3-D Turbulent Particle Dispersion Submodel Development

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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 has yet to be accurately and efficiently modeled for these industrial applications.

On 15 May 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 a 3-D submodel for turbulent particle dispersion,
3. Evaluation of the 3-D submodel for turbulent particle dispersion,
4. Exploration of extensions of the Lagrangian dispersion theory to other applications including chemistry-turbulence interactions.

During this quarter work on task 1 has been essentially completed and the framework of a 3-D model has been initiated as per task 2. This report summarizes that work. Our review and model formulation has include coal combustion in dilute (as in p.c.-boilers) and dense (as in recirculating bed boilers) systems.

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 has 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 [10] and Fletcher [5]. 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 applica-

ble numerical technique. The computer model will be based on an extension of previous laboratory research performed in the development of two-dimensional combustion codes, for example [1985].

A three-dimensional gas combustion computational model has been developed. Simulations made with the 3-D model for nearly axisymmetric cases was initially evaluated through a comparison of solutions with a 2-D flow code's predictions. The key issue in producing an economical code was identified as numerical efficiency and an investigation into improving existing mathematical techniques was initiated.

Several furnace configurations have been successfully converged with the 3-D model. These have included wall-fired and corner-fired furnaces. For illustrative purposes, a test case is shown in the next few figures. The test case configuration is that of the International Flame Foundation's single burner, wall-fired furnace burning natural gas. The grid spacing used for this case is illustrated in Figure 1

Figure 1 Three-dimensional computational mesh using 111,375 (55x45x45) grid points. This view shows a slice off the near side and off the exit to illustrate the flow field (note the arched roof and the refined mesh through the centerline).

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 field is shown with a temperature field for the plane cutting the center of the burner in Figure 2

Figure 2 Three-dimensional view of velocity vectors along one plane in the IFRF furnace (note strong forward flow along burner centerline and reverse flow around the outside of the jet) and temperature in shaded colors in another plane. The computational mesh is illustrated at the outlet

A three-dimensional volume rendered view of the temperature field and of the CO concentration field are shown in Figure 3 and Figure 4.

Figure 3 Volume rendered view of the temperature field in the IFRF furnace.

Figure 4 Volume rendered view of the CO concentration field in the IFRF furnace

tle 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 Work Statements

The work to be accomplished under this contract over a two year period is to develop a new three-dimensional par-

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 review of past methods and the development of new methods is 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

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 has yet to be understood and accurately modelled.

A computationally efficient model describing the stochastic transport of particles in a turbulent flow, referred to as the STP model, has been developed and incorporated in a two dimensional comprehensive pulverized coal combustion simulation previously. The model currently approximates the particle turbulence characteristics, i.e., the particle velocity correlation function and the mean square particle velocity, by relationships which are not fundamental.

In this program we plan to implement a physically realistic method, which has been recently developed, for obtaining the particle turbulence characteristics from available Eulerian flow properties, in the STP model. The derived relationships take into account particle inertia and drag effects and at the same time are mathematically simple. It is shown that implementation of this methodology will be an improvement in the STP model. The model will be evaluated by comparison with the best available experimental data.

A non linear sensitivity analysis is planned to be performed on this model. A two-step methodology previously developed specifically for computationally complex simulations will be used. This will involve an initial screening design and then a global non-linear sensitivity analysis considering only those parameters identified in the first step as having a significant effect on the model predictions. The results of this study will provide an insight into the mechanism of turbulent particle dispersion and provide fundamental direction for future model development.

3.1 Background

3.1.1 Problem Definition

The dispersion of particles by turbulent motion has been an active field of research in recent years. Practical interests are widespread and include, the combustion of particulate and droplet fuels, the pneumatic transport of particles, the mixing and settling of industry emissions, particle deposition, electrostatic precipitation, and particle fluid separations. Practical combustion processes like spray combustion, pulverized coal and coal slurry combustion, fluidized beds, sorbent injection, and hazardous waste incineration, introduce the fuel as particles, liquid droplets, or slurries into turbulent environments.

Despite its practical importance, an accurate description of particle dispersion in turbulent flows has not been found. The reason for this is not just the lack of understanding of turbulence itself, but the inherent complexity involved in dealing with gas and particulate phases at the same time. There is a need for a physically realistic model for particle dispersion and a better understanding of the physical significance and importance of the parameters used and assumptions made in the model.

