Three-Dimensional Turbulent Particle Dispersion Submodel Development

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1 Introduction

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 environments in such applications 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. Even when the turbulence characteristics are known, computational methods for coupling the dynamics of the particulate phase with the continuous phase have not been well established. Several new theoretical descriptions of the turbulent dispersion of particles and droplets have been proposed over the past few years. It has been the purpose of this project to explore the potential of these theories for coupling with the other aspects of three-dimensional, reacting, turbulent, particle-laden systems, to provide computational simulations that could be useful for addressing industrial problems.

Two different approaches were explored in this project. The major thrust of this project was on identifying a suitable dispersion submodel for dilute dispersed flows, implementing it in a comprehensive three-dimensional CFD code framework for combustion simulation and evaluating its performance rigorously. In another effort the potential of a dispersion submodel for densely loaded systems was analyzed. This report discusses the main issues that were resolved as part of this project.

2 Dilute Particle Phase Dispersion Model Development

This analysis, as currently implemented, is valid for describing the dispersion of well-defined dispersed phase elements, e.g. particles, entrained in a turbulent flowfield, with particle mass loadings of less than unity and corresponding relatively small local dispersed phase volume fractions (generally $< 0.1\%$). Under such conditions particle-to-particle interaction can be neglected [Oesterle, 1991].

The mechanistic aspect of the dispersion of the condensed phase, in turbulent systems, is not just the transport along the mean flow, but also the turbulent fluctuations, of the continuous phase. Also, the effect of particles on the fluid phase due to exchange of mass (especially important for combusting particles) and momentum, between the phases, needs to be included in the continuous phase calculations as appropriate sources and sinks, to provide two-way coupling. Modification of continuous-phase turbulence properties due to particle transport, called turbulence modulation, is considered a less important aspect. The objective is to provide a dispersion model which can adequately incorporate these phenomena within the framework of a 3D comprehensive combustion computation, in a relatively efficient manner, so that industrial flows can be simulated.

In the next section various dispersion models used in the past will be reviewed. The following sections describe the important aspects of dilute particle system submodel theory and implementation. Finally results and conclusions are presented.

Background

Several reviews available in the literature address various aspects of turbulent particle dispersion [Faeth, 1987; Hinze, 1975; Baxter, 1989]. Different analyses can broadly be classified, either as those which assume infinitely fast interphase transport rates resulting in locally homogeneous flow (LHF) or separated flow (SF) analyses where finite interphase transport rates are considered and then again on the basis of the frame of reference in which the condensed phase is considered (Eulerian or Lagrangian). Advantages and disadvantages of different formulations for dispersion in turbulent flows will be discussed here briefly.

The continuous phase is almost exclusively cast in an Eulerian reference frame. The LHF analysis [Faeth, 1983; Kuo, 1986] treats the condensed phase as a mixture fraction and is easy to implement in this Eulerian framework. However the assumptions of phase equilibrium and molecular diffusion of particles are not realistic and result in overprediction of dispersion (Fig. 1).

SF models can be looked at as those that treat the dispersed phase as a continuum (in an Eulerian reference frame) and those that track discrete particle elements (in a Lagrangian frame of reference). Continuum formulations can involve treating the gas and dispersed phase as interpenetrating continua, in conjunction with empirical interphase transport rates [Drew, 1983]. Considerable effort was spent looking into the potential of this formulation applied to densely loaded systems [Smith, 1992]. However numerical instabilities inherent to this approach and the prohibitive storage requirements for applying this approach to polydisperse flows made it difficult to implement. Further discussion of this analysis will be considered in Section 3. Alternatively, in the continuous particle model, as described by Williams [1985], a multi-dimensional statistical distribution function describes the particle properties. This function is obtained by solving its Eulerian transport equation along with the gas phase equations containing source terms. However, dispersed phase/turbulence interaction for these analyses have not been satisfactorily resolved and this approach becomes computationally intensive for polydisperse flows involving interphase heat and mass transfer.

The discrete element formulation involves dividing the dispersed phase into representative groups, whose motion and transport are tracked through the flow field using a Lagrangian formulation, a distinct advantage since numerical diffusion is minimized and also particle life history information can be maintained. The continuous phase is resolved in an Eulerian reference frame. A simplified discrete particle formulation is the Particle Source in Cell Technique (PSICT) of Crowe et al [1977], in which each representative computational parcel is characterized by a single particle, which is tracked using a Lagrangian formulation and particle source terms are introduced, into the Eulerian gas-phase conservation equations, according to the distribution of parcels, to account for mass and momentum transfer between the phases. However, the point source representation of particles can introduce computational shot noise. Also, turbulent particle dispersion has to be introduced into the scheme. In an oversimplified approach the computational parcels follow deterministic trajectories interacting with mean gas flow properties only. Obviously, these Lagrangian ballistic methods underestimate dispersion of the condensed phase (Fig. 1).

Because of the large number of particles we are dealing with, the effect of dispersion of particles due to turbulent gas velocity fluctuations must be included in the Lagrangian discrete particle formulation in a stochastic manner. Early ideas for stochastic models introduced by Yuu et al. [1978], Dukowicz [1980], Hutchinson et al. [1979], are essentially random-walk approaches to particle dispersion. Gosman and Ioannides [1981] extended these ideas to come up with the Stochastic Separated Flow (SSF) model. The SSF methods involve tracking individual particle trajectories similar to Lagrangian ballistic models, except that now particles get entrained in eddies and interact with instantaneous gas velocities, obtained by random sampling of the turbulent gas velocity fluctuation distribution in that eddy. Implementations of this basic methodology have been demonstrated to provide a sufficiently accurate description of turbulent dispersion by Shuen et al. [1986] for different experimental setups, like the measurements of Yuu et al. [1978] in a round, turbulent jet (Fig. 1). However, typically nearly 5000 trajectories had to be calculated to achieve statistically stable and converged solutions in the simulations of these simplified flowdomains with monosized particles. Computational costs can be prohibitive for the large number of trajectories required to be simulated in an industrial furnace.

In another effort, Smith [1985] used a gradient diffusion approach to resolve turbulent dispersion effects while tracking mean particle properties in a Lagrangian reference frame. However, parameters fitted for obtaining a gas-particle exchange coefficient cannot be justified or trusted to work for different cases.

From the above discussion it is evident that these traditional methods fail to meet our need for a turbulent particle dispersion submodel. An approach outlined by Baxter and Smith [1989,1994] has shown potential to accurately model the stochastic transport of particles (STP model) in turbulent flows in a computationally efficient manner. Some of its basic features were implemented in two-dimensional computations and its performance was promising. Litchford et al. [1992] recently reported satisfactory performance of a similar approach for dispersion computations in test cases. The STP model was chosen for implementation and testing in the framework of a three-dimensional comprehensive computer code.

The 3DSTP Submodel

The approach we have developed to model particle dispersion in lightly loaded systems involves tracking particle clouds in a Lagrangian frame of reference. Lagrangian methods have the advantage of being able to account for time-temperature histories of reacting particles. This is important since particles arriving at any given spatial position in the system may have different histories and properties. However, as discussed in the previous section Lagrangian methods developed in the past, at best, perform Monte-Carlo simulations of particle trajectories which require simulation of a large number of trajectories to arrive at a numerically accurate and stable solution. The computational effort involved in predicting particle dispersion in industrial coal combustors by this method makes it inadvisable to use these models. We have developed a technique for computationally tracking clouds of particles, rather than individual particles, in which we calculate mean particle trajectories and the stochastic turbulent dispersion of the cloud about this mean position. The method deals with the reaction of coal particles and also coupling with the continuous phase using source terms for mass, momentum

and energy exchanges. Detailed analysis of this model for the stochastic transport of particles (STP model) can be found in previous quarterly reports [Smith, 1991]. In the following discussion we shall summarize some important aspects of its theory and implementation.

Mathematical Description

In the STP model, the time evolution of a probability density function (pdf) for particle position is modelled. The value of this time evolving pdf, at any location, represents the probability of finding particles of the corresponding type and starting position, with that residence time, at that location in the flow field. This probability is used to obtain the expected number density of particles with the corresponding properties in each computational volume. The contribution to mass, momentum and energy by these particles in each Eulerian computational cell is added dynamically while tracking the particle pdf, to provide source terms, which are coupled into the Eulerian gas phase transport equations. Particles represented by different pdf's with various residence times contribute to the overall particle contribution of the cell. Thus, the total source term for an Eulerian cell is obtained as the summation of the following over all particle type trajectories.

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

where $\dot{q}$ is the particle number flowrate, r_p^{ϕ} is the rate of particle property change, the time integral is with respect to residence time, W is a weighting term based on the pdf, ijk represent the coordinates of the Eulerian cell 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

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

where lb and ub represent the lower and upper bounds of the cell, respectively. Table 1 defines the specific variables for which these source terms are calculated.

