D particle dispersion model incorporated on a unix-based engineering workstation at PETC and made available in the public domain. 2) User's manual. 3) Technical report and papers on a 3-D particle dispersion model theory.

2.2.3 Task 3: Evaluation of 3-D Particle Dispersion Submodel

Upon completion of the development of the 3-D dispersion model, evaluation of its applicability will be initiated. The evaluation will proceed from simple, well defined systems to complex industrial applications. The assumptions and theory of the dispersion model will be tested independent of other comprehensive modeling assumptions as much as possible then proceed to increasingly more coupling with the comprehensive model. This will include coal flow particle mixing cases to fully reacting coal combustion furnaces. The best available data for model testing will be sought as a part of this evaluation.

- Duration: 1 year
- Deliverables: A report and technical papers enumerating the applicability and limitations of 3-D particle dispersion predictability.

2.2.4 Task 4: Extension of Lagrangian Dispersion Theory to other Applications

An effort will be made to explore the applicability of the new Lagrangian particle dispersion model to other physical situations. Particle dispersion is a turbulence interaction process much like gaseous fluid element turbulent interaction. There is a potential for computing interactions between fluid turbulence and chemical kinetics by using the same theory. This potential will be explored. Other turbulence interaction processes will be examined to evaluate the potential for application of this new theory.

- Duration: 1.25 years
- Deliverables: A report on the applications of the pdf Lagrangian dispersion theory to turbulence interaction processes.

2.3 Outline of Remainder of Report

In the remainder of this report the results of the algorithm development of the two new methods are outlined in two major sections. Here the discussion is broken into two approaches, one for lightly loaded particle systems the other for densely loaded systems. The applicability of the two methods necessarily has some overlap, the range of each method is discussed within each section. First we discuss lightly loaded systems in section 3. Then we discuss dense systems in section 4. A statement of status and plans follows in section 5.

3.0 Dilute Particle Phase Dispersion Model Development

3.1 Introduction

A major obstacle in the development of a three dimensional predictive computer program to simulate the combustion process in industrial, pulverized coal fired furnaces has been the inability to incorporate an adequate submodel describing the turbulent dispersion of the particle phase. A three dimensional comprehensive combustion

code [Smith,1990] has been developed over the past few years for gaseous combustion.

As discussed in the previous quarterly report, a particle cloud model for predicting the stochastic transport of particles was presented that has the potential for accurately and efficiently describing turbulent particle dispersion within the framework of a comprehensive combustion code. Some of the basic attributes of this model have been previously incorporated in a comprehensive simulation of coal combustion for a *two dimensional* axisymmetric case, called the reacting, mixing limited flow model or REMIF.

The primary goal of this research effort is to incorporate a theoretically sound particle submodel into a *three dimensional* combustion model applicable to practical, industrial furnaces. Preliminary work in this direction has been done in the last quarter and this section outlines the proposed algorithm for achieving these goals.

Section 3.2 describes the framework of the calculations in REMIF which will be the same as in the 3D model and discusses the extension of the turbulent particle dispersion calculations to three dimensions. Section 3.3 discusses the formulation and algorithm of the REMIF code and identifies the particle phase submodel. Section 3.4 briefly discusses the incorporation of this submodel in the 3D combustion code.

3.2 Framework of the 3D Particle Dispersion Submodel Coupled to a Combustion Code

The algorithmic structure of the test code in two-dimensions (REMIF) will be used as the framework for incorporating the 3D particle dispersion theory described in the previous quarterly report. This section gives the algorithm for that model. A full description of the REMIF computer model will not be given here, but some relevant points of its formulation will be briefly discussed. A flow chart of the overall calculations is shown in Figure 3.

3.2.1 Gas Phase Calculations

The gas phase portion of the model is cast in a grid-oriented, Eulerian reference frame. The transport equations for total gas mass, the three components of velocity, turbulent kinetic energy and its dissipation, two mixture fractions and their variances, and gas phase enthalpy are written in the form of a single transport equation. This

general equation for the three dimensional Cartesian coordinates is discussed subsequently in Section 4.2 (EQ 41). Substitutions indicated in Table 4, describe the transport of the scalar quantities identified above. All terms designated S are to be calculated in the particle portion of the code.

Radiation in the gas phase and between the particles and the gas phase is handled, optionally, by either a flux method or a discrete ordinates method. A k- ϵ turbulence model has been used above to predict the gas phase turbulence properties.

Finite difference equations are derived using nodal upwind differencing for convection terms and generalized arbitrary mesh central differencing for diffusive terms. These are solved for each variable independently in an iterative fashion. A single iteration in which new estimates of each of the variables in the table are generated is called a microiteration. During these microiterations, the particle source terms are not changed.

After the Eulerian equations are converged for a given set of particle source terms, the particle portion of the model is activated. New source terms are produced from the particle portion of the code. One cycle, in which the gas phase is converged and the particle portion of the code calculates new source terms is called a macroiteration.

The boundary conditions, methods of solution, and accuracy of this description of the gas phase of reacting flows will not be discussed here, nor will the specific correlations describing the reaction and heat transfer rates of the particles. The immediate purpose of the discussion is to extend the particle dispersion calculations to three dimensions.

3.2.2 Overview of Particle Calculations

The particle phase is handled in a Lagrangian reference frame. A primary motivation for choosing different reference frames for different portions of the model is to account for the history effect of the particles. In dilute systems the particles do not form a continuum. That is, while gases sampled at a point or small region and at given instant of time may reasonably be expected to be in local equilibrium, this is not true of the particles. Two particles in very close proximity at the same time in the reactor may have markedly different properties due to their different histories. Gases can be characterized by a single tempera-

Figure 3 Overall flowchart for the coupled code with fluid-dynamics, combustion and particle dispersion.

ture, for example. While this temperature may vary with time as a result of turbulent fluctuations, at any instant a single temperature should be characteristic of the gases at a point in the reactor. Two particles in close proximity, however, may have temperatures which differ by many hundreds of degrees, depending on their extents of burnout and other aspects of their history. This history effect is difficult to capture in an Eulerian formulation of the condensed phase but is a natural consequence of the Lagrangian formulation.

The particle portion of the code allows considerable detail in describing the rates of reaction and heat transfer between the gases and the condensed phases. Condensed phases ranging from liquids to slurries can be modelled. Specific modelled transfer rates include vaporization, devolatilization, heterogeneous reaction, and heat transfer.

This formulation allows the simulation to calculate local characteristics in a large variety of reacting and nonreacting flows. These include nonreacting turbulent flows both with and without entrained particles, gaseous diffusion flames, coal combustion and gasification, fuel oil combustion, coal slurry combustion, and spray drying.

A general flowchart for the particle calculations is shown in Figure 4. Particles are started from up to ten starting locations in the reactor. In addition, up to fifteen different particle types or sizes can be modelled. These are used primarily to simulate the range of particle sizes fed to the coal reactor. Having selected a starting location and initial particle size, the equations describing the development of the pdf for particle location are solved as a function of residence time.

In addition to the pdf for particle position, the particle temperature, composition, size and density are predicted as functions of time. The particle properties are used to calculate source terms for the gas phase calculations.

3.2.3 Calculation of Particle Source Terms in 3-D

From the perspective of the Eulerian framework, the purpose of the particle model is to generate particle source terms for each variable in each computational cell. This section describes the calculation of these source terms in three dimensional Cartesian coordinates. The proposed methodology is analogous to that used in REMIF for the two dimensional axisymmetric case.