This proposal outlines a mathematically simple model with a sound physical basis, for the dispersion of particles in a turbulent flow. It discusses its application within the framework of a comprehensive simulation code for pulverized coal combustion and gasification. Also, it is proposed to perform a sensitivity analysis of this model. Besides providing an error analysis of the model, the sensitivity analysis will be used as a tool to get an insight into the dispersion process and help identify critical parameters and approximations in the model.

3.1.2 Relevant Literature

The various approaches used for modelling turbulent particle dispersion can be broadly classified by the reference frame used to describe particle transport, i.e., Eulerian, Lagrangian or mixed.

Models cast in Eulerian reference frames

Models cast in a reference frame which is fixed with respect to the experimental device, i.e., an Eulerian reference frame, are the easiest to implement. This is because the concepts of turbulent fluid mechanics (which is nearly exclusively cast in an Eulerian framework) can be

extended to the particle phase. The simplest Eulerian models treat the condensed phase as a mixture fraction. Kuo [1986] and Faeth [1983] have reviewed such Eulerian models. Other Eulerian models fit into the category of multifluid models. Such models employ separate transport equations for condensed and gas phases, allowing for finite rates of heat and mass transfer between the phases. Melville and Bray [1979] proposed this approach and others [Genchev and Karpuzov, 1980; Elgobashi and Abou-Arab, 1983] have offered more sophisticated models based on it. Eulerian particle dispersion models, though easy to use, are practically unsuitable because of three major deficiencies.

Equilibrium Behavior: Continuum Eulerian models assume equilibration of properties (such as temperature) in each computational cell. However, particles do not equilibrate, with either local gases or each other, as they move through the fulfilled.

History Effects: Eulerian models do not account for particles with different histories arriving at the same location, having different properties.

Gradient Diffusion: A gradient diffusion law analogous to Fick's law is used to model turbulent particle dispersion. This is difficult to justify and results in overprediction of dispersion.

The first two shortcomings are a result the reference frame rather than a lack of understanding of particle behavior and are taken care of easily by shifting to a Lagrangian reference frame. The gradient diffusion assumption must be replaced by a more accurate mechanism for particle dispersion.

Models cast in Lagrangian reference frames

The Lagrangian reference frame follows the particle flow. Particle properties like position, at any time, can be obtained by integrating ordinary differential equations based on particle physics. The equation of motion for a reacting coal particle is given by

$$\frac{d}{dt}(m_p V_i) = \sum_{l=1}^n f_{i,l} \quad (\text{EQ 1})$$

Typical particle and gas properties in a pulverized coal combustor are tabulated in Table 1.i, Table 1.ii lists various forces relevant to pulverized coal particle dispersion, with

their typical fractional contributions. It can be seen that steady state aerodynamic drag and weight of the particle account for all but about 2 percent of the total force

The simpler Lagrangian particle dispersion models neglect the effect of fluctuations in gas phase velocity on particle motion. Particle trajectories are found by substituting average values in the equation of motion. These type of models, referred to as ballistic Lagrangian models, resolve the first two deficiencies of the Eulerian models by virtue of tracking each particle through the flowfield. However, not accounting for the effects of gas velocity fluctuations on the particle trajectories, results in a lack of dispersion and in general these models underpredict the rate of particle dispersion. These models are coupled to the Eulerian gas phase calculations by adding source terms to the gas transport equations. These terms account for mass, momentum, and energy transfer between the phases and are computed by the particle source in cell (PSIC) technique described by Crowe et al [1977]. Representative examples of these models have been discussed by Faeth [1983], Shuen et al [1983], and Kuo [1986] among others.

From the results of ballistic Lagrangian models and also from a theoretical viewpoint, it can be shown that an accurate Lagrangian model must account for fluctuations in the gas velocity. However, this is not trivial, since most current gas phase turbulence models (i.e. $k-\epsilon$ model) do not provide actual time variation of velocity. Accurate predictions of the mean gas properties and reasonable estimates of the root mean square (rms) of their fluctuations, including their anisotropic nature, is the best one can hope to get. Consequently, Lagrangian models must account for fluctuations in some statistical way. These models are referred to as stochastic models.