The term $W(x_i, t)$ is a weight function defined in terms of the pdf for particle position, $P(x_i, t)$.

$$W(x_i, t) \equiv \frac{P(x_i, t)}{\int_{V(min-max)} P(x_i, t) dV} \quad (\text{EQ 3})$$

The pdf's for particle position are assumed to be multivariate Gaussian or normal pdf's. These are completely described by their means, μ_i , and variances, σ_i , and are of the form

$$P(x_i, t) = \frac{1}{(8\pi)^{3/2} \prod_{i=1}^3 \sigma_i} e^{-s^2/2} \quad (\text{EQ 4})$$

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 $S_p^m = S_p^f + S_p^\eta$		

$$s = s(x_i, t) = \sum_{i=1}^3 \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2. \quad (\text{EQ 5})$$

The mean particle position and its variance are expressed as ODE's, with the aerodynamic drag force and weight providing the main driving force for mean particle position change and the fluctuating component of velocity determining the variance about this value. The expected mean particle position is given by

$$\langle x_i(t) \rangle = \int_0^t \langle V_i(t_1) \rangle dt_1 + \langle x_i(0) \rangle = \mu_i \quad (\text{EQ 6})$$

$$\frac{d\langle V_i \rangle}{dt} = \beta (\langle U_i \rangle - \langle V_i \rangle) + g_i \quad (\text{EQ 7})$$

where $\langle U \rangle$ and $\langle V \rangle$ are the ensemble averaged gas and particle phase velocities respectively. β is calculated from Stoke's law as

$$\beta = \frac{3\pi d_p \mu_g}{m_p}. \quad (\text{EQ 8})$$

Note that the above equations are written in terms of ensemble averaged properties. These can be understood by thinking of them as the statistical average value obtained if the same experiment is performed repeatedly. This expected mean value can be calculated, for the gas velocity for example, as

$$\langle U_i \rangle = \left(\iiint U(x_i) \langle n(x_i) \rangle dx_i \right) / \langle n_T \rangle \quad (\text{EQ 9})$$

where n represents particle number density. Its expected value can be obtained from the particle position pdf by definition as follows,

$$\langle n(x_i) \rangle = qP(x_i, t) \quad (\text{EQ 10})$$

The covariance matrix for a stationary field is written in terms of the particle velocity correlation function $R_{ij}^p(t_1, t_2)$ as

$$\sigma_{ij}(t) = 2 \int_0^t (t - \tau) R_{ij}^p(\tau) d\tau \quad (\text{EQ 11})$$

$$R_{ij}^p(t_1, t_2) \equiv \langle v_i(t_1) v_j(t_2) \rangle. \quad (\text{EQ 12})$$

In the STP model this correlation function is computed by assuming that its behavior is represented by a class of stochastic processes called Markovian processes. Under this Markovian approximation the particle autocorrelation function takes the form

$$R_{ij}^p(\tau) = \langle v^2 \rangle e^{-\frac{\tau}{T_L(\tau)}} \quad (\text{EQ 13})$$

The mean square of particle velocity fluctuations is computed from the gas velocity fluctuations, u , as

$$\langle v^2 \rangle = \langle u^2 \rangle (1 - e^{-\beta T_g}) \quad (\text{EQ 14})$$

where T_g is a characteristic time scale of the gas turbulence and in the case of a k - ϵ model is derived by Corrsin [1963] as

$$T_g = \frac{C_\mu^{3/4} k^{3/2}}{\epsilon (\frac{2}{3}k)} \quad (\text{EQ 15})$$

The mean square gas velocity fluctuations depend on the turbulent kinetic energy as follows.

$$u_i^2 = \frac{2k}{3} \quad (\text{EQ 16})$$

T_L is the Lagrangian integral time constant. This time constant has been approximated as

$$T_L = \max(T_g, \beta^{-1}) \quad (\text{EQ 17})$$

Framework of the 3D Comprehensive Combustion Computer Code

The STP model has been incorporated in a three-dimensional comprehensive combustion computer code previously developed by the authors. A flow chart of the solution algorithm for performing the overall calculations in series (as opposed to parallel computations) is shown in Fig. 2.

The gas phase portion of the calculations 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 the gas phase enthalpy are written in the form of a single transport equation (in the form: convection - diffusion = source):

$$(\nabla \cdot (\rho v \phi)) - (\nabla \cdot (\Gamma_{\phi} \nabla \phi)) = S^{\phi} \quad (\text{EQ 18})$$

This generalized equation along with the variable substitutions for the different transport properties is presented in Table 2. All terms designated by a S, are source terms, to be calculated in the particle portion of the code.

After initialization, finite difference forms of the transport equations for the gas phase are solved for each variable independently using a line-by-line Tri-Diagonal Matrix Algorithm (TDMA) iterative technique (microiterations). A single overall iteration in which new estimates of each of the main dependent variables in the Table 1 are generated, is called a macroiteration. Fluid properties and radiation properties are also updated in every macroiteration. During these macroiterations, 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 particle iteration. This algorithm can be modified to allow parallel processing of the particle and gas phase calculations on two CPU's with exchange of information taking place through direct data transfer, resulting in improved memory and run time efficiency.

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. Particles clouds are initiated from several (typically about ten) starting locations in the reactor. In addition, heterogeneity of inlet particle-laden streams is accounted for by tracking separate clouds for several (typically about fifteen) different particle types. 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 for a cloud, the equations describing the development of the pdf for particle location are solved as a function of residence time until the particle trajectory reaches the reactor exit or stagnates. In addition to the pdf for particle position, the particle temperature, composition, size and density are predicted as functions of time. Exchanges of mass, momentum and energy for a particle cloud are dynamically evaluated at discrete time steps from these properties and the particle number density given by the particle pdf and added to the source terms in each computational cell in which the particles are located, similar to the PSIC technique described by Crowe et al. [1977]. The calculation of the cloud dispersion allows these source

Figure 2 Algorithm for running the 3DSTP code in series

Table 2 3D Cartesian Differential Equation Set for Continuous Phase

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

Equation ϕ Γ_ϕ S^ϕ

Continuity 1 0 S_p^m

X-Momentum

$$\bar{u}_s = \mu_s^g \left[-\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}(\mu_s^g \frac{\partial \bar{u}_s}{\partial x}) + \frac{\partial}{\partial y}(\mu_s^g \frac{\partial \bar{v}_s}{\partial x}) + \frac{\partial}{\partial z}(\mu_s^g \frac{\partial \bar{w}_s}{\partial x}) - \frac{2}{3}\bar{\rho}k + \bar{\rho}g_x + \bar{u}_s S_p^m + S_p^u \right]$$

Y-Momentum

$$\bar{v}_s = \mu_s^g \left[-\frac{\partial p}{\partial y} + \frac{\partial}{\partial x}(\mu_s^g \frac{\partial \bar{u}_s}{\partial y}) + \frac{\partial}{\partial y}(\mu_s^g \frac{\partial \bar{v}_s}{\partial y}) + \frac{\partial}{\partial z}(\mu_s^g \frac{\partial \bar{w}_s}{\partial y}) - \frac{2}{3}\bar{\rho}k + \bar{\rho}g_y + \bar{v}_s S_p^m + S_p^v \right]$$

Z-Momentum

$$\bar{w}_s = \mu_s^g \left[-\frac{\partial p}{\partial z} + \frac{\partial}{\partial x}(\mu_s^g \frac{\partial \bar{u}_s}{\partial z}) + \frac{\partial}{\partial y}(\mu_s^g \frac{\partial \bar{v}_s}{\partial z}) + \frac{\partial}{\partial z}(\mu_s^g \frac{\partial \bar{w}_s}{\partial z}) - \frac{2}{3}\bar{\rho}k + \bar{\rho}g_z + \bar{w}_s S_p^m + S_p^w \right]$$

Turbulent Kinetic Energy

$$\bar{k} = \frac{\mu_s^g}{\sigma_k} G - \bar{\rho}\bar{\epsilon}$$

Dissipation Rate

$$\bar{\epsilon} = \left(\frac{\bar{\epsilon}}{\bar{k}} \right) (c_1 G - c_2 \bar{\rho}\bar{\epsilon})$$

where

$$G = \mu_s^g \left[2 \left(\left(\frac{\partial \bar{u}_s}{\partial x} \right)^2 + \left(\frac{\partial \bar{v}_s}{\partial y} \right)^2 + \left(\frac{\partial \bar{w}_s}{\partial z} \right)^2 \right) + \left(\frac{\partial \bar{u}_s}{\partial y} + \frac{\partial \bar{v}_s}{\partial x} \right)^2 + \left(\frac{\partial \bar{u}_s}{\partial z} + \frac{\partial \bar{w}_s}{\partial x} \right)^2 + \left(\frac{\partial \bar{v}_s}{\partial z} + \frac{\partial \bar{w}_s}{\partial y} \right)^2 \right]$$

terms to be distributed spatially throughout the Eulerian mesh. Also, as discussed in Quarterly Progress Report #4 [Smith, 1992], any particle property (number density, temperature, residence time, burnout, etc.) can be displayed as an Eulerian field. Ensemble average Eulerian properties needed for solving the next time-step of the particle ODE's, are calculated dynamically while distributing source terms over three standard deviations of the pdf. Also the algorithm for the distribution of sources has been improved so that it handles the distribution in the three coordinate directions more efficiently and interacts with walls more realistically.

The Lagrangian nature of this particle model 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, pulverized coal combustion and gasification, fuel oil combustion, coal slurry combustion, and spray drying.

Evaluation and Results

In the past the two-dimensional implementation of the STP model has been shown to compare well with exact solutions [Baxter, 1989] for a hypothetical system with a constant diffusion coefficient. However as pointed out by the same author because of the inherent assumptions in these cases these comparisons are of little practical significance. Hence the emphasis of the evaluation was put on comparison with experimental data. A literature search was done to come up with appropriate and reliable experimental data, to be used to evaluate the performance of the 3D STP dispersion model and its implementation within the framework of a comprehensive coal combustion simulation. Some of the dilute dispersed flows considered were, measurements in turbulent particle-laden jets by Yuu et al. [1978], Modarres et al. [1984], and Shuen et al. [1985], PIV measurements by Lee, Hanratty and Adrian [1989], and combustion measurements by Lockwood et. al. [1988]. The following two cases were chosen for comparison. One is the the measurements of particle velocity autocorrelation functions for various spherical beads in a grid generated homogeneous turbulent flow by Snyder and Lumley [1971], which have been used by others in the past for comparing dispersion models [Berlemont, 1987; Litchford, 1991; Shuen, 1983; Zhuang, 1989] and is accepted as a reliable base case for validation of the dispersion model. The other is the coal-fired International Flame Research Foundation (IFRF) furnace case for which detailed combustion measurements have been made [Michels and Payne, 1991] and can be consequently used to demonstrate the applicability of the dispersion model for describing pulverized coal combustion environments.

Dispersion in Homogeneous Turbulent flow

The experiments of Snyder and Lumley involved measurement of the ensemble average dispersion of spherical beads (46.5 μ hollow glass, 87 μ glass, 87 μ corn pollen, and 46.5 μ copper) introduced isokinetically, downstream in a natural grid generated turbulent flow. Eulerian turbulence data taken indicated homogeneous turbulence in planes parallel to the grid and mild inhomogeneity in the streamwise direction due to decay of turbulent energy. The turbulence was also nearly isotropic.