The contribution of particles with a specific residence time to the Eulerian particle source term in a given computational cell will be evaluated by integrating the product of the instantaneous values of the particle number flowrate, particle reaction rate, and a weighting term based on the pdf between the limits of cell boundaries. That is, for the specific example of the continuity equation,

$$S_{p,ijk}^m = \int_{-\infty}^{\infty} \int_{V(ijk)} \dot{q} r_p^m W(x_p, t) dV dt \quad (\text{EQ } 1)$$

where ijk represent the coordinates of the Eulerian cell, the time integral is with respect to residence time, $\dot{q}$ represents the number flowrate of particles, r_p^m represents the total rate of mass evolved from an average particle to the gas as a function of time, and $\int_{V(ijk)} dV$ represents a volume integral between the boundaries of the Eulerian cell with coordinates ijk . That is, in the Cartesian coordinate system

$$\int_{V(ijk)} f(x_p, t) dV = \int_{x_{1,lb}}^{x_{1,ub}} \int_{x_{2,lb}}^{x_{2,ub}} \int_{x_{3,lb}}^{x_{3,ub}} f(x_p, t) dx_1 dx_2 dx_3 \quad (\text{EQ } 2)$$

where lb and ub represent the lower and upper bounds of the cell, respectively. The factor $W(x_p, t)$ will be discussed shortly.

Note that the time integral is particle residence time. That is, the time dependence of the integrand is a residence time dependence. In any given cell, particles with a range of residence times are present. Contributions from each of these are integrated to obtain the total particle source term. At many residence times, the value of W will not be significant. Therefore, the definite integral is finite even though its limits are not.

The other source terms can be similarly computed. In general, the source terms are calculated from

$$S_{p,ijk}^{\phi} = \int_{-\infty}^{\infty} \int_{V(ijk)} \dot{q} r_p^{\phi} W(x_p, t) dV dt \quad (\text{EQ } 3)$$

where Table 1 defines the specific variables.

Figure 4 Flowchart for particle dispersion submodel

Table 1 Variable Substitutions to compute source terms

Source Term	ϕ	Description
S_p^m	m	total mass from condensed phase
S_p^u	u	axial momentum
S_p^v	v	radial momentum
S_p^w	w	tangential momentum
S_p^f	f	vapor evolved from liquid phase
S_p^η	η	mass evolved from solid phase
S_p^h	h	enthalpy exchanged with condensed phase
where	$S_p^m = S_p^f + S_p^\eta$	

In principle, there should be source terms for k, ϵ , and both variances g_f and g_η . The derivation of the transport equations for these quantities is, in itself, largely empirical. Additional empiricism to accommodate these source terms seems unjustified.

The term r_p^ϕ in (EQ 3) is calculated from supporting particle equations. These equations describe the motion of the particles, the rates of devolatilization and oxidation, and the rate of heat exchange. The number of independent differential equations which are solved to calculate the source terms varies from 9, for nonreacting cold flow calculations, to several hundred for combusting particle calculations using the most sophisticated descriptions of coal reaction processes. A minimum of 12 equations must be solved when reacting particles are included.

The term $\dot{q}$ in (EQ 3) is independent of position, and therefore can be taken outside the volume integral. If the particles do not fragment, as will be assumed here, it can also be taken outside the time integral.

The only remaining factor in the volume integral in (EQ 3) is $W(x_i, t)$. This term is defined in terms of the pdf.

$$W(x_i, t) \equiv \frac{P(x_i, t)}{\int_{V(\min-\max)} P(x_i, t) dV} \quad (\text{EQ 4})$$

where

$$\int_{V(\min-\max)} P(x_i, t) dV \equiv \int_{x_{1,\min}}^{x_{1,\max}} \int_{x_{2,\min}}^{x_{2,\max}} \int_{x_{3,\min}}^{x_{3,\max}} P(x_i, t) dx_1 dx_2 dx_3 \quad (\text{EQ 5})$$

The denominator is a constant with respect to position and can be evaluated outside of the volume integral in (EQ 3). The limits of integration are at least $\pm 3\sigma$ and in most cases are effectively $\pm\infty$ in each coordinate direction. With the latter limits, the factor is identically unity in a Cartesian coordinate system. It is convenient to rename this normalization factor as follows.

$$\int_{V(\min-\max)} P(x_i, t) dV \equiv \frac{1}{A(t)} \quad (\text{EQ 6})$$

Differences between $P(x_i, t)$ and $W(x_i, t)$ are trivial in a Cartesian reference frame. In this reference frame, W is used to account for the finite limits of integration over P . Otherwise, the functions are identical. Values of $A(t)$ will always lie between 1.008 and 1.0 in a three dimensional Cartesian system in which the integrals are evaluated over at least $\pm 3\sigma$ in each direction.

An example of the volume integral of $W(x_i, t)$ is given here for the case of a bivariate normal distribution with correlation coefficient of 0 in a Cartesian coordinate system. Both a time and a volume integral are indicated in (EQ 3). The time integral is performed numerically. For constant $\dot{q}$ and r_p^ϕ , the volume integral need only address the spatial variation of W . This integral, for a Cartesian coordinate system, is given by

$$\int_V W(x_i, t) dV = A(t) \int_{x(lb)}^{x(ub)} \int_{y(lb)}^{y(ub)} \int_{z(lb)}^{z(ub)} P(x, y, z, t) dx dy dz \quad (\text{EQ 7})$$

The designations lb and ub refer to the values of the variables at the lower and upper bounds, respectively.

The right side of (EQ 7) is evaluated as follows. The function $A(t)$ is divided into three factors a_x, a_y , and a_z . These factors depend on the upper and lower bounds of integration in their respective coordinate directions but are otherwise independent of both space and time. The remainder

of the right side of the equation is also separated into three functions, namely, w_x , w_y , and w_z , which depend on x , y , and z respectively. Thus

$$\int_V W(x, y, z, t) = a_x a_y a_z w_x w_y w_z \quad (\text{EQ 8})$$

The functions w_x , w_y , and w_z are discussed first. They are then used to evaluate a_x , a_y , and a_z .

The function w_x is the difference between two standard normal distribution functions.

$$w_x = N(\zeta(x/ub)) - N(\zeta(x/lb)) \quad (\text{EQ 9})$$

The standard normal distribution function is defined as

$$N(\zeta) = \int_{-\infty}^{\zeta} \frac{1}{\sqrt{2\pi}} e^{-0.5\zeta'^2} d\zeta' \quad (\text{EQ 10})$$

where ζ , a dummy variable, is given by

$$\zeta(s) = \frac{s - \bar{s}}{\sigma_s} \quad (\text{EQ 11})$$

Here, s would be either x , y , or z , depending on the coordinate direction under consideration.

The functions w_y and w_z can be similarly calculated. The limits for w_x , w_y , and w_z correspond to individual Eulerian cell boundaries. One also has to limit the number of Eulerian cells included in the volume integration. That is, it is not practical to evaluate the source terms in all of the Eulerian cells over the limits x , y , $z = \pm\infty$. In practice, the integrals are carried out for a distance of at least ± 3 standard deviations in each coordinate direction. The functions a_x , a_y , and a_z in (EQ 7) are defined by substituting these limits in the formulas for w_x , w_y , and w_z . Cell boundaries do not generally fall at precisely ± 3 standard deviations from the mean position, therefore the integrals are carried out for more than 3 standard deviations and less than $\pm\infty$ in each direction. The maximum error associated with limiting the volume integral to 3 standard deviations instead of $\pm\infty$ is 0.54%.