Early stochastic models proposed by Hutchinson et al [1971] and Yuu et al [1978] were essentially random walk approaches to particle dispersion, with particles assumed to be entrained in a series of eddies in the gas flow. The particles spent a time equal to the eddy lifetime before becoming entrained in another eddy. Later Brown and Hutchinson [1981] included an eddy crossing effect allowing the particle to shift to another eddy before the eddy dissipated. Gosman and Ioannides [1981] modified the gas phase transport equations to include particle effects. Faeth,

Shuen, and coworkers have developed and evaluated this model [Faeth, 1983; Shuen et al, 1986; Sun and Faeth,

1986]. Faeth and coworkers have named this model the Stochastic Separated Flow or SSF model. This model performs a Monte-Carlo simulation of the particle trajectories. However, predicting the dispersion of monosized particles being emitted from a single source in a turbulent flowfield requires 2000 to 5000 particle trajectories. In a pulverized coal combustor particle sizes vary from 0.1 to 150 μ m and particles may be emitted from many different locations in the flowfield. The computational effort involved in predicting particle dispersion in a coal combustor by this method makes it inadvisable to use this model. Baxter [1990] has outlined a model to describe the stochastic transport of particles, referred to as the STP model, which is much more efficient computationally. The model has been incorporated in a comprehensive simulation code for pulverized coal combustion called the reacting, mixing limited flow model or REMIF. The discussion in this proposal is developed around the STP model and it shall be considered in detail later

Models cast in mixed Lagrangian-Eulerian reference frames
A look at the shortcomings of the Eulerian and ballistic Lagrangian models suggests forming a model using features of both reference frames, i.e., track the particle trajectory in a Lagrangian reference frame to account for particle history, and at the same time use Eulerian diffusion concepts analogous to Fick's law to account for particle dispersion. Such a model was used by Smith [1980] in a comprehensive simulation of pulverized coal combustion and gasification. This code referred to as PCGC was the predecessor to the REMIF combustion code developed by the principal investigator. These models have reasonable success in the range over which the parameters have been fit. However, they cannot be trusted to work over wider ranges. Furthermore, there is no theoretical basis for the assumption of particle dispersion being analogous to Fickian diffusion.

From the above discussion it is evident that stochastic Lagrangian models, particularly the STP model, have the potential of accurately and efficiently predicting particle dispersion in complex turbulent flows.

Property	Typical Value	Typical Range of Values
Particle Properties		
Diameter	50 μm	0.01 - 150 μm
Specific Gravity	1.2	0.3 - 1.6
Blowing Factor ^a	0.95	0.6 - 1.0
Sphericity ^b	0.7	0.2 - 1.0
Velocity	5 m/s	0 - 40 m/s
Rate of Rotation	200 cycles/s	10 - 1000 cycles/s
Mass Flux	0.5 kg/(m ² s)	0 - 1 kg/(m ² s)
Velocity Adjustment ^c	5 m/s ²	0-100 m/s ²
Temperature	1600 K	300 - 2100 K
Gas Properties		
Velocity	5.5 m/s	0 - 40 m/s
Velocity Gradient	10000 s ⁻¹	0 - 60000 s ⁻¹
Viscosity	6 x 10 ⁻⁵ (N s)/m ²	0.15 - 5 x 10 ⁻⁵ (N s)/m ²
Specific Gravity	2 x 10 ⁻⁴	1.5 - 12 x 10 ⁻⁴
Pressure Gradient	100 N/m ³	0 - 1000 N/m ²
Temperature	1600 K	300 - 2100 K

Table 1.1: Particle and gas properties typical of a full scale pulverized coal combustor [Baxter, 1989]

Force	Typical Relative Contribution
Steady aerodynamic drag	0.93
Buoyancy	0.001
Virtual mass	0.01
Magnus	< 0.0001
Bassett	0.001
Weight	0.05
Saffman	< 0.0001
Thrust	0.01

Table 1.11: A summary of the contribution of several forces in the particle equation of motion [Baxter, 1989].

3.2 The STP Model

The STP model as described here has been developed by Larry Baxter and a detailed analysis of the model can be found in his Ph.D. thesis [Baxter, 1989].

In the STP model, the time evolution of a probability density function (pdf) for particle position is modelled. Figure 5 through Figure 7 illustrate pictorially the development of a pdf for particle position for an initially concentrated group of particles released from a source near the origin in a two dimensional coordinate system. The mean position of the particles represented by the pdf in any one figure (or at any particular residence time) corresponds to the most probable position, and is at the peak of the pdf. In practice, particles with many different residence times will be within the same Eulerian computational cell. This is illustrated in Figure 8, which is essentially a top view of pdf's shown in Figure 5 through Figure 7. The circles circumscribe the region of the flowfield included within one standard deviation of the mean particle position, which is at the center of each circle.