The reported flow turbulence characteristics were used to simulate the turbulent gas flow field. A single trajectory corresponding to each particle type was computed and the dispersion associated with each trajectory was evaluated using the STP model. Since the particle loading was low, coupling of particle momentum in the gas phase solution could be neglected. In Fig. 3, mean square displacements as a function of residence time obtained from experiments and STP model predictions are shown. Good agreement is obtained from the STP model by computing just one trajectory and its associated dispersion, whereas similar predictions by the SSF model required computation of more than 1000 particle trajectories for a stable solution. Pulverized coal particles are typically $\sim 100\mu$ size and their density is ~ 1.4 g/cc, so their behavior is represented closely by the corn and glass beads, whereas the hollow glass is more typical of the behavior of fluid elements. It should be noted that the probability densities of particle position produced by the experimental results and the SSF model are Gaussian, thus providing justification for the normal pdf used to describe the particle cloud in the STP model.

Coal combustion in the IFRF furnace

Detailed input, output and in-flame measurements in long pulverized coal flames, in the IFRF furnace no. 1, which is a refractory tunnel furnace of approximate dimensions $6.25 * 1.9 * 1.9$ m., have been reported [Michels and Payne, 1991]. The primary and secondary ducts are concentric and located at one end of the reactor and the overall flow is essentially axisymmetric even though the roof of the furnace is dome shaped. Trials with various flow rates and burner dimensions have been analyzed. The flame A1, which is characterized by high (>25 m/s) secondary air velocity and a flame attached to the burner, was selected for detailed comparison with combustion simulation predictions. Table 3 lists the general characteristics of the experimental conditions in which the flame A1 was obtained.

Table 3 General characteristics of IFRF pulverized coal combustion case

Variables	Values
Combustor length, width, height	2.0, 0.2, 0.2 m
Primary, Secondary diameters	70.3, 260 mm
Primary, Secondary air flowrate	.07, 0.57 kg/s
Particle loading in primary	0.83
Initial particle size, density	25 - 200 μ m, 1340 kg/m ³
Primary, Secondary temp.	423, 763 K

The simulations for this case were started off by initializing the particle mass source terms such that all the coal off-gas was distributed in the first quarter of the reactor. The final solutions were found to be independent of this guess. Particle clouds of five types (different sizes to adequately represent the particle size distribution) were started from six different locations in the primary inlet, with an initial dispersion width (particle pdf variance) such that an approximately uniform distribution of particles

Figure 1 Predicted particle concentrations in a particle-laden round jet using three types of particle dispersion models. Measurements from Yuu et al.

Figure 3 Comparison of 3D STP model predictions with measurements by Snyder and Lumley of particle dispersion in a grid-generated turbulent flow.

over the inlet was simulated. A converged solution was obtained in less than ten particle iterations in a total cpu time of ~10 hrs. with the particle calculations taking 20% of that time on an IBM Model 560 RISC System 6000 workstation. Computations were performed with 4 different mesh resolutions. Grid independent simulations of this case were obtained by resolving the furnace with a $32 \times 30 \times 30$ three-dimensional mesh. However the results are displayed for a $46 \times 36 \times 36$ mesh (Fig. 4), with 46 nodes in the axial direction and providing a better resolution in the near-burner region, to show more detail of the flame characteristics (Fig. 5).

This mesh is illustrated in Fig. 4, along with the velocity fields in the reactor. In Fig. 5, a picture of the actual experimental flame is presented alongside the simulated flame. One can see that we simulate the general structure of this attached flame very well. Since this flame is mixing-controlled, flame characteristics depend on the degree of mixing between the coal off-gas and the oxygen in the secondary air stream and are a good indication of how well we simulate the particle dispersion process.

Simulated axial and radial temperature profiles are compared with in-flame point measurements in Fig. 6. Overall predicted temperature fields are reasonable and duplicate observed trends remarkably well. Some discrepancy is seen in the axial profile very close to the burner. However, temperatures in the flame are ~2000 K and measuring the temperature in this extremely turbulent environment is difficult. Also temperatures in the near-burner region vary drastically within a short distance as we move away from the axis. With our fine resolution we are able to report an axial temperature which is the local temperature within 1 cm. from the axis. Experimental results with such spatial resolution are not available. The initial peak that we see in the axial profile actually corresponds to the computational cell in which the oxygen in the primary stream achieves stoichiometric combustion with the coal off gas.

Another variable which is a good indication of the overall performance of the comprehensive simulation is the particle burnout. In fact, a converged particle burnout in consecutive particle iterations is used as one of the criterion for deciding overall computational convergence. Particle burnouts, calculated as an Eulerian field by the 3DSTP model, are plotted along the axis in Fig. 7 and are in excellent agreement with the reported values.

Predicted species concentration and other properties compared favorably with the experimental results and showed trends as expected. This case study has proven that this comprehensive computer code we have developed is capable of accurately and efficiently simulating industrial processes involving turbulent particle dispersion.

Figure 4 Computational mesh used to resolve the IFRF furnace. Velocity fields in the reactor are displayed.

Figure 5 Actual picture of the Flame A1 in the IFRF furnace alongside the simulated flame.

Figure 6 Computed axial (above left) and radial (above right) temperature profiles are compared to the reported experimental values. Figure on top shows the lines in the reactor along which these plots have been made

Figure 7 Comparison of line plot of computed particle burnouts along the reactor axis with experimentally obtained values.

3 Dense-Phase Dispersion Submodel

The second approach to describing the turbulent transport of particles is to use a pure Eulerian description. In this section the progress is described in the development of a dense-phase particle dispersion submodel which can be used to predict the flow behavior of multiphase mixtures for potentially all void fractions but particularly in situations where the mixture is more dense. The work done focuses primarily on the development of a computer model which can couple the important processes to predict steady-state enclosed flow patterns of gas-solid mixtures in an arbitrary three-dimensional geometry.

Review of Theory Development

The main thrust of this effort is to develop a code applicable to industrial scale particle-laden combustors over a wide range of loadings including circulating fluidized bed combustors. The solid fractions in these more dense situations are typically in the range of 0.3 - 0.6, in which case a Lagrangian approach which is based on the assumption of non-interacting particles starts to break down. The Eulerian description considers the mixture to be comprised of mutually interpenetrating phases. In what follows, we first describe the theory for a two-phase (gas-solid) mixture with uniform monodisperse particles. Extensions to multiple sizes are described in a later section.

Review of Constitutive Equations for the Granular Phase

In the first quarterly report (Smith, 1991a) 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. It was then decided to adopt the constitutive equations of Jenkins and Savage (1983), modified to include the kinetic contribution of Lun et al. (1984) for the situation under consideration. For convenience these are summarized below (in these equations, tensile stresses are taken as positive) :

$$\sigma = -\rho_p \bar{v} T I - \frac{\pi^{1/2} \kappa T^{1/2}}{d} I + \left(\frac{1}{5}\right) \kappa (2 + \alpha) [(tr D) I + 2D] \quad (\text{EQ 19})$$

$$\kappa = 2\rho_p \bar{v}^2 g_0(\bar{v}) d (1 + e) \left(\frac{T}{\pi}\right)^{1/2} \quad (\text{EQ 20})$$

$$\left(\frac{3}{2}\right) \bar{\rho} \frac{DT}{Dt} = -(\nabla \cdot q) + tr(\sigma \nabla \bar{v}) - \gamma \quad (\text{EQ 21})$$

$$q = -\kappa \nabla T \quad (\text{EQ 22})$$

Harlow and Amsden, 1975b; Crowe, 1975). More recently, Ding and Gidaspow (1990) have derived governing equations from a more fundamental viewpoint, starting from the same ensemble-averaged form of the balance equation as Jenkins and Savage (1983). However, for the force acting on an individual particle, F , they used the following expression:

$$F = g + \frac{D}{m} (c_g - c) - \frac{1}{\rho_p} \nabla p \quad (\text{EQ 27})$$

The first term on the right-hand side of (EQ 27) is gravity, the second is the drag, and the third is the pressure force due to the gas phase. Substituting this in the ensemble averaged balance equation for the particle phase, Ding and Gidaspow (1990) obtained the governing equations (for a single particle size), which are shown here in steady-state form:

Continuity:

$$\nabla \cdot (\bar{\rho} \bar{v}) = 0 \quad (\text{EQ 28})$$

Momentum:

$$\nabla \cdot (\bar{\rho} \bar{v} \bar{v}) = -\bar{v} \nabla p + \nabla \cdot \sigma + \bar{\rho} g + \beta (\bar{v}_g - \bar{v}) \quad (\text{EQ 29})$$

Fluctuating Energy:

$$\frac{3}{2} \nabla \cdot (\bar{\rho} \bar{v} T) = \sigma : \nabla \bar{v} - \nabla \cdot q - \gamma - 3\beta T \quad (\text{EQ 30})$$

where p is the thermodynamic pressure due to the gas. β is the exchange coefficient between the two phases (per unit volume of the particle phase) due to interphase drag. The term involving the drag appears in the governing equations of both gas and particle phases, but with opposite signs (the exact form of this exchange coefficient is discussed in a later section.) In this formulation the pressure gradient is distributed among the gas and particle phases. Harlow and Amsden (1975a) have shown that this is the correct way of interpreting the effect of the pressure gradient on the particles, i.e., with the solid fraction outside the gradient rather than inside it.

As the present work aims at the solution of flow problems involving several grain sizes, the present theory needs extension. The inclusion of additional particle sizes is handled by considering each grain size as a phase, and writing equations similar to (EQ 28) - (EQ 30) for each phase. However, the presence of an extra granular phase will generate extra source terms on the right hand sides of (EQ 29) and (EQ 30). The source term for the momentum equation is modeled by considering the particle-particle interaction to be analogous to a fluid-particle interaction. In other words, since the particle phase has a Newtonian constitutive relation, it is treated as one, and the particle-particle situation is mod-

eled analogous to that of a Newtonian fluid moving around a particle. The “drag” force acting on one phase due to the motion of the second phase relative to it is calculated analogous to the way the drag is calculated in a fluid-particle system (see discussion in a later section.) Thus, for the interaction between two phases, the momentum exchange coefficient may be written as:

$$\beta_{12} = \frac{18\mu_{e2}\bar{v}_1}{d_1^2} , \quad (\text{EQ 31})$$

where the subscripts refer to the particle phases 1 and 2.