The evaluation of the standard normal distribution function, (EQ 10), will be performed with the following approximation [Abramowitz and Stegun, 1972]:

$$N(x) = 1 - Z(x) (b_1 y + b_2 y^2 + b_3 y^3 + b_4 y^4 + b_5 y^5) + (EQ 12)$$

where

$$y = \frac{1}{1 + px} \quad (\text{EQ 13})$$

and $Z(x)$ is the standard normal probability density function. The constants b_i and p are as follows.

$$b_1 = 0.319381530 \quad (\text{EQ 14})$$

$$b_2 = -0.356563782 \quad (\text{EQ 15})$$

$$b_3 = 1.784177937 \quad (\text{EQ 16})$$

$$b_4 = -1.821255978 \quad (\text{EQ 17})$$

$$b_5 = 1.330274429 \quad (\text{EQ 18})$$

$$p = 0.2316419 \quad (\text{EQ 19})$$

The argument x of (EQ 12) is assumed positive. In practice, negative arguments will be handled by combining (EQ 12) with the following property of symmetrical probability distribution functions.

$$P(-x) = 1 - P(x) \quad (\text{EQ 20})$$

where P is any symmetrical distribution function and x is an arbitrary argument.

These equations, combined with the continuity, momentum, and energy equations for the particle phase, complete the coupling of the particle model to the gas model.

3.3 Algorithm Information Flow

Having defined the source terms the next task is to trace the flow of information in the computational algorithm to be used in the computer program and to identify the specific particle-phase submodel.

3.3.1 The Overall Structure

An overall information flow diagram of algorithm to be used in the 3D model was given in Figure 3. A tree diagram of the structure of the program showing the actual computer routines is given in Figure 5 through Figure 15.

Figure 5 Subroutines called by main driver

Figure 6 Subroutines called by COAL0

Figure 7 Subroutines called by CREE

Figure 8 Subroutines called by TABLE

Figure 9 Subroutines called by PROPS

Figure 10 Subroutines called by PLTWRT

Figure 11 CALC subroutines called by the main driver

Figure 12 Subroutines called by EOLP

Figure 13 Subroutines called by PSOLVE

Figure 14 Subroutines called by FLUX

Figure 15 Subroutines called by NOXMN

The calling routines are on the left, and the called routines are on the right. The routines are generally given in the order in which they are called, however each called routine is shown only once for a given calling routine. Not shown in the figures are calls to programs CPUTIM and FLUSH, which are used to keep track of execution time for various portions of the program, and to download stored output to output files, respectively. The calls to CPUTIM and FLUSH are numerous and would clutter the figures if shown.

The main calling routine is REMIF, and the subroutines it calls are shown in Figure 5 and Figure 11. INFLOW reads the input data for the inlet streams. GRID generates the numerical grid. GRMAP modifies the numerical grid if a grid datafile is being used and writes a new grid datafile. GRDGRF writes a schematic showing the grid locations in the output file. CREE0 reads the reactant composition data and thermochemical datafile. INIT initializes arrays used in the code. PRTRST reads the particle phase restart files.

PSICT0, COAL0, and FLUX0 read input data and perform initial calculations for the particle trajectory calculations, particle reaction scheme, and radiation submodel respectively. Routines called by COAL0 are shown in Figure 6. Other input data are read primarily by the driver program for the nitrogen oxide submodel (NOXMN).

TABLE is the driver program for generating the table of equilibrium gas properties for lookup. Routines called by TABLE are shown in Figure 8.

PROFIL reads input data and sets the boundary values for the gas inlet streams. RESTRT reads and writes gas-phase restart files. Particle phase restart files are read and written by the main program. FLINT initializes the flow field variables and calculates the gas density field. EULINT is an entry in PSICT0 that calculates the particle number flow rate for each particle trajectory.

PROPS calculates the time-mean gas properties, incorporating the effects of turbulence. Routines called by PROPS are shown in Figure 9.

STREAM calculates the velocity streamlines for plotting. PLTWRT writes plotting files. PRINT is a routine that is called frequently to print values of field variables to the output file.

The CALC routines calculate the flowfield variables such as velocities, turbulence properties, mixture fraction, and pressure at each node throughout the flowfield. These routines are shown in Figure 11. Each CALC routine calls an entry point in PROMOD to modify the coefficients and source terms in the appropriate finite difference equation in order to account for the boundary conditions. LISOLV is the solver that uses the TDMA algorithm.

EOLP is the driver program for the particle calculations. Routines called by EOLP are shown in Figure 12. CALCNJ calculates the particle number densities from Eulerian calculations. EULINT initializes variables for Eulerian calculations. FLUX is the driver program for the radiation submodel. BVALIN is an entry point in BPROPS that inserts reasonable values into boundary intrusions in order to allow for interpolation of gas properties. XYINDX returns the appropriate indices of the cell containing the particle. BVALOUT is an entry point in BPROPS that substitutes the original values of properties back into the boundary intrusions after the particle trajectory calculations are complete.

FREUND obtains the source terms and the Eulerian particle description for use in the Eulerian calculation. REACT initializes the reactivity and reference enthalpy for coals of different starting size or different type. PRTSTR initializes variables used in the particle trajectory calculations. PSOLVE integrates the particle trajectory.

Routines called by PSOLVE are shown in Figure 13. EULPRP interpolates the required properties of the gas phase to obtain their local values for the Lagrangian calculations. TRNPRP updates transport properties used in COALRX. COALRX calculates other particle properties. Subroutine SOURCE calculates source terms for each time step. PWRITE writes the Lagrangian information to files for plotting and debugging. TIMSTP determines the size for the upcoming integration step. STPRST resets the independent variables to the values they had at the beginning of this time step. PRTTMP calculates the particle temperature and enthalpy. BOUNCE calculates particle interactions with walls or intrusions.

FLUX is the driver program for the radiation submodel. Routines called by FLUX are shown in Figure 14.

PROG monitors the progress of the calculation towards convergence by recording the values of the variables at a specified location for each iteration.

NOXMN is the driver program for the pollutant submodel. Routines called by NOXMN are shown in Figure 15.

3.3.2 The Particle Phase Submodel

The particle submodel begins with the call to subroutine EOLP. CALCNJ first calculates the Eulerian number density field for each particle size. This is used by the FLUX routines to calculate the radiation fluxes. Subroutine FREUND interfaces the particle (Lagrangian) model with the gas (Eulerian) model.

XYINDEX, REACT, and PRTSTR initialize calculation of the trajectory of a particle type, by calculating the initial location, initial reactivity and initial particle properties respectively. Then PSOLVE integrates the Lagrangian differential equations and obtains the particle trajectory. FREUND calls these routines for all particle types and starting locations. At the completion of all particle simulations it corrects the variances and correlation coefficients for the mean values and writes the plotting information and particle restart files.

To integrate the particle trajectory subroutine PSOLVE first calls EULPRP to interpolate the local Eulerian properties at the particle position. Next, the particle properties like reaction rates, heat transfer, temperature, diameter etc. are calculated by COALRX and TRNPRP. Subroutine SOURCE then calculates the source terms for that particular time step and sums them up at the same time. Routines TIMSTP, STPRST, PRTTMP, and XYINDEX initialize the integration for the next time step by calculating the size of the next time step, resetting independent variables, calculating particle enthalpy, and new location indices, respectively. PSOLVE calls all these routines iteratively and integrates the trajectory for that particle type until the end of the reactor is reached.

This particle submodel has yet to be coded and incorporated into the 3D code.