The particle concentration (number density, n) can be obtained from the pdf by definition, as follows

$$\langle n(x_i) \rangle = qP(x_i, t) \quad (\text{EQ 2})$$

where q is the total number of particles released from a point at time, $t=0$, and $\langle n(x_i) \rangle$ is the ensemble average number density of particle with residence time t at location x_i (relative to the Eulerian reference frame). For a steady flowrate of particles $\dot{q}$, the average number density at the Eulerian location x_i is

$$\langle n(x_i) \rangle = \dot{q} \int_0^t P(x_i, t') dt' \quad (\text{EQ 3})$$

Thus, the average concentration of particles at a given location in a steady flowfield can be predicted if the function P is known. The multivariate pdf, $P(x_i, t)$ can be defined in terms of its moments. The STP model is a means of getting these.

Theoretical description of particle dispersion given the turbulence characteristics was developed by Taylor as early as 1921. More relevant discussions can be found in the works of Hinze [1975], Tennekes and Lumley [1972], and

Csanady [1973]. The STP model is an extension of these theories.

3.2.1 Mathematical Description

The path of an individual particle is given by

$$x(t) = \int_0^t V(t_1) dt_1 + x(0) \quad (\text{EQ 4})$$

An ensemble average of (EQ 4) gives the expected value, $\langle x(t) \rangle$, of the pdf for particle position in terms of the average particle velocity $\langle V(t_1) \rangle$.

$$\langle x(t) \rangle = \int_0^t \langle V(t_1) \rangle dt_1 + \langle x(0) \rangle = \mu_x \quad (\text{EQ 5})$$

The mean particle velocity is related to the mean gas velocity using (EQ 1). As is evident from Table 1.ii, the only significant forces on the particle are the steady state aerodynamic drag and the weight. In the Stokes regime (EQ 1) becomes

$$\frac{d\langle V \rangle}{dt} = \beta (\langle U \rangle - \langle V \rangle) + g \quad (\text{EQ 6})$$

where U and V are the gas and particle velocities, respectively and g is the component of acceleration due to gravity in this coordinate direction. β is calculated from Stoke's law as

$$\beta = \frac{3\pi d_p \mu_g}{m_p} \quad (\text{EQ 7})$$

Thus the first moment, μ , of the pdf (expected value of particle position) can be predicted.

The second moment of the particle position pdf, or the variance, can also be derived. The time derivative of the variance is given by

$$\frac{d\langle x'^2 \rangle}{dt} = \frac{d\sigma_x^2}{dt} = 2 \int_0^t \langle v(t) v(t_1) \rangle dt_1 \quad (\text{EQ 8})$$

where v is the fluctuating component of the particle velocity. This fundamental result can be expressed in terms of more tractable and classical turbulence properties, namely, the local rms velocity fluctuations and the Lagrangian

Figure 5 Illustration of a pdf for particle position in a two-dimensional coordinate system shortly after a group of particles are released. The development of the pdf with time can be seen by comparing with Figure 6 and Figure 7.

Figure 6 Illustration of a pdf for particle position in a two-dimensional coordinate system at an intermediate time after a group of particles are released. The development of the pdf with time can be seen by comparing with Figure 5 and Figure 7

Figure 7 Illustration of a pdf for a particle position in a two-dimensional coordinate system at a long time after a group of particles are released. The development of the pdf with time can be seen by comparing with Figure 5 and Figure 6.

Figure 8 A Lagrangian view of dispersion in a one-dimensional flow. Each circle is a measure of the spatial extent of a pdf for particle position at successive and equally spaced residence times.

autocorrelation function. The particle Lagrangian autocorrelation function is defined as

$$R^p(t_1, t) = \langle v(t_1) v(t) \rangle \quad (\text{EQ 9})$$

Substituting (EQ 9) into (EQ 8) and integrating with respect to time yields

$$\sigma_{ij}(t) = 2 \int_0^t \int_0^{t_2} (R^p(t_2, t_1)) dt_1 dt_2 \quad (\text{EQ 10})$$