The additional source term in the fluctuation energy (granular temperature) equation due to the presence of more than one solid phase is modeled based on the extra source term in the energy equation arising from the gas phase motion. In (EQ 30), this is the last term on the right side. Ding and Gidaspow (1990) originally obtained this term as

$$\beta (\overline{C_g \cdot C} - \overline{C} \cdot \overline{C}) , \quad (\text{EQ 32})$$

for the case of a single particle phase.

They then assumed that the correlation between the gas velocity fluctuation and the particle velocity fluctuation was zero, and, using Eq. (46) in Chapter 2, reduced this term to $-3\beta T$. Here it is assumed that the source term in the energy equation due to particle-particle interactions has the same form as (EQ 32), i.e.,

$$\beta_{ij} (\overline{C_i \cdot C_j} - \overline{C_i} \cdot \overline{C_j}) , \quad (\text{EQ 33})$$

where the i and j refer to two different particle phases.

Further, it is assumed that the fluctuating velocities are almost perfectly correlated, so that the source term from (EQ 33) vanishes. Of course, this implies the restriction that the variation in sizes of the mixture not be too great, for it would be unrealistic to expect that the fluctuating velocities of a very small particle and a very large particle would be perfectly correlated.

With these modeling assumptions, the governing equations for the i^{th} particle phase become:

Continuity:

$$\nabla \cdot (\bar{\rho}_i \bar{v}_i) = 0 . \quad (\text{EQ 34})$$

Momentum:

$$\nabla \cdot (\bar{\rho}_i \bar{v}_i \bar{v}_i) = -\bar{v}_i \nabla p + \nabla \cdot \sigma_i + \bar{\rho}_i g + \beta_i (\bar{v}_g - \bar{v}_i) + \sum_{j=1, i}^l \beta_{ij} (\bar{v}_j - \bar{v}_i) \quad . \quad (\text{EQ 35})$$

Fluctuating Energy:

$$\frac{3}{2} \nabla \cdot (\bar{\rho}_i \bar{v}_i T_i) = \sigma_i : \nabla \bar{v}_i - \nabla \cdot q_i - \gamma_i - 3\beta_i T_i \quad . \quad (\text{EQ 36})$$

Here l is the number of particle sizes, and ρ_i , $\bar{v}_i$, $\bar{v}_i$ and T_i are the bulk density, velocity vector, solid fraction and granular temperature of the i^{th} phase respectively. The β_{ij} are of the form of (EQ 31), and the quantities σ_i , q_i , and γ_i for each phase are obtained from the constitutive relations given in (EQ 19)-(EQ 23), written for each phase. The β_i are the exchange coefficients for the gas-solid drag. The evaluation of this term is discussed in a later section.

One does not need to solve (EQ 36) for each of the l phases, since, as Farrell et al. (1986) point out, the principle of equipartition of energy can be utilized if all grains are composed of the same material, and hence possess the same coefficient of restitution. Mathematically, this may be expressed as:

$$\frac{3}{2} \bar{v}_i T_i = \frac{3}{2} \bar{v}_j T_j \quad \forall \quad i, j = 1, \dots, l \quad . \quad (\text{EQ 37})$$

Thus, knowing the relative proportions of two grain phases and the value of the granular temperature of one phase, the granular temperature of the other phase can be determined.

Governing Equations for Gas Phase Flow

The description of the gas-phase dynamics that follows is brief and details can be found in many sources (e.g. Rodi, 1982.)

The gas phase is turbulent and assumed to be Newtonian. As a result of the large variation in the length and time scales in turbulent flow, the gas-phase momentum equations cannot be solved in their instantaneous form. Hence the instantaneous variables are assumed to be composed of mean and fluctuating parts as shown:

$$\phi_k = \bar{\phi}_k + \phi'_k \quad , \quad (\text{EQ 38})$$

where the mean is an ensemble average. The resulting equations are then averaged to obtain equations for statistical means. These are given below:

Continuity:

$$\nabla \cdot (\bar{\rho}_g \bar{\mathbf{v}}_g) = 0 . \quad (\text{EQ 39})$$

Momentum:

$$\nabla \cdot (\bar{\rho}_g \bar{\mathbf{v}}_g \bar{\mathbf{v}}_g) = -\bar{\varepsilon}_g \nabla p + \nabla \cdot (\mu_g (\nabla \bar{\mathbf{v}}_g + (\nabla \bar{\mathbf{v}}_g)^T) - \bar{\rho}_g \overline{\mathbf{v}'_g \mathbf{v}'_g}) + \bar{\rho}_g \mathbf{g} + \sum_{i=1}^I \beta_i (\bar{\mathbf{v}}_i - \bar{\mathbf{v}}_g) . \quad (\text{EQ 40})$$

In these equations $\bar{\rho}_g$ is the bulk density of the gas, defined as

$$\bar{\rho}_g = \rho_g \bar{\varepsilon}_g , \quad (\text{EQ 41})$$

where $\bar{\varepsilon}_g$ is the void fraction of the gaseous phase, related to the solid fraction by

$$\bar{\varepsilon}_g = 1 - \bar{v} . \quad (\text{EQ 42})$$

Note that (EQ 41) incorporates the implicit assumption that the gas-phase density and voidage are independent variables [statistically speaking.]

However, as can be seen, the averaged equations involve correlations of fluctuating quantities ($\overline{\mathbf{v}'_g \mathbf{v}'_g}$) which do not directly depend on the mean flow quantities - often referred to as the closure problem of turbulence. To solve this, use here is made of an eddy viscosity hypothesis, whereby the velocity fluctuation correlations are expressed as linear functions of the deformation rate tensor, analogous to the molecular viscosity. The eddy kinematic viscosity ν_t , defined by

$$-\overline{\mathbf{v}'_g \mathbf{v}'_g} = \nu_t \left(\frac{\partial \bar{v}_{gi}}{\partial x_j} + \frac{\partial \bar{v}_{gj}}{\partial x_i} \right) - \frac{2}{3} (\nu_t (\nabla \cdot \bar{\mathbf{v}}_g) + \bar{k}) \delta_{ij} \quad (\text{EQ 43})$$

is assumed to be related to mean-flow quantities via the Prandtl-Kolmogorov hypothesis,

$$\nu_t = \frac{C_\mu \bar{k}^2}{\bar{\varepsilon}} , \quad (\text{EQ 44})$$

where $\bar{k}$ is the ensemble-averaged turbulent kinetic energy, defined as the trace of the Reynolds stress tensor (the fluctuating velocity correlation tensor), $\bar{\varepsilon}$ is the (averaged) dissipation of turbulent kinetic energy (not to be confused with $\bar{\varepsilon}_g$, the void fraction) and C_μ is a constant. The turbulent kinetic energy and the dissipation are obtained from transport equations similar in form to the equations for mean motion:

Turbulent Kinetic Energy:

$$\nabla \cdot (\bar{\rho}_g \bar{v}_g \bar{k}) - \nabla \cdot \left(\frac{v_t}{\sigma_k} \nabla \bar{k} \right) = G - \bar{\epsilon} \quad . \quad (\text{EQ 45})$$

Dissipation Rate of Kinetic Energy:

$$\nabla \cdot (\bar{\rho}_g \bar{v}_g \bar{\epsilon}) - \nabla \cdot \left(\frac{v_t}{\sigma_\epsilon} \nabla \bar{\epsilon} \right) = c_1 G \left(\frac{\bar{\epsilon}}{\bar{k}} \right) - c_2 \left(\frac{\bar{\epsilon}^2}{\bar{k}} \right) \quad . \quad (\text{EQ 46})$$

Here G is the rate of production of turbulent kinetic energy, given by:

$$G = \left(\frac{1}{2} \right) \bar{\rho}_g v_t \left[\sum_i \sum_j \left(\frac{\partial \bar{v}_{gi}}{\partial x_j} + \frac{\partial \bar{v}_{gj}}{\partial x_i} \right)^2 \right] \quad , \quad (\text{EQ 47})$$

σ_k and σ_ϵ are turbulent Prandtl numbers for the $\bar{k}$ and $\bar{\epsilon}$ equations, whose standard values are 0.9 and 1.22 respectively. The constants c_1 , c_2 , and C_μ have the values 1.44, 1.92 and 0.09 in the standard model (Rodi, 1982.) The form of the equations for the gas-phase turbulence are assumed not to be highly affected by the presence of particles. One expects the presence of particles in the flow to damp the turbulence in the gas phase, and to account for this, a modification of a correction proposed by Melville and Bray (1979) is adopted:

$$v_{t(\text{particles})} = \frac{v_{t(\text{no_particles})}}{\left(1 + \frac{\sum_{i=1}^I \rho_i}{\rho_g} \right)^{0.5}} \quad (\text{EQ 48})$$

Treatment of Hydrodynamic Drag

The drag force on a spherical particle is defined (Bird, et al., 1960) by the following relation:

$$F_d = \left(\frac{1}{2} \rho_g v_0 |v_0| \right) C_d A_p \quad (\text{EQ 49})$$

where A_p is the projected area of the particle, v_0 is the fluid approach velocity relative to the particle,

$$v_0 = \bar{v}_g - \bar{v} \quad , \quad (\text{EQ 50})$$

ρ_g is the fluid density, and C_d is the drag coefficient.