3.4 Incorporation Into the 3D code

The three dimensional model to be used as a basis for this particle dispersion work has yet to be named, but is a gen-

eralized, three-dimensional, steady state model for describing a variety of reactive and non-reactive flows in Cartesian and cylindrical coordinate systems. The approach to the gas phase calculations is conceptually the same as that in the two dimensional model. New and more efficient numerical methods have been implemented to handle the large number of nodes needed for three dimensional industrial systems. However this code does not have any particle phase description yet.

The particle phase submodel will be interfaced with the gas phase calculations through source terms which will be calculated after the completion of each "macroiteration", analogous to the two dimensional calculations.

Radiation calculations have been substantially changed over the past few years. The coupling between the radiation submodel and the other processes in the simulation is much more tightly coupled. A new algorithm has been incorporated which requires updating the energy equation radiation source terms at each iteration through the computation.

The algorithm for the rest of the particle submodel calculations will essentially be the same as that described for the REMIF code. Work is currently being done on modifying the subroutines identified in Section 3 as the particle phase submodel of the REMIF code, to do the calculations for a three dimensional Cartesian coordinate system as per the discussion in Section 2. The modified subroutines will then be incorporated in the 3D code with small changes to the 3D code itself.

4.0 Dense-Phase Dispersion Submodel Development

In this section the progress made in the development of a three-dimensional code for predicting turbulent particle dispersion in densely loaded systems is reported, for the period of July 15th to October 15th, 1991. In the first Quarterly Progress Report the various constitutive equations for predicting the stress-strain behavior in rapid shear flows of granular materials were presented and the advantages and disadvantages of each were elaborated upon. In the present report the constitutive equations of Jenkins and Savage (1983) are chosen to model the situation under consideration and the solution method for the resulting governing equations are described.

In the first quarterly report (Smith, 1991), it was pointed out that owing to the large number of particles in a densely loaded system such as a fluidized bed, a Lagrangian approach to modeling the motion of particles would not be computationally feasible. Hence it was decided to consider the particles as a "continuous phase" in the Eulerian sense of the term, and use constitutive equations to describe the stress-strain behavior of this "continuous phase" to enable an accurate fluid-mechanical description of the gas-solid two-phase system. The theoretical models available to predict constitutive equations for granular flow were also discussed. It was then seen that among the various approaches to the problem, the kinetic model of Jenkins and Savage (1983) and related kinetic theories had the advantage of being the most fundamental in their incorporation of the microstructure of the particle flow, while still preserving simplicity in the resulting constitutive equations.

We thus have a two-phase system of gas and solid in an Eulerian frame of reference, and need to solve the equations of the gas and particle phases simultaneously.

It needs to be mentioned here that the aim of this code is not merely the prediction of the fluid mechanics of the resulting complex system, but also the heat and mass transfer that would result in a reacting system such as a fluidized bed combustor (FBC). The model for the fluid mechanics discussed herein is intended to be part of a more general comprehensive 3-dimensional combustion code developed by the principal investigator, which, at present, has been developed only for lightly loaded systems, but includes submodels for the prediction of such important processes as chemical reaction and radiative heat transfer, in completely arbitrary configurations (Smith, 1990). Hence the aim here is to incorporate this fluid mechanical submodel for the particle phase in a densely loaded system into the 3-dimensional code in such a way that the resulting overall code would be capable of predicting fluid mechanics, heat transfer and chemical reaction in a reactive/nonreactive system of arbitrary flow geometry. The intention is also to develop a code that would be capable of handling a range of particle sizes in the input solid phase, so that one can accurately simulate the behavior of actual feed mixtures consisting of several grain sizes.

Hence in the description that follows, we describe the general equations of change, for reacting systems with heat exchange, and the methodology we intend to adopt to ef-

fect the solution of these equations. However, we restrict, for the purposes of this report, our discussion to that of mixtures containing just one particle size.

4.1 Governing Equations for Particle Phase Flow

The basic governing equations for particle phase flow, in a reacting system, in accordance with the Jenkins and Savage (1983) model are:

Continuity:

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = S_g^m \quad (\text{EQ 21})$$

where S_g^m is the mass source term for the particle equation (i.e. rate of mass addition to the particle phase from the gas phase per unit volume), and is given by:

$$S_g^m = \sum_{j=1}^l r_j \quad (\text{EQ 22})$$

where l is the number of components which make up the solid phase (e.g., in coal combustion, these would be the coal, char, ash and volatile matter), r_j is the rate of mass production of each component per unit volume, ρ is the ensemble-averaged local particle density, i.e. the bulk density of the particle phase (and not the bulk density of the gas-solid mixture) and $\mathbf{v}$ is the local ensemble averaged velocity.

If we assume steady state, then (EQ 21) reduces to:

$$(\nabla \cdot \rho \mathbf{v}) = S_g^m \quad (\text{EQ 23})$$

In addition, we have individual species continuity equations for the l species,

$$(\nabla \cdot \rho_j \mathbf{v}) = r_j \quad (\text{EQ 24})$$

whereupon, on summing over all j we obtain (EQ 23).

Momentum:

$$\rho \frac{D\mathbf{v}}{Dt} = -(\nabla \cdot \boldsymbol{\sigma}) + \mathbf{v}f \quad (\text{EQ 25})$$

where f is the external force per unit volume of the particle phase. This would include the weight of the particle as well as the drag force acting on the particle phase.

The constitutive equations may be written as (Smith, 1991):

$$\sigma = \frac{\pi^{1/2} \kappa T^{1/2}}{d} I - \left(\frac{1}{5}\right) \kappa (2 + \alpha) [(tr D) I + 2D] \quad (\text{EQ 26})$$

$$\kappa = 2\rho v g_0(v) d (1 + e) \left(\frac{T}{\pi}\right) \quad (\text{EQ 27})$$

$$\left(\frac{3}{2}\right) \rho \frac{DT}{Dt} = -(\nabla \cdot q) - tr(\sigma \nabla v) - \gamma \quad (\text{EQ 28})$$

$$q = -\kappa \nabla T \quad (\text{EQ 29})$$

$$\gamma = \frac{\kappa(1 - e)}{2d^2} \left[12T - (3\pi + 4\alpha) d \left(\frac{T}{\pi}\right) (tr D) \right] \quad (\text{EQ 30})$$

where T is defined as the "granular temperature", and is actually the ensemble average of the square of the fluctuating velocity of individual particles:

$$T = \frac{1}{3} \langle C^2 \rangle \quad (\text{EQ 31})$$

in which

$$C = |C| = |c - v| \quad (\text{EQ 32})$$

where c is the velocity of an individual particle, v is the ensemble averaged velocity, and C is the fluctuating velocity whose magnitude is C , d is the diameter of the particles (assumed spherical and uniform), e is the coefficient of restitution for collisions between particles, ρ is the bulk density of the particle phase, defined as:

$$\rho = \rho_p v \quad (\text{EQ 33})$$

where v is the ensemble-averaged local solid fraction in the mixture.

γ is defined as the dissipation due to "viscous" drag, i.e. the energy dissipation due to collisions, q is the flux of T (the "diffusive flux" of the granular "temperature"), κ is the "thermal conductivity" of the granular material in rapid shear flow (and is not a constant), σ is the stress tensor, α is a constant, tr denotes the trace of a matrix, D is the rate of deformation tensor, I is the identity tensor, α is a

constant, and $g_0(v)$ is a function of the solid fraction v which may be of the form (Smith, 1991):

$$g_0(v) = \frac{1}{1-v} + \frac{3v}{2(1-v)^2} + \frac{v^2}{2(1-v)^3} \quad (\text{EQ 34})$$

The net external force, f , may be written as:

$$f = \rho g + S_g^u \quad (\text{EQ 35})$$

where S_g^u is the momentum source term added to the particle phase equation due to momentum exchange with the gas phase, viz. the drag force.

One can see from inspection of (EQ 26) that the form of this constitutive equation is very reminiscent of that of a Newtonian fluid. In fact, if we define a particle pressure:

$$p_e = \frac{\pi^{1/2} \kappa T^{1/2}}{d} \quad (\text{EQ 36})$$

i.e.,

$$p_e = 2 \left(\frac{T}{\pi}\right)^{1/2} T \rho g_0(v) v (1 + e) \quad (\text{EQ 37})$$

and a particle diffusivity:

$$\mu_e = \left(\frac{2}{5}\right) \kappa (2 + \alpha) \quad (\text{EQ 38})$$

i.e.,

$$\mu_e = \left(\frac{4}{5}\right) \rho v g_0(v) d (1 + e) (2 + \alpha) \left(\frac{T}{\pi}\right) \quad (\text{EQ 39})$$

then the resulting equations of motion (EQ 25) become identical to the Newtonian case, with the one difference that in rapid granular flow, the pressure and viscosity are not constant but functions of the granular temperature, which, unlike the thermodynamic temperature, varies much more rapidly in the flow. The balance equation for the "granular temperature" is similar to the equation of change of the turbulent kinetic energy of a turbulent Newtonian fluid.

In addition, for a complete description of the particle phase one needs the energy equation, which can be written as:

$$\frac{D(\rho h)}{Dt} - (\nabla \cdot K \nabla h) = q'_{rg} + (\nu \cdot \nabla p_g) + S_g^h + h_{gp} S_g^m \quad (\text{EQ 40})$$

where S_g^h represents the source addition for enthalpy to the particle phase from the gas phase per unit volume, and h_{gp} is the relative enthalpy of the gas with respect to the particle phase. The $h_{gp} S_g^m$ term represents loss of enthalpy from the particle phase to the gas phase as the particles react and burn off into the gas phase. q'_{rg} is the radiative heat transfer from the gas phase to the particle phase, and K is the actual thermal conductivity of the particle phase.

4.2 Generalized Equations of Change

(EQ 25), (EQ 28) and (EQ 40) can be written, after simplification, in the following general form (assuming steady state):

$$(\nabla \cdot (\rho \nu \phi)) - (\nabla \cdot (\Gamma_\phi \nabla \phi)) = S^\phi \quad (\text{EQ 41})$$

(i.e., in the form: convection - diffusion = source.)

Here ϕ is a variable associated with the flow (such as density, the three velocity components, and enthalpy.) In Table 2 and Table 3 we give a summary of the fluid mechanical equations for the particle phase, which were shown earlier, in this simplified form, with the appropriate expressions for the source terms.

These equations are solved in conjunction with the gas phase equations. We also provide the gas phase equations (Smith, 1990) in their Cartesian and cylindrical forms, for reference, in Table 4 and Table 5. A look at Table 2 and Table 4 clearly shows that the gas-phase equations have a form similar to that of the particle phase equations. In these gas-phase equations k is the turbulent kinetic energy, $\bar{\epsilon}$ is the dissipation of kinetic energy, and μ_g^* is the effective viscosity in the turbulent gas-phase, given by:

$$\mu_g^* = \mu + \mu_t \quad (\text{EQ 42})$$

where μ is the viscosity of the gas and μ_t is the eddy viscosity, defined by (Smith, 1990):

$$\mu_t = \frac{C_\mu \bar{k}^2}{\bar{\epsilon}} \quad (\text{EQ 43})$$

where C_μ is a constant. The particle mass source terms, S_p^m , are related to the gas phase mass source terms, S_g^m , in the following way:

$$S_p^m = -S_g^m \quad (\text{EQ 44})$$

The constants, c_1 and c_2 , and the parameters σ_k and σ_ϵ , are discussed in detail by Smith (1990).

4.3 Treatment of Hydrodynamic Drag

The drag force on a spherical particle is defined (Bird, et al.) by the following relation:

$$F_d = \left(\frac{1}{2} \rho_g u_0^2\right) C_d A_p \quad (\text{EQ 45})$$

where A_p is the projected area of the particle, u_0 is the fluid approach velocity relative to the particle, ρ_g is the fluid density, and C_d is the drag coefficient. This force acts in the direction opposing the motion of the particle. For example, for the x -component of the velocity (i.e., the u -velocity), at any point in the flow field, one would use:

$$u_0 = u - u_g \quad (\text{EQ 46})$$

where the subscript g refers to the gas phase.

At low particle Reynolds numbers the drag coefficient is modeled using Stokes' drag (Bird, et al., 1960), i.e.

$$C_d = \frac{24}{Re} \quad (\text{EQ 47})$$

for $Re < 2$.

At higher Reynolds numbers, the intermediate region law (Bird, et al., 1960) is used, viz.:

$$C_d = \frac{18.5}{(Re)^{3/5}} \quad (\text{EQ 48})$$

for $Re > 2$.

The switch from Stokesian drag to the intermediate regime is determined by the particle Reynolds' number, which in turn is based on the approach velocity, u_0 , in the following way (McCabe, et al., 1985):

Table 2 Cartesian differential equation set for particle phase

$$\frac{\partial}{\partial x}(\rho u \phi) + \frac{\partial}{\partial y}(\rho v \phi) + \frac{\partial}{\partial z}(\rho w \phi) - \frac{\partial}{\partial x}(\Gamma_\phi \frac{\partial \phi}{\partial x}) - \frac{\partial}{\partial y}(\Gamma_\phi \frac{\partial \phi}{\partial y}) - \frac{\partial}{\partial z}(\Gamma_\phi \frac{\partial \phi}{\partial z}) = S_\phi$$

Equation	ϕ	Γ_ϕ	S_ϕ
Continuity	1	0	S_g^m
X-Momentum	u	μ_s	$-\frac{\partial p_s}{\partial x} + \frac{\partial}{\partial x}(\mu_s \frac{\partial u}{\partial x}) + \frac{\partial}{\partial y}(\mu_s \frac{\partial v}{\partial x}) + \frac{\partial}{\partial z}(\mu_s \frac{\partial w}{\partial x}) + \rho_p v g_x + u S_g^m + S_g^u$
Y-Momentum	v	μ_s	$-\frac{\partial p_s}{\partial y} + \frac{\partial}{\partial x}(\mu_s \frac{\partial u}{\partial y}) + \frac{\partial}{\partial y}(\mu_s \frac{\partial v}{\partial y}) + \frac{\partial}{\partial z}(\mu_s \frac{\partial w}{\partial y}) + \rho_p v g_y + v S_g^m + S_g^v$
Z-Momentum	w	μ_s	$-\frac{\partial p_s}{\partial z} + \frac{\partial}{\partial x}(\mu_s \frac{\partial u}{\partial z}) + \frac{\partial}{\partial y}(\mu_s \frac{\partial v}{\partial z}) + \frac{\partial}{\partial z}(\mu_s \frac{\partial w}{\partial z}) + \rho_p v g_z + w S_g^m + S_g^w$

Equation	ϕ	Γ_ϕ	S_ϕ
Granular Temperature			
	T	$\frac{2}{3} \kappa$	$T S_g^m - \frac{2}{3} (p_s) (\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}) + \frac{2\mu_s}{r} (\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z})^2 + \frac{2\mu_s}{3} [2 (\frac{\partial u}{\partial x})^2 + (\frac{\partial v}{\partial y})^2 + (\frac{\partial w}{\partial z})^2 + (\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})^2 + (\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x})^2 + (\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y})^2] + (-\frac{2}{3}) \frac{\rho_p v^2 g_0(v) (1-e^2)}{\pi d} \bullet T^2 \bullet (12 - (3\pi + 4\alpha) d (\frac{T}{\pi}) \bullet (\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}))$