Here an empirical law is used (Crowe, 1979), for C_d :

$$C_d = \frac{24}{Re_p} (1 + 0.15 Re_p^{0.687}) \quad , \quad (EQ 51)$$

valid for $0 < Re_p < 1000$,

where Re_p is the particle Reynolds number,

$$Re_p = \frac{d|\vec{v}_0|\rho_g}{\mu_g} \quad . \quad (EQ 52)$$

At higher Reynolds numbers (up to $Re_p = 200000$), Newton's law is used (Bird et al., 1960):

$$C_d = 0.44 \quad . \quad (EQ 53)$$

Hence in the present work use is made of (EQ 51) in conjunction with (EQ 53) to determine the drag coefficient. The momentum exchange coefficient, β , is related to C_d in the following manner:

$$\beta = \frac{3}{4} \frac{\bar{v}\rho_g|\vec{v}_0|C_d}{d} \quad (EQ 54)$$

Generalized Equations of Change

(EQ 34) - (EQ 36), (EQ 39), (EQ 40), (EQ 45) and (EQ 46) can be written, after simplification, in the following general form (assuming steady state):

$$\nabla \bullet (\bar{\rho} \vec{v} \phi) - \nabla \bullet (\Gamma_\phi \nabla \phi) = S^\phi \quad (EQ 55)$$

(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,) Γ_ϕ is the corresponding diffusion coefficient for ϕ , and S^ϕ is the corresponding source/sink term.

Table 1 and Table 2 show the values of the diffusion coefficients and source terms, in Cartesian and cylindrical co-ordinates respectively, obtained when the particle-phase equations are cast into the general form of (EQ 55). Table 3 and Table 4 present the corresponding terms for the gas phase. The similarity between the momentum equations of the gas and particle phases, and the close correspon-

Table 4 Cartesian differential equation set for the i^{th} particle phase

$\frac{\partial}{\partial x}(\bar{\rho}_i \bar{u}_i \phi) + \frac{\partial}{\partial y}(\bar{\rho}_i \bar{v}_i \phi) + \frac{\partial}{\partial z}(\bar{\rho}_i \bar{w}_i \phi) - \frac{\partial}{\partial x}(\Gamma_\phi \frac{\partial \phi}{\partial x}) - \frac{\partial}{\partial y}(\Gamma_\phi \frac{\partial \phi}{\partial y}) - \frac{\partial}{\partial z}(\Gamma_\phi \frac{\partial \phi}{\partial z}) = S^\phi$			
Equation	ϕ	Γ_ϕ	S^ϕ
Continuity	1	0	0
X-Momentum	$\bar{u}_i$	μ_{ei}	$-\frac{\partial p_{ei}}{\partial x} - \bar{v}_i \frac{\partial p}{\partial x} + \frac{\partial}{\partial x}(\mu_{ei} \frac{\partial \bar{u}_i}{\partial x}) + \frac{\partial}{\partial y}(\mu_{ei} \frac{\partial \bar{v}_i}{\partial x}) + \frac{\partial}{\partial z}(\mu_{ei} \frac{\partial \bar{w}_i}{\partial x}) + \rho_p \bar{v}_i g_x + S_d^{\mu_i}$
Y-Momentum	$\bar{v}_i$	μ_{ei}	$-\frac{\partial p_{ei}}{\partial y} - \bar{v}_i \frac{\partial p}{\partial y} + \frac{\partial}{\partial x}(\mu_{ei} \frac{\partial \bar{u}_i}{\partial y}) + \frac{\partial}{\partial y}(\mu_{ei} \frac{\partial \bar{v}_i}{\partial y}) + \frac{\partial}{\partial z}(\mu_{ei} \frac{\partial \bar{w}_i}{\partial y}) + \rho_p \bar{v}_i g_y + S_d^{\nu_i}$
Z-Momentum	$\bar{w}_i$	μ_{ei}	$-\frac{\partial p_{ei}}{\partial z} - \bar{v}_i \frac{\partial p}{\partial z} + \frac{\partial}{\partial x}(\mu_{ei} \frac{\partial \bar{u}_i}{\partial z}) + \frac{\partial}{\partial y}(\mu_{ei} \frac{\partial \bar{v}_i}{\partial z}) + \frac{\partial}{\partial z}(\mu_{ei} \frac{\partial \bar{w}_i}{\partial z}) + \rho_p \bar{v}_i g_z + S_d^{\omega_i}$
Granular Temperature	T_i	$\frac{2}{3} \kappa_i$	$-\frac{2}{3} p_{ei} \left(\frac{\partial \bar{u}_i}{\partial x} + \frac{\partial \bar{v}_i}{\partial y} + \frac{\partial \bar{w}_i}{\partial z} \right) + \frac{2\mu_{ei}}{3} \left(\frac{\partial \bar{u}_i}{\partial x} + \frac{\partial \bar{v}_i}{\partial y} + \frac{\partial \bar{w}_i}{\partial z} \right)^2$ $+ \frac{2\mu_{ei}}{3} \left[2 \left(\left(\frac{\partial \bar{u}_i}{\partial x} \right)^2 + \left(\frac{\partial \bar{v}_i}{\partial y} \right)^2 + \left(\frac{\partial \bar{w}_i}{\partial z} \right)^2 \right) + \left(\frac{\partial \bar{u}_i}{\partial y} + \frac{\partial \bar{v}_i}{\partial x} \right)^2 + \left(\frac{\partial \bar{u}_i}{\partial z} + \frac{\partial \bar{w}_i}{\partial x} \right)^2 + \left(\frac{\partial \bar{v}_i}{\partial z} + \frac{\partial \bar{w}_i}{\partial y} \right)^2 \right] - \frac{2\rho_p \bar{v}_i^2 g_0 (\bar{v}_i) (1-e^2)}{3\pi d_i} \bullet T_i^2 \bullet$ $(12 - (3\pi + 4\alpha) d_i \left(\frac{T_i}{\pi} \right) \bullet \left(\frac{\partial \bar{u}_i}{\partial x} + \frac{\partial \bar{v}_i}{\partial y} + \frac{\partial \bar{w}_i}{\partial z} \right)) - 3\beta_i T_i$

Table 5 Cylindrical differential equation set for the i^{th} particle phase

$r \frac{\partial}{\partial x} (\bar{\rho}_i \bar{u}_i \phi) + \frac{\partial}{\partial r} (\bar{\rho}_i \bar{v}_i r \phi) + \frac{\partial}{\partial \theta} (\bar{\rho}_i \bar{w}_i \phi) - r \frac{\partial}{\partial x} (\Gamma_\phi \frac{\partial \phi}{\partial x}) - \frac{\partial}{\partial r} (r \Gamma_\phi \frac{\partial \phi}{\partial r}) - \frac{\partial}{\partial \theta} \left(\frac{\Gamma_\phi \partial \phi}{r \partial \theta} \right) = S^\phi$			
Equation	ϕ	Γ_ϕ	S^ϕ
Continuity	1	0	0
X-Momentum	$\bar{u}_i$	μ_{ei}	$-r \frac{\partial p_{ei}}{\partial x} - r \bar{v}_i \frac{\partial p}{\partial x} + r \frac{\partial}{\partial x} (\mu_{ei} \frac{\partial \bar{u}_i}{\partial x}) + \frac{\partial}{\partial r} (\mu_{ei} r \frac{\partial \bar{v}_i}{\partial x}) + \frac{\partial}{\partial \theta} (\mu_{ei} \frac{\partial \bar{w}_i}{\partial x}) +$ $r \rho_p \bar{v}_i g_x + r S_d^{u_i}$
R-Momentum	$\bar{v}_i$	μ_{ei}	$-r \frac{\partial p_{ei}}{\partial r} - r \bar{v}_i \frac{\partial p}{\partial r} + r \frac{\partial}{\partial x} (\mu_{ei} \frac{\partial \bar{u}_i}{\partial r}) + \frac{\partial}{\partial r} (\mu_{ei} r \frac{\partial \bar{v}_i}{\partial r}) + \frac{\partial}{\partial \theta} (\mu_{ei} \frac{\partial \bar{w}_i}{\partial r} - \frac{\bar{w}_i}{r})$ $- \frac{2\mu_{ei}}{r} \frac{\partial \bar{w}_i}{\partial \theta} - \frac{2\bar{v}_i \mu_{ei}}{r} + \rho_i \bar{w}_i^2 + r \rho_p \bar{v}_i g_r + r S_d^{v_i}$
θ -Momentum	$\bar{w}_i$	μ_{ei}	$- \frac{\partial p_{ei}}{\partial \theta} - \bar{v}_i \frac{\partial p}{\partial \theta} + r \frac{\partial}{\partial x} \left(\mu_{ei} \frac{\partial \bar{u}_i}{r \partial \theta} \right) + \frac{\partial}{\partial r} (\mu_{ei} \frac{\partial \bar{v}_i}{\partial \theta} - \mu_{ei} \bar{w}_i) - \bar{\rho}_i \bar{v}_i \bar{w}_i +$ $+ \frac{\partial}{\partial \theta} \left(\frac{\mu_{ei}}{r} \left(\frac{\partial \bar{w}_i}{\partial \theta} + 2\bar{v}_i \right) \right) + \mu_{ei} \left(\frac{\partial \bar{w}_i}{\partial r} + \frac{1}{r} \frac{\partial \bar{v}_i}{\partial \theta} - \frac{\bar{w}_i}{r} \right)$ $r \rho_p \bar{v}_i g_\theta + r S_d^{w_i}$
Granular Temperature	T_i	$\frac{2}{3} \kappa_i$	$- \frac{2}{3} \rho_{ei} r \left(\frac{\partial \bar{u}_i}{\partial r} + \frac{1}{r} \frac{\partial}{\partial r} (r \bar{v}_i) + \frac{1}{r} \frac{\partial \bar{w}_i}{\partial \theta} \right) + \frac{2\mu_{ei} r}{3} \left(\frac{\partial \bar{u}_i}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} (r \bar{v}_i) \right.$ $\left. + \left(\frac{1}{r} \frac{\partial \bar{w}_i}{\partial \theta} \right)^2 \right) + \frac{2\mu_{ei} r}{3} \left[2 \left(\left(\frac{\partial \bar{u}_i}{\partial x} \right)^2 + \left(\frac{1}{r} \frac{\partial}{\partial r} (r \bar{v}_i) \right)^2 + \left(\frac{1}{r} \frac{\partial \bar{w}_i}{\partial \theta} \right)^2 \right) \right.$ $\left. + \left(\frac{\partial \bar{u}_i}{\partial r} + \frac{\partial \bar{v}_i}{\partial x} \right)^2 + \left(\frac{1}{r} \frac{\partial \bar{u}_i}{\partial \theta} + \frac{\partial \bar{w}_i}{\partial x} \right)^2 + \left(\frac{1}{r} \frac{\partial \bar{v}_i}{\partial \theta} + \frac{\partial \bar{w}_i}{\partial r} \right)^2 \right] +$ $\frac{2\mu_{ei} r}{3} \left(\frac{\bar{w}_i^2}{r^2} - \frac{\bar{w}_i \partial \bar{v}_i}{r \partial \theta} - \frac{2\bar{w}_i \partial \bar{v}_i}{r \partial \theta} - \frac{2\bar{w}_i \partial \bar{w}_i}{r \partial r} - \frac{\bar{w}_i^2 \partial \bar{v}_i}{r^2 \partial \theta} + 4 \frac{\bar{v}_i \partial \bar{w}_i}{r^2 \partial \theta} - 4 \frac{\bar{v}_i \partial \bar{v}_i}{r \partial r} \right)$