Table 3 Cylindrical differential equation set for particle phase

$$r \frac{\partial}{\partial x} (\rho u \phi) + \frac{\partial}{\partial r} (\rho v r \phi) + \frac{\partial}{\partial \theta} (\rho w \phi) - r \frac{\partial}{\partial x} \left(\Gamma_\phi \frac{\partial \phi}{\partial x} \right) - \frac{\partial}{\partial r} \left(r \Gamma_\phi \frac{\partial \phi}{\partial r} \right) - \frac{\partial}{\partial \theta} \left(\frac{\Gamma_\phi \partial \phi}{r \partial \theta} \right) = S^\phi$$

Equation	ϕ	Γ_ϕ	S^ϕ
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Continuity 1 0 $r S_t^m$

X-Momentum u μ_s $-r \frac{\partial}{\partial x} (p_s) + r \frac{\partial}{\partial x} \left(\mu_s \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial r} \left(\mu_s r \frac{\partial}{\partial x} (v) \right) + \frac{\partial}{\partial \theta} \left(\mu_s \frac{\partial w}{\partial x} \right) + r \rho_p v g_x + r u S_t^m + r S_t^x$

R-Momentum v μ_s $-r \frac{\partial}{\partial y} (p_s) + r \frac{\partial}{\partial x} \left(\mu_s \frac{\partial v}{\partial r} \right) + \frac{\partial}{\partial r} \left(\mu_s r \frac{\partial v}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\mu_s \frac{\partial w}{\partial r} - \frac{w}{r} \right) - \frac{2 \mu_s \partial w}{r \partial \theta} - \frac{2 v \mu_s}{r} + \rho w^2 + r \rho_p v g_r + r v S_t^m + r S_t^y$

θ -Momentum w μ_s $-\frac{\partial p_s}{\partial \theta} + r \frac{\partial}{\partial x} \left(\frac{\mu_s \partial w}{r \partial \theta} \right) + \frac{\partial}{\partial r} \left(\mu_s \frac{\partial v}{\partial \theta} - \mu_s w \right) - \rho v w + \frac{\partial}{\partial \theta} \left(\frac{\mu_s}{r} \right) \left(\frac{\partial w}{\partial \theta} + 2v \right) + \mu_s \left(\frac{\partial w}{\partial r} + \frac{1}{r} \frac{\partial v}{\partial \theta} - \frac{w}{r} \right) + r \rho_p v g_\theta + r w S_t^m + r S_t^w$

Equation	ϕ	Γ_ϕ	S^ϕ
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Granular Temperature

$$T = \frac{2}{3} \kappa \left[r T S_t^m - \frac{2}{3} (p_s r) \left(\frac{\partial u}{\partial r} + \frac{1}{r} \frac{\partial}{\partial r} (r v) + \frac{1}{r} \frac{\partial w}{\partial \theta} \right) + \frac{2 \mu_s r}{3} \left(\frac{\partial u}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} (r v) + \frac{1}{r} \frac{\partial w}{\partial \theta} \right)^2 + \frac{2 \mu_s r}{3} \left[2 \left(\frac{\partial u}{\partial x} \right)^2 \left(\frac{1}{r} \frac{\partial}{\partial r} (r v) \right)^2 + \left(\frac{1}{r} \frac{\partial w}{\partial \theta} \right)^2 \right] + \left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right)^2 + \left(\frac{1}{r} \frac{\partial u}{\partial \theta} + \frac{\partial w}{\partial x} \right)^2 + \left(\frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{\partial w}{\partial r} \right)^2 \right] + \frac{2 \mu_s r}{3} \left(\frac{w^2}{r^2} - \frac{w \partial v}{r \partial \theta} - \frac{2 w \partial v}{r \partial \theta} - \frac{2 w \partial w}{r \partial r} - \frac{w^2 \partial v}{r^2 \partial \theta} + \frac{4 v \partial w}{r^2 \partial \theta} - \frac{4 v \partial v}{r \partial r} \right) - \frac{2}{3} \frac{\rho_p v^2 g_\theta (v) (1 - e^2)}{\pi d} T^2 (12 - (3\pi + 4\alpha) d \left(\frac{T}{\pi} \right) \left(\frac{\partial u}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} (r v) + \frac{\partial w}{\partial \theta} \right))$$

Table 4 Cartesian differential equation set for gas phase

$$\frac{\partial}{\partial x}(\bar{\rho}\bar{u}_t\phi) + \frac{\partial}{\partial y}(\bar{\rho}\bar{v}_t\phi) + \frac{\partial}{\partial z}(\bar{\rho}\bar{w}_t\phi) - \frac{\partial}{\partial x}(\Gamma_t \frac{\partial \phi}{\partial x}) - \frac{\partial}{\partial y}(\Gamma_t \frac{\partial \phi}{\partial y}) - \frac{\partial}{\partial z}(\Gamma_t \frac{\partial \phi}{\partial z}) = S^{\phi}$$

Equation	ϕ	Γ_t	S^{ϕ}
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Continuity 1 0 S_p^m

$$\begin{aligned} \text{X-Momentum } \bar{u}_t \quad \mu_t^s & - \frac{\partial p}{\partial x} + \frac{\partial}{\partial x}(\mu_t^s \frac{\partial \bar{u}_t}{\partial x}) + \frac{\partial}{\partial y}(\mu_t^s \frac{\partial \bar{v}_t}{\partial x}) + \\ & \frac{\partial}{\partial z}(\mu_t^s \frac{\partial \bar{w}_t}{\partial x}) - \frac{2}{3}\bar{\rho}\bar{k} + \bar{\rho}g_x \\ & \bar{u}_t S_p^m + S_p^u \end{aligned}$$

$$\begin{aligned} \text{Y-Momentum } \bar{v}_t \quad \mu_t^s & - \frac{\partial p}{\partial y} + \frac{\partial}{\partial x}(\mu_t^s \frac{\partial \bar{u}_t}{\partial y}) + \frac{\partial}{\partial y}(\mu_t^s \frac{\partial \bar{v}_t}{\partial y}) + \\ & + \frac{\partial}{\partial z}(\mu_t^s \frac{\partial \bar{w}_t}{\partial y}) - \frac{2}{3}\bar{\rho}\bar{k} + \bar{\rho}g_y \\ & \bar{v}_t S_p^m + S_p^v \end{aligned}$$

$$\begin{aligned} \text{Z-Momentum } \bar{w}_t \quad \mu_t^s & - \frac{\partial p}{\partial z} + \frac{\partial}{\partial x}(\mu_t^s \frac{\partial \bar{u}_t}{\partial z}) + \frac{\partial}{\partial y}(\mu_t^s \frac{\partial \bar{v}_t}{\partial z}) + \\ & + \frac{\partial}{\partial z}(\mu_t^s \frac{\partial \bar{w}_t}{\partial z}) + \bar{\rho}g_z + \bar{w}_t S_p^m + S_p^w \end{aligned}$$