Table 6 Cartesian differential equation set for gas phase

$\frac{\partial}{\partial x}(\bar{\rho}_g \bar{u}_g \phi) + \frac{\partial}{\partial y}(\bar{\rho}_g \bar{v}_g \phi) + \frac{\partial}{\partial z}(\bar{\rho}_g \bar{w}_g \phi) - \frac{\partial}{\partial x}(\Gamma_\phi \frac{\partial \phi}{\partial x}) - \frac{\partial}{\partial y}(\Gamma_\phi \frac{\partial \phi}{\partial y}) - \frac{\partial}{\partial z}(\Gamma_\phi \frac{\partial \phi}{\partial z}) = S_\phi$			
Equation	ϕ	Γ_ϕ	S_ϕ
Continuity	1	0	0
X-Momentum	$\bar{u}_g$	μ_g^s	$-\bar{\epsilon}_g \frac{\partial p}{\partial x} + \frac{\partial}{\partial x}(\mu_g^s \frac{\partial \bar{u}_g}{\partial x}) + \frac{\partial}{\partial y}(\mu_g^s \frac{\partial \bar{v}_g}{\partial x}) + \frac{\partial}{\partial z}(\mu_g^s \frac{\partial \bar{w}_g}{\partial x}) - \frac{2}{3} \frac{\partial}{\partial x}(\bar{\rho}_g \bar{k}) +$ $\bar{\rho}_g g_x + S_d^u$
Y-Momentum	$\bar{v}_g$	μ_g^s	$-\bar{\epsilon}_g \frac{\partial p}{\partial y} + \frac{\partial}{\partial x}(\mu_g^s \frac{\partial \bar{u}_g}{\partial y}) + \frac{\partial}{\partial y}(\mu_g^s \frac{\partial \bar{v}_g}{\partial y}) + \frac{\partial}{\partial z}(\mu_g^s \frac{\partial \bar{w}_g}{\partial y}) - \frac{2}{3} \frac{\partial}{\partial y}(\bar{\rho}_g \bar{k}) +$ $\bar{\rho}_g g_y + S_d^v$
Z-Momentum	$\bar{w}_g$	μ_g^s	$-\bar{\epsilon}_g \frac{\partial p}{\partial z} + \frac{\partial}{\partial x}(\mu_g^s \frac{\partial \bar{u}_g}{\partial z}) + \frac{\partial}{\partial y}(\mu_g^s \frac{\partial \bar{v}_g}{\partial z}) + \frac{\partial}{\partial z}(\mu_g^s \frac{\partial \bar{w}_g}{\partial z}) - \frac{2}{3} \frac{\partial}{\partial z}(\bar{\rho}_g \bar{k}) +$ $\bar{\rho}_g g_z + S_d^w$
Turbulent Kinetic Energy			
	$\bar{k}$	$\frac{\mu_g^s}{\sigma_k}$	$G - \bar{\rho}_g \bar{\epsilon}$
Dissipation Rate			
	$\bar{\epsilon}$	$\frac{\mu_g^s}{\sigma_\epsilon}$	$(\frac{\bar{\epsilon}}{\bar{k}}) (c_1 G - c_2 \bar{\rho}_g \bar{\epsilon})$

where

$$G = \mu_g \left[2 \left(\left(\frac{\partial \bar{u}_g}{\partial x} \right)^2 + \left(\frac{\partial \bar{v}_g}{\partial y} \right)^2 + \left(\frac{\partial \bar{w}_g}{\partial z} \right)^2 + \left(\frac{\partial \bar{u}_g}{\partial y} + \frac{\partial \bar{v}_g}{\partial x} \right)^2 + \left(\frac{\partial \bar{u}_g}{\partial z} + \frac{\partial \bar{w}_g}{\partial x} \right)^2 + \left(\frac{\partial \bar{v}_g}{\partial z} + \frac{\partial \bar{w}_g}{\partial y} \right)^2 \right]$$

Table 7 Cylindrical differential equation set for gas phase

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

Equation ϕ Γ_ϕ S^ϕ

Continuity 1 0 0

X-Momentum $\bar{u}_g$ μ_g^s

$$-r \bar{\epsilon}_g \frac{\partial p}{\partial x} + r \frac{\partial}{\partial x} (\mu_g^s \frac{\partial \bar{u}_g}{\partial x}) + \frac{\partial}{\partial r} (\mu_g^s r \frac{\partial \bar{v}_g}{\partial x}) + \frac{\partial}{\partial \theta} (\mu_g^s \frac{\partial \bar{w}_g}{\partial x}) + r \bar{\rho}_g g_x$$

$$- \frac{2}{3} r \frac{\partial}{\partial x} (\bar{\rho}_g \bar{k}) + r S_d^u$$

R-Momentum $\bar{v}_g$ μ_g^s

$$-r \bar{\epsilon}_g \frac{\partial p}{\partial r} + r \frac{\partial}{\partial x} (\mu_g^s \frac{\partial \bar{u}_g}{\partial r}) + \frac{\partial}{\partial r} (\mu_g^s r \frac{\partial \bar{v}_g}{\partial r}) + \frac{\partial}{\partial \theta} (\mu_g^s \frac{\partial \bar{w}_g}{\partial r} - \frac{\bar{w}_g}{r})$$

$$- \frac{2 \mu_g^s \partial \bar{w}_g}{r \partial \theta} - \frac{2 \bar{v}_g \mu_g^s}{r} + \bar{\rho}_g \bar{w}_g^2 + r \bar{\rho}_g g_r - \frac{2}{3} r \frac{\partial}{\partial r} (\bar{\rho}_g \bar{k}) + r S_d^v$$

Z-Momentum $\bar{w}_g$ μ_g^s

$$-r \bar{\epsilon}_g \frac{\partial p}{\partial \theta} + r \frac{\partial}{\partial x} (\frac{\mu_g^s}{r} \frac{\partial \bar{u}_g}{\partial \theta}) + \frac{\partial}{\partial r} (\mu_g^s \frac{\partial \bar{v}_g}{\partial \theta} - \mu_g^s \bar{w}_g) - \bar{\rho}_g \bar{v}_g \bar{w}_g$$

$$+ \frac{\partial}{\partial \theta} (\frac{\mu_g^s}{r} (\frac{\partial \bar{w}_g}{\partial \theta} + 2 \bar{v}_g)) + \mu_g^s (\frac{\partial \bar{w}_g}{\partial r} + \frac{1}{r} \frac{\partial \bar{v}_g}{\partial \theta} - \frac{\bar{w}_g}{r})$$

$$+ r \bar{\rho}_g g_\theta - \frac{2}{3} \frac{\partial}{\partial \theta} (\bar{\rho}_g \bar{k}) + r S_d^w$$

Turbulent kinetic energy

$$\bar{k} \quad \frac{\mu_g^s}{\sigma_k} \quad r (G' - \bar{\rho}_g \bar{\epsilon})$$

Dissipation rate

$$\bar{\epsilon} \quad \frac{\mu_g^s}{\sigma_\epsilon} \quad r (\frac{\bar{\epsilon}}{\bar{k}}) (c_1 G' - c_2 \bar{\rho}_g \bar{\epsilon})$$

where

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

$$\lambda_p = \frac{1}{\sqrt{1/3}} d . \quad (\text{EQ 60})$$

Ding and Gidaspow (1990) also used a zero wall granular temperature boundary condition.

Louge et al. (1991) used a momentum balance equating the shear stress at the wall to the Coulomb friction at the wall,

$$\sigma_{ij} = \mu_w \sigma_{ii} , \quad (\text{EQ 61})$$

to get a boundary condition on the velocity. For the granular temperature, they equated the diffusion of fluctuation energy to the wall to the dissipation of fluctuation energy due to particle-wall collisions:

$$q_i = \frac{3}{8} \sigma_{ii} (3T)^{\frac{1}{2}} \left[\frac{7}{2} (1 + e_w) \mu_w^2 - (1 - e_w) \right] . \quad (\text{EQ 62})$$

Here e_w is the coefficient of restitution for wall-particle collisions and μ_w is the coefficient of sliding friction between particles and the wall.

From simple mean free path arguments, Hui et al. (1984) proposed that boundary conditions for the particle velocity should be of the form:

$$v_j \propto \frac{d}{\phi_s} \frac{\partial v_j}{\partial x_i} , \quad (\text{EQ 63})$$

Here ϕ_s is the fraction of diffuse collisions. If ϕ_s is close to unity, then a significant fraction of particle momentum is transferred to the wall in each collision- this corresponds to a rough wall, and the slip velocity will then be negligible. If U is a representative velocity scale and L is a typical length over which U changes, then (EQ 63) reduces to (Hui et al., 1984)

$$v_j \propto \frac{d}{L} \frac{U}{\phi_s} . \quad (\text{EQ 64})$$

Thus provided that the particle diameter is small relative to the dimensions of the flow domain, and provided that the fraction of diffuse collisions is not too small (i.e. ϕ_s not too close to zero,) we can use the no-slip boundary condition with negligible error.