Equation	ϕ	Γ_t	S^{ϕ}
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Turbulent Energy

$$\bar{k} \quad \frac{\mu_t^s}{\sigma_k} G - \bar{\rho}\bar{\epsilon}$$

Dissipation Rate

$$\bar{\epsilon} \quad \frac{\mu_t^s}{\sigma_{\epsilon}} \left(\frac{\bar{\epsilon}}{\bar{k}} \right) (c_1 G - c_2 \bar{\rho}\bar{\epsilon})$$

where

$$\begin{aligned} G = \mu_t^s & \left[2 \left(\left(\frac{\partial \bar{u}_t}{\partial x} \right)^2 + \left(\frac{\partial \bar{v}_t}{\partial y} \right)^2 + \left(\frac{\partial \bar{w}_t}{\partial z} \right)^2 + \left(\frac{\partial \bar{u}_t}{\partial y} + \frac{\partial \bar{v}_t}{\partial x} \right)^2 \right. \right. \\ & \left. \left. + \left(\frac{\partial \bar{u}_t}{\partial z} + \frac{\partial \bar{w}_t}{\partial x} \right)^2 + \left(\frac{\partial \bar{v}_t}{\partial z} + \frac{\partial \bar{w}_t}{\partial y} \right)^2 \right] \end{aligned}$$

Table 5 Cylindrical differential equation set for gas phase

$r \frac{\partial}{\partial x} (\bar{\rho} \bar{u}_g \phi) + \frac{\partial}{\partial r} (\bar{\rho} \bar{v}_g r \phi) + \frac{\partial}{\partial \theta} (\bar{\rho} \bar{w}_g \phi) - r \frac{\partial}{\partial x} \left(\Gamma_g \frac{\partial \phi}{\partial x} \right) - \frac{\partial}{\partial r} \left(r \Gamma_g \frac{\partial \phi}{\partial r} \right) - \frac{\partial}{\partial \theta} \left(\frac{\Gamma_g}{r} \frac{\partial \phi}{\partial \theta} \right) = S^\phi$			
Equation	ϕ	Γ_g	S^ϕ
Continuity	1	0	$r S_p^m$
X-Momentum	$\bar{u}_g$	μ_g	$-r \frac{\partial}{\partial x} (p) + r \frac{\partial}{\partial x} \left(\mu_g \frac{\partial \bar{u}_g}{\partial x} \right) + \frac{\partial}{\partial r} \left(\mu_g r \frac{\partial \bar{v}_g}{\partial x} \right) + \frac{\partial}{\partial \theta} \left(\mu_g \frac{\partial \bar{w}_g}{\partial x} \right) + r \bar{\rho} g_x - \frac{2}{3} r \bar{\rho} \bar{k} + r \bar{u}_g S_p^m + r S_p^u$
R-Momentum	$\bar{v}_g$	μ_g	$-r \frac{\partial}{\partial y} (p) + r \frac{\partial}{\partial x} \left(\mu_g \frac{\partial \bar{u}_g}{\partial r} \right) + \frac{\partial}{\partial r} \left(\mu_g \frac{\partial \bar{v}_g}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\mu_g \frac{\partial \bar{w}_g}{\partial r} - \frac{\bar{w}_g}{r} \right) - \frac{2 \mu_g}{r} \frac{\partial \bar{w}_g}{\partial \theta} - \frac{2 \bar{v}_g \mu_g}{r} + \bar{\rho} \bar{w}_g^2 + r \bar{\rho} g_r - \frac{2}{3} r \bar{\rho} \bar{k} + r \bar{v}_g S_p^m + r S_p^v$
Z-Momentum	$\bar{w}_g$	μ_g	$- \frac{\partial p}{\partial \theta} + r \frac{\partial}{\partial x} \left(\frac{\mu_g}{r} \frac{\partial \bar{u}_g}{\partial \theta} \right) + \frac{\partial}{\partial r} \left(\mu_g \frac{\partial \bar{v}_g}{\partial \theta} - \mu_g \bar{w}_g \right) - \bar{\rho} \bar{v}_g \bar{w}_g + \frac{\partial}{\partial \theta} \left(\left(\frac{\mu_g}{r} \right) \left(\frac{\partial \bar{w}_g}{\partial \theta} + 2 \bar{v}_g \right) \right) + \mu_g \left(\frac{\partial \bar{w}_g}{\partial r} + \frac{1}{r} \frac{\partial \bar{v}_g}{\partial \theta} - \frac{\bar{w}_g}{r} \right) + r \bar{\rho} g_\theta - \frac{2}{3} r \bar{\rho} \bar{k} + r \bar{w}_g S_p^m + r S_p^w$
Turbulent kinetic energy	$\bar{k}$	$\frac{\mu_g}{\sigma_k}$	$r (G' - \bar{\rho} \bar{\epsilon})$
Dissipation rate	$\bar{\epsilon}$	$\frac{\mu_g}{\sigma_\epsilon}$	$r \left(\frac{\bar{\epsilon}}{\bar{k}} \right) (c_1 G' - c_2 \bar{\rho} \bar{\epsilon})$

where

$$G' = \mu_g \left[2 \left(\left(\frac{\partial \bar{u}_g}{\partial x} \right)^2 + \left(\frac{\partial \bar{v}_g}{\partial r} \right)^2 + \left(\frac{1}{r} \frac{\partial \bar{w}_g}{\partial \theta} + \frac{\bar{v}_g}{r} \right)^2 \right) + \left(\frac{\partial \bar{u}_g}{\partial r} + \frac{\partial \bar{v}_g}{\partial x} \right)^2 + \left(\frac{1}{r} \frac{\partial \bar{u}_g}{\partial \theta} + \frac{\partial \bar{w}_g}{\partial x} \right)^2 + \left(\frac{1}{r} \frac{\partial \bar{v}_g}{\partial \theta} + \frac{\partial \bar{w}_g}{\partial r} - \frac{\bar{w}_g}{r^2} \right)^2 \right]$$

$$Re = \frac{du_0 \rho_g}{\mu} \quad (\text{EQ 49})$$

where μ is the viscosity of the fluid. A switching condition will therefore be employed in the code to switch from one law to the other. This is made necessary by the fact that in fluidized bed combustors, unlike pulverized coal combustors, the particles may be very large, of the order of 1000 microns and the assumption of Stokesian drag does not always hold true in this range of particle sizes.

The approach velocity, u_0 , is usually some multiple of the minimum fluidization velocity, or the gas velocity at incipient fluidization, v_{mf} . The minimum fluidization velocity may be obtained from the following equation (McCabe, et al., 1985):

$$\left(\frac{1.75 \rho_g}{\phi_s d \epsilon_M^3} \right) v_{mf}^2 + \left(\frac{150 \mu}{\phi_s^2 d^2} \right) \left(\frac{1 - \epsilon_M}{\epsilon_M^3} \right) v_{mf} = g (\rho_p - \rho_g) \quad (\text{EQ 50})$$

in which ϕ_s is the average sphericity of the particles, and ϵ_M is the bed void fraction at minimum fluidization.

Hence the momentum source terms for the gas and solid phases will be:

$$S_g^M = F_d \quad (\text{EQ 51})$$

$$S_p^M = -S_g^M \quad (\text{EQ 52})$$

4.4 Boundary conditions for the particle phase

The boundary conditions for the particle velocity are taken to be

$$(\mathbf{v} \cdot \mathbf{n}) = 0 \quad (\text{EQ 53})$$

at any wall (or intrusion), where $\mathbf{n}$ is the vector normal to the wall (or intrusion) at that point. In addition, the shear stress at the wall is specified as the "viscosity" multiplied by the velocity gradient based on the distance between the wall and the node nearest to it. The inlet velocity boundary condition is the specified inlet velocity; and the conditions for the thermal energy (or enthalpy) equation are the specified temperatures at the boundary, or, more often, a specified heat flux at the wall. The conditions for the granular "temperature" are taken to be:

$$T = 0 \quad (\text{EQ 54})$$

at any wall (or intrusion), in accordance with the analysis of Hui et al. (1988) and

$$\frac{dT}{dx_i} = 0 \quad (\text{EQ 55})$$

at any center of symmetry.