Hui et al. (1984) also performed an energy balance, equating the fluctuation energy flux at the wall to the dissipation due to particle-wall collisions, and arrived at a boundary condition of the form:

$$T \propto \frac{d}{1 - e_w^2} \frac{\partial T}{\partial x_i} \quad (\text{EQ 65})$$

From this it can be seen that if $\frac{d}{L} \ll 1$ and if the collisions with the wall are not too elastic (Hui et al., 1984) then from (EQ 65) it is reasonable to assume a zero wall-granular temperature boundary condition.

Thus in the present thesis, the no-slip boundary condition for the velocity and the zero wall-value boundary condition for the granular temperature are adopted. However, for completeness, mention must be made here of other approaches in the literature to this problem.

Several workers have attempted to write boundary conditions for granular flow in a more rigorous manner without assuming the limiting behavior sketched above. In all these, the boundary condition on the velocity results from a momentum balance of the form:

$$\bar{M} = \sigma \cdot n \quad (\text{EQ 66})$$

while the granular temperature boundary condition results from an energy balance of the form:

$$\bar{M} \cdot v - \gamma_w = q \cdot n \quad (\text{EQ 67})$$

where M is the momentum transferred to the flow from the wall in collisions, γ_w is the dissipation of fluctuation energy due to inelastic particle-wall collisions, and n is a unit vector normal to the boundary. The expressions for $\bar{M}$ and γ_w are obtained using the same rigorous kinetic theory-based averaging used to arrive at the constitutive relations, and thus no further approximations are needed. The wall momentum flux and dissipation rate are necessarily functions of the coefficient of restitution and the geometry of the particles and the wall roughness. Jenkins and Richman (1986), Hanes et al. (1988) and Pasquarell (1991) developed boundary conditions for flows of smooth circular disks near bumpy walls, while Richman (1988) and Jenkins (1992) considered flows of inelastic spheres. Johnson and Jackson (1987) and Jenkins and Aksari (1991) also consider the interesting (and practically relevant) case where a layer of granular fluid may be in rapid motion adjacent to a layer of particles at rest.

At inlets, a uniform velocity profile is assumed and calculated based on the given flow rate. The inlet void/solid fraction is also needed at the inlet. A "granular fluctuation intensity" is also needed to specify the granular temperature at the inlet:

$$I_{T_{in}} = \frac{T_{in}^{0.5}}{\bar{v}_{in}} \quad (\text{EQ 68})$$

Gas-Phase Boundary Conditions

The no-slip boundary condition is applied to the velocity at any solid boundary. However, to reduce computational labor, the turbulence model is not integrated down to the wall. Instead, use is made of wall-functions (Launder and Spalding, 1972; Rodi, 1982) for the mean velocity as well as the $\bar{k}$ and $\bar{\epsilon}$ values at the point in the flow-field grid nearest a boundary. Thus the law-of-the-wall (Launder, 1986) is used:

$$v_{gj}^+ = \frac{1}{\kappa'} \ln(Ex_i^+) \quad , \quad (\text{EQ 69})$$

where

$$v_{gj}^+ = \frac{\bar{v}_{gj}}{u_\tau} \quad , \quad (\text{EQ 70})$$

u_τ is related to the wall shear stress τ_w as

$$u_\tau = \sqrt{\frac{\tau_w}{\rho_g}} \quad , \quad (\text{EQ 71})$$

x_i^+ is defined as

$$x_i^+ = \frac{x_i u_\tau \rho_g}{\mu_g} \quad , \quad (\text{EQ 72})$$

and E and κ' have the standard values of 9.8 and 0.42 respectively. Here i is the direction normal to the wall and j is a direction parallel to the wall.

This semi-empirical relation is used to calculate the wall shear stress τ_w , and this, rather than the velocity itself, is used as a boundary condition for the first computational cell. This formulation was originally devised for two-dimensional flows, where the definition of τ_w would be unambiguous. In a three-dimensional formulation there are two orthogonal directions at a wall and hence, in general, two non-zero components of the shear stress at a wall. Hence the procedure used in the current code is:

$$\tau_{wj} = \rho_g u_\tau u_{\tau j} \quad (\text{EQ 73})$$

where u_τ is given by (Launder, 1986)

$$u_{\tau} = c_{\mu}^{\frac{1}{4}} \bar{k}^{\frac{1}{2}}, \quad (\text{EQ 74})$$

and $u_{\tau j}$ is obtained from the law-of-the-wall applied in the j direction parallel to the wall:

$$u_{\tau j} = \frac{\bar{v}_{sj} K'}{\ln(E x_i^+)} \quad (\text{EQ 75})$$

The boundary conditions for the kinetic energy are Neumann boundary conditions, with the derivative in the direction normal to the wall set to zero. The production and dissipation of kinetic energy near a wall also need modification. For example, for a wall normal to the i direction, the boundary condition for k would be:

$$\frac{\partial \bar{k}}{\partial x_i} = 0, \quad (\text{EQ 76})$$

while the expression for the production given in (EQ 47) would be rewritten as:

$$G = \bar{\rho}_s v_i \left[2 \left(\left(\frac{\partial \bar{v}_{si}}{\partial x_i} \right)^2 + \left(\frac{\partial \bar{v}_{sj}}{\partial x_j} \right)^2 + \left(\frac{\partial \bar{v}_{sk}}{\partial x_k} \right)^2 \right) + \left(\frac{\partial \bar{v}_{sj}}{\partial x_j} + \frac{\partial \bar{v}_{sk}}{\partial x_k} \right)^2 \right] + \bar{\epsilon}_s \frac{\tau_{wj}^2 + \tau_{wk}^2}{\mu_s} \quad (\text{EQ 77})$$

The dissipation $\bar{\epsilon}$ used in (EQ 45) at the node next to the wall is not the $\bar{\epsilon}$ obtained from (EQ 46) at the same node. Rather, the dissipation is evaluated as:

$$\bar{\epsilon} = \frac{c_{\mu}^{\frac{3}{4}} \bar{k}^{\frac{3}{2}}}{K x_i}, \quad (\text{EQ 78})$$

where x_i is once again the distance from the wall to the first node in the flow field.

At inlets the flow rate is specified, and a uniform velocity based on this flow rate is calculated. The inlet turbulent kinetic energy is calculated from a supplied inlet turbulent intensity,

$$I_{in} = \frac{(2 \bar{k}_{in})^{\frac{1}{2}}}{\bar{v}_{gin}}, \quad (\text{EQ 79})$$

while a turbulence length scale, l_{in} , has also to be specified in order to calculate the inlet value of the dissipation:

$$\bar{\epsilon}_{in} = \frac{c_{\mu}^{\frac{3}{4}} \bar{k}_{in}^{\frac{3}{2}}}{\kappa' l_{in}} \quad (\text{EQ 80})$$

At outlets, the velocity boundary conditions are obtained either by setting the derivative of the velocity in the direction of the outflow to zero, or by a mass balance. The boundary conditions for $\bar{k}$ and $\bar{\epsilon}$ too are zero streamwise gradient at the outlet.

Current State of Development

For the purposes of comparison with experiments the data obtained by Ai (1990) at the University of Illinois at Urbana-Champaign would be useful. Currently the algorithm is capable of handling both continuous and semibatch operation (i.e. with respect to the particle phase), multiple inlets and outlets, and permits specification of inlet profiles for gas and particle velocities, solid fractions, and granular temperatures.

An appropriate numerical method needs to be identified to solve the highly coupled partial differential equations developed in this research. Many new solution techniques have been developed by the applied mathematics community over the past five years. Higher level tools have also been compiled for exploring many of these numerical techniques. For example, Argonne National Laboratory (Gropp and Smith, 1993) have distributed a package called PETSc (Portable, Extensible Toolkit for Scientific computing) to allow users to try different algorithms (both serial and parallel) for solving such systems.

Our research work in dense phase particle dispersion has identified an algorithm for describing Eulerian dispersion of multiple particle sizes in gases. We have not yet identified the optimum numerical solver.

4 Conclusion

Two algorithms have been developed for computing the turbulent dispersion of particles. One, a pure Lagrangian algorithm has the advantage of tracking more accurate time temperature histories for clouds of homogeneous particles and seems most applicable to dilute mixtures. The other, a pure Eulerian approach, more readily allows for the local effects of the other phases including particle-particle interactions. This approach seems most applicable to denser systems. Issues of computational efficiency and model accuracy have been explored. These computational models will be helpful in describing turbulent multiphase systems of industrial significance. This was demonstrated for the Lagrangian approach. Applications for the dense-phase Eulerian approach have yet to be proven.