4.5 Solution Methodology

The equations given in Table 2 through Table 5 need to be solved simultaneously. This will be done by discretizing the differential equations as done previously for 3D flows (Smith, 1990), and solving the resulting system of equations by a planar, vectorizable tridiagonal matrix algorithm. The coupling of the pressure and velocity fields, is accomplished by using one of the many variants of the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm (for a detailed discussion see Smith (1990)). The only significant difference between the gas and solid phase equations lies in the source terms, as can be seen from Table 2-Table 5.

4.6 Concluding Observations Regarding Densely Loaded Systems

A constitutive theory for rapid granular flow has been selected to model the flow behavior of the particle phase in a flowing 2-phase Eulerian gas-solid mixture for applications in flow systems such as fluidized beds. It is seen that this constitutive equation has the form of that of a Newtonian fluid in turbulent flow. The governing equations resulting from the incorporation of these constitutive equations into the equations of motion are given. The boundary conditions for the variables of interest are also briefly discussed and the source terms appearing in the various equations are elaborated upon.

These governing equations are shown to be reducible to the standard convection-diffusion-source format, and hence potentially soluble by the use of finite-differencing techniques similar to those employed in the rest of the combustion code.

5.0 Project Plans

This report has summarized the second 3 month effort on a project to develop a computationally accurate and efficient turbulent particle dispersion model for incorporation in computational fluid dynamical and combustion codes. We have reviewed possible approaches outlined the theory for a proposed model that would include components for dealing with dilute systems as well as dense systems and during this quarter have developed the computer algorithm for solving the equations for such a system.

We have started the computer coding to solve the outlined equations. This coding will continue over the next quarter. This computer coding involves the incorporation of this model into our three-dimensional combustion code. Evaluation will proceed from that point according to the tasks outlined in Section 1.

6.0 Nomenclature

Symbol	Units	Definition
a	varies	weighting function
A	varies	weighting function
A_p	m^2	projected area of particle normal to fluid velocity
b	-	constant
C	$\frac{m}{s}$	fluctuating velocity vector defined by (EQ 32)
C	$\frac{m}{s}$	magnitude of fluctuating velocity
C_d	m^{-3}	drag coefficient
C_μ	-	dimensionless constant used in $k - \epsilon$ model
c	$\frac{m}{s}$	velocity vector of individual grains
D	s^{-1}	rate of deformation tensor
d	m	particle diameter
e	-	coefficient of restitution
F_d	$\frac{kg}{m^2 \cdot s^2}$	drag force per unit volume acting on each particle
f	$\frac{kg}{m^2 \cdot s^2}$	net external force acting on particle phase (vector)
g	$\frac{m}{s^2}$	acceleration due to gravity
g_r	$\frac{m}{s^2}$	r-component of acceleration due to gravity
g_x	$\frac{m}{s^2}$	x-component of acceleration due to gravity
g_y	$\frac{m}{s^2}$	y-component of acceleration due to gravity

Nomenclature

g_z	$\frac{m}{s^2}$	z-component of acceleration due to gravity	S_g^u	$\frac{kg}{m^2 \cdot s^2}$	gas phase momentum source term for particle momentum equation
g_0	-	function of the solid fraction to account for particle distribution	S_p^u	$\frac{kg}{m^2 \cdot s^2}$	particle momentum source term for gas phase momentum equation
g_θ	$\frac{m}{s^2}$	θ -component of acceleration due to gravity	T	$\frac{m^2}{s^2}$	"granular temperature"
h_{gp}	$\frac{m^2}{s^2}$	specific enthalpy of gas with respect to particle	t	s	time
I	-	identity tensor	u	$\frac{m}{s}$	x-component of particle velocity
K	$\frac{kg \cdot m}{s^2 \cdot ^\circ K}$	thermal conductivity	$\bar{u}_g$	$\frac{m}{s}$	x-component of gas velocity
$\bar{k}$	$\frac{m^2}{s^2}$	mass-averaged turbulent kinetic energy	u_0	$\frac{m}{s}$	velocity of gas with respect to particle
n	-	vector normal to any surface	v	$\frac{m}{s}$	y- or r-component of particle phase velocity
N	-	normal distribution	$\bar{v}_g$	$\frac{m}{s}$	y- or r-component of gas velocity
P	varies	probability density function	v_{mf}	$\frac{m}{s}$	minimum fluidization gas velocity
p	$\frac{kg}{m \cdot s^2}$	thermodynamic pressure	V	m^3	volume
p_s	$\frac{kg}{m \cdot s^2}$	particle pressure	w	varies	weighting function
q	$\frac{kg}{m \cdot s^4}$	diffusive flux of granular temperature, defined by (EQ 29)	w	$\frac{m}{s}$	z- or θ -component of gas velocity
$\dot{q}$	#/s	particle number flowrate	W	varies	weighting function
q'_{rg}	$\frac{kg^2}{m^4 \cdot s^2}$	radiative heat transfer from gas phase to particle phase per unit volume per unit time	x	m	x-coordinate length
Re	-	particle Reynolds number defined by	y	m	y-coordinate length
r	m	r-direction length coordinate	z	m	z-coordinate length
r_j	$\frac{kg}{m^3 \cdot s}$	rate of mass production per unit volume of j^{th} component of solid phase	Greek		
S_g^m	$\frac{kg}{m^3 \cdot s}$	gas phase mass source term for particle continuity equation	α	-	constant used in (EQ 26) and (EQ 30)
S_p^m	$\frac{kg}{m^3 \cdot s}$	particle mass source term for gas phase continuity equation	γ	$\frac{kg}{m \cdot s^3}$	dissipation of kinetic energy due to collisions between particles, defined by (EQ 30)
			Γ_ϕ	varies	diffusion coefficient in the generalized equation of change, (EQ 41)
			ϵ_M	-	void fraction of fluidized bed at mini-

		min fluidization velocity
ϵ	$\frac{m^2}{s}$	dissipation rate of turbulent energy
η	-	coal gas mixture fraction
κ	$\frac{kg^2}{s^2}$	diffusive coefficient for granular temperature
θ	°	θ -coordinate length
μ	$\frac{kg}{m \cdot s}$	laminar viscosity of gas phase
μ_e	$\frac{kg}{m \cdot s}$	effective particle phase "viscosity"
μ_g	$\frac{kg}{m \cdot s}$	effective gas turbulent viscosity
μ_i	$\frac{kg}{m \cdot s}$	eddy viscosity of gas phase
v	-	ensemble averaged solid fraction
π	-	constant
ρ	$\frac{kg}{m^3}$	ensemble averaged density of particle phase
$\bar{\rho}$	$\frac{kg}{m^3}$	time-averaged density of gas phase
ρ_g	$\frac{kg}{m^3}$	density of gas phase
ρ_p	$\frac{kg}{m^3}$	actual particle density
σ	m	standard deviation, covariance matrix
σ	$\frac{kg}{m \cdot s^2}$	total particle stress tensor
σ_k	-	constant required in the equation for the turbulent kinetic energy
σ_ϵ	-	constant required in the equation for the eddy dissipation in Table 4 and Table 5
ϕ	varies	a general flow variable
ϕ_s	-	sphericity of solid particles

Special Symbols

$\frac{D}{Dt}$ s^{-1} substantial derivative

∇ m^{-1} gradient

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