5 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 of individual grains
c_k	$\frac{m}{s}$	fluctuating velocity vector of gas phase at the same location as that of the individual grains
C	$\frac{m}{s}$	magnitude of fluctuating velocity
C_g	$\frac{m}{s}$	magnitude of fluctuating velocity of gas phase
C_d	m^{-3}	drag coefficient
C_μ	-	dimensionless constant used in $k-\varepsilon$ model
c	$\frac{m}{s}$	velocity vector of individual grains
c_g	$\frac{m}{s}$	velocity vector of gas phase at the same location as that of the individual grains mentioned above
c_1	-	model constant in the $\bar{\varepsilon}$ -equation
c_2	-	model constant in the $\bar{\varepsilon}$ -equation
c_{12}	$\frac{m}{s}$	velocity vector of particle 1 relative to particle 2
D	s^{-1}	rate of deformation tensor
D	$\frac{kg}{s}$	drag force acting on a single particle (see (67))
d	m	particle diameter
d_i	m	particle diameter of i^{th} particle phase

E	-	constant used in the law of the wall, (109)
e	-	coefficient of restitution
F	$\frac{kg}{m^2 \cdot s^2}$	total external force acting on each particle, per unit volume, in (35)
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	$\frac{kg}{m \cdot s^3}$	generation of turbulent kinetic energy
G'	$\frac{kg}{m \cdot s^3}$	generation of turbulent kinetic energy, in cylindrical co-ordinates
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
g_z	$\frac{m}{s^2}$	z-component of acceleration due to gravity
g_θ	$\frac{m}{s^2}$	θ -component of acceleration due to gravity
$g_0(\bar{v})$	-	radial distribution function at equilibrium in a homogeneous system
I	-	identity tensor
I_{in}	-	inlet turbulent intensity, defined by (119)
$I_{T_{in}}$	-	inlet granular fluctuation intensity, defined by (108)
I_2	$\frac{1}{s^2}$	second principal invariant of deformation rate tensor
$\bar{k}$	$\frac{m^2}{s^2}$	ensemble-averaged turbulent kinetic energy
$\tilde{k}$	$\frac{m^2}{s^2}$	mass-averaged turbulent kinetic energy
k_{in}	$\frac{m^2}{s^2}$	inlet turbulent intensity
L	m	typical length scale
l	-	number of particle phases

l_{in}	m	inlet turbulence length scale
$\bar{M}$	$\frac{kg \cdot m}{s^2}$	momentum transferred to the wall in particle-wall collisions, per unit area
m	kg	mass of an individual particle
n	-	unit vector normal to wall
n	$\frac{1}{m^3}$	average number density of particles
N	-	normal distribution
p	$\frac{kg}{m \cdot s^2}$	thermodynamic pressure
p_p	$\frac{kg}{m \cdot s^2}$	particle pressure
$p_{e,i}$	$\frac{kg}{m \cdot s^2}$	particle pressure of the i^{th} particle phase
P	varies	probability density function
q	$\frac{kg}{m \cdot s^4}$	diffusive flux of granular temperature, defined by (44)
$\dot{q}$	#/s	particle number flowrate
Re_p	-	particle Reynolds number defined by (92)
r	m	r-direction length coordinate
r_j	$\frac{kg}{m^3 \cdot s}$	rate of mass production per unit volume of j^{th} component of solid phase
S_d^u	$\frac{kg}{m^2 \cdot s^2}$	source term due to drag in the $\bar{u}_i$ -momentum equation
S_d^v	$\frac{kg}{m^2 \cdot s^2}$	source term due to drag in the $\bar{v}_i$ -momentum equation
S_d^w	$\frac{kg}{m^2 \cdot s^2}$	source term due to drag in the $\bar{w}_i$ -momentum equation
S_d^u	$\frac{kg}{m^2 \cdot s^2}$	source term due to drag in the $\bar{u}_g$ -momentum equation
S_d^v	$\frac{kg}{m^2 \cdot s^2}$	source term due to drag in the $\bar{v}_g$ -momentum equation
S_d^w	$\frac{kg}{m^2 \cdot s^2}$	source term due to drag in the $\bar{w}_g$ -momentum equation
S_g^m	$\frac{kg}{m^3 \cdot s}$	gas phase mass source term for particle continuity equation

S_p^m	$\frac{kg}{m^3 \cdot s}$	particle mass source term for gas phase continuity equation
S_g^u	$\frac{kg}{m^2 \cdot s^2}$	gas phase momentum source term for particle momentum equation
S_p^u	$\frac{kg}{m^2 \cdot s^2}$	particle momentum source term for gas phase momentum equation
S^ϕ	varies	source term for variable ϕ in the generalized equation of change, (95)
S_1^ϕ	varies	sum of source terms for variable ϕ excluding the pressure gradient term
$S_{\bar{u}_i}$	$\frac{kg}{m^2 \cdot s^2}$	source term for the $\bar{u}_i$ equation
$S_{\bar{u}_g}$	$\frac{kg}{m^2 \cdot s^2}$	source term for the $\bar{u}_g$ equation
$S_1^{\bar{u}_i}$	$\frac{kg}{m^2 \cdot s^2}$	sum of all source terms except the pressure gradient term for the $\bar{u}_i$ equation
$S_1^{\bar{u}_g}$	$\frac{kg}{m^2 \cdot s^2}$	sum of all source terms except the pressure gradient term for the $\bar{u}_g$ equation
S_p^M	$\frac{kg}{m^3 \cdot s}$	mass source (residual of continuity equation)
s	m	interparticle distance
T	$\frac{m^2}{s^2}$	"granular temperature"
T	s	integral time scale
T_i	$\frac{m^2}{s^2}$	"granular temperature" of i^{th} particle phase
t	s	time
U	$\frac{m}{s}$	typical velocity scale
U	$\frac{m}{s}$	fluid velocity
u	$\frac{m}{s}$	fluctuating component of fluid velocity
$\bar{u}$	$\frac{m}{s}$	x -component of particle velocity
$\bar{u}_g$	$\frac{m}{s}$	x -component of gas velocity
u_τ	$\frac{m}{s}$	friction velocity, defined by (111)

$u_{\tau j}$	$\frac{m}{s}$	friction velocity in the j -direction, defined by (115)
v	$\frac{m}{s}$	fluctuating component of particle velocity
V	$\frac{m}{s}$	particle velocity
V	m^3	volume
$\bar{v}$	$\frac{m}{s}$	ensemble-averaged particle phase velocity vector
$\bar{v}_g$	$\frac{m}{s}$	ensemble-averaged gas phase velocity vector
$\bar{v}$	$\frac{m}{s}$	Favre-averaged particle-phase velocity vector, defined by (19)
v''	$\frac{m}{s}$	fluctuating part of particle phase velocity vector based on Favre average, defined by (18)
$\bar{v}_{gin}$	$\frac{m}{s}$	gas phase inlet velocity, based on given flow rate and a flat velocity profile
v_{in}	$\frac{m}{s}$	particle phase inlet velocity, based on given flow rate and a flat velocity profile
$\bar{v}$	$\frac{m}{s}$	y - or r -component of particle phase velocity
$\bar{v}_g$	$\frac{m}{s}$	y - or r -component of gas velocity
v_{gj}^+	$\frac{m}{s}$	wall-normalized velocity in the j -direction given by (110)
v_0	$\frac{m}{s}$	fluid approach velocity relative to the particle
w	varies	weighting function
W	varies	weighting function
$\bar{w}$	$\frac{m}{s}$	z - or θ -component of particle phase velocity
$\bar{w}_g$	$\frac{m}{s}$	z - or θ -component of gas velocity
x	m	x -coordinate length
x_i^+	m	distance from the wall, in wall units, given by (112)
y	m	y -coordinate length
z	m	z -coordinate length

Greek

α	-	constant used in (EQ 23)
β	$\frac{kg}{m^3 \cdot s}$	momentum exchange coefficient between gas and particle phases
β_i	$\frac{kg}{m^3 \cdot s}$	momentum exchange coefficient between gas and i^{th} particle phase
β_{ij}	$\frac{kg}{m^3 \cdot s}$	momentum exchange coefficient between i^{th} and j^{th} particle phases
Γ_ϕ	varies	diffusion coefficient for variable ϕ in the generalized equation of change, (95)
γ	$\frac{kg}{m \cdot s^3}$	dissipation of particle fluctuation kinetic energy due to collisions between particles, defined by (45)
γ_w	$\frac{kg}{m \cdot s^3}$	dissipation of particle fluctuation kinetic energy due to collision between particles and walls
$\bar{\epsilon}$	$\frac{m^2}{s^3}$	dissipation rate of turbulent energy (ensemble-averaged)
$\bar{\epsilon}_g$	-	ensemble-average void fraction of gas phase
$\bar{\epsilon}_{in}$	$\frac{m^2}{s^3}$	inlet turbulent kinetic energy dissipation rate
η	-	coal gas mixture fraction
θ	°	θ -coordinate length
κ	$\frac{kg^2}{s^2}$	diffusive coefficient for granular temperature
κ'	-	constant used in the law of the wall, (109)
κ_i	$\frac{kg^2}{s^2}$	diffusive coefficient of i^{th} particle phase
λ_p	m	mean distance between particles, as given by (100)
μ	-	coefficient of sliding friction between particles
μ_w	-	coefficient of sliding friction between particles and wall
μ_g	$\frac{kg}{m \cdot s}$	laminar viscosity of gas phase
μ_e	$\frac{kg}{m \cdot s}$	effective particle phase "viscosity"
μ_{ei}	$\frac{kg}{m \cdot s}$	effective "viscosity" of the i^{th} particle phase

Nomenclature

μ_e^g	$\frac{kg}{m \cdot s}$	effective gas turbulent viscosity
μ_t	$\frac{kg}{m \cdot s}$	eddy viscosity of gas phase
$\bar{v}$	-	ensemble averaged solid fraction
ν_t	$\frac{m^2}{s}$	eddy turbulent kinematic viscosity of gas phase
π	-	constant (universal)
$\bar{\rho}$	$\frac{kg}{m^3}$	ensemble averaged density of particle phase
$\bar{\rho}_i$	$\frac{kg}{m^3}$	ensemble averaged density of i^{th} particle phase
$\bar{\rho}_g$	$\frac{kg}{m^3}$	time-averaged bulk density of gas phase
ρ_g	$\frac{kg}{m^3}$	density of gas phase
ρ_p	$\frac{kg}{m^3}$	actual particle density
σ	$\frac{kg}{m \cdot s^2}$	total particle stress tensor
σ_k	-	turbulent Prandtl number for turbulent kinetic energy
σ_ϵ	-	turbulent Prandtl number for dissipation of turbulent kinetic energy
τ_w	$\frac{kg}{m \cdot s^2}$	wall shear stress
τ_{wj}	$\frac{kg}{m \cdot s^2}$	wall shear stress in the j -direction
ϕ	varies	a general flow variable
ϕ'	varies	fluctuating part of variable ϕ with respect to its ensemble average $\bar{\phi}$ (see (78))
ϕ''	varies	fluctuating part of a variable ϕ with respect to its Favre average $\bar{\phi}$
ϕ_s	-	fraction of diffuse collisions of particles with wall

Special Symbols

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

δ_{ij}	-	Kronecker delta
tr	varies	trace of a matrix
ϵ_{ijk}	-	alternating unit tensor

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