The multidimensional derivation of these relationships are similar to the above derivation in all respects and the results are as follows. The mean position is given by multi-dimensional analogs of (EQ 5) and (EQ 6)

$$\langle x_i(t) \rangle = \int_0^t \langle V_i(t_1) \rangle dt_1 + \langle x_i(0) \rangle = \mu_i \quad (\text{EQ 11})$$

and

$$\frac{d\langle V_i \rangle}{dt} = \beta (\langle U_i \rangle - \langle V_i \rangle) + g_i \quad (\text{EQ 12})$$

The multidimensional particle velocity correlation function is given by

$$R_{ij}^p(t_1, t_2) = \langle v_i(t_1) v_j(t_2) \rangle \quad (\text{EQ 13})$$

The function $R_{ij}^p(t_1, t_2)$ can be used to generate the tensorial covariance matrix

$$\sigma_{ij}(t) = \int_0^t \int_0^{t_2} (R_{ij}^p(t_2, t_1) + R_{ji}^p(t_1, t_2)) dt_1 dt_2 \quad (\text{EQ 14})$$

For a stationary velocity field (EQ 14) can be written as

$$\sigma_{ij}(t) = 2 \int_0^t (t - \tau) R_{ij}^p(\tau) d\tau \quad (\text{EQ 15})$$

where $\tau = |t_2 - t_1|$.

The pdf's for particle position are assumed to be multivariate Gaussian or normal pdf's. These are completely described by their means and variances, which are pre-

dicted by (EQ 11) and (EQ 15). The general formula for a multivariate Gaussian pdf of any dimensionality is

$$P(x_p, t) = \frac{|\sigma_{ij}|^{-1/2}}{(2\pi)^{n/2}} e^{-\frac{1}{2} (x_p - \langle x_p \rangle)^T \sigma^{-1} (x_p - \langle x_p \rangle)} \quad (\text{EQ 16})$$

where,

$$g(x_i) = \sum_{i,j=1}^n (x_i - \langle x_i \rangle) (x_j - \langle x_j \rangle) (\sigma_{ij})^{-1} \quad (\text{EQ 17})$$

This is the function used to generate the pdf's shown in Figure 5 - Figure 8 to illustrate the STP model. However, there is rarely enough information about a turbulent flow-field to evaluate the off diagonal terms in σ_{ij} . If they are assumed to be zero, the resulting pdf has the following form

$$P(x_p, t) = \frac{1}{(8\pi)^{3/2} \prod_{i=1}^3 \sigma_i} e^{-\frac{1}{2} \sum_{i=1}^3 \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2} \quad (\text{EQ 18})$$

where,

$$s = s(x_p, t) = \sum_{i=1}^3 \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2 \quad (\text{EQ 19})$$

This completes the description of the model for particle dispersion except for the turbulence properties required to compute the variance, i.e., the rms particle velocity fluctuations and the particle Lagrangian autocorrelation function.

The mean square of particle velocity fluctuations is computed assuming that the fluctuations in particle velocity are caused by the gas velocity fluctuations, u . This yields the following approximate relationship

$$\langle v^2 \rangle = \langle u^2 \rangle (1 - e^{-\beta T_g}) \quad (\text{EQ 20})$$

where T_g is a characteristic time scale of the gas turbulence. In the comprehensive combustion simulation the gas phase turbulence is modelled by the k - ϵ model. T_g is calculated from the k - ϵ parameters as

$$T_s = \frac{C_\mu^{3/4} k^{3/2}}{\varepsilon \left(\frac{2}{3}k\right)^{1/2}} \quad (\text{EQ 21})$$

This relation has been derived previously by Corrsin [1963], Shuen et al [1983], and Gosman and Ioannides [1981]. The mean square gas velocity fluctuations are assumed to be isotropic in this model, and are calculated from the turbulent kinetic energy, k , as

$$u_i^2 = \frac{2k}{3} \quad (\text{EQ 22})$$

The STP model computes the particle velocity correlation function assuming that its behavior is represented by a class of stochastic processes called Markovian processes. The Markovian approximation to stochastic processes assumes that the fluctuations of the random variables is determined entirely by the current value of the variable. In this approximation, the particle autocorrelation function, as used in the STP model, takes the form

$$R_{ij}^p(\tau) = \langle v^2 \rangle e^{-\frac{\tau}{T_L(\tau)}} \quad (\text{EQ 23})$$

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

$$T_L = \max(T_g, \beta^{-1}) \quad (\text{EQ 24})$$

3.2.2 Conclusions

Comparison of the STP model with the SSF model has been done for simplified cases where an analytical solution for particle dispersion has been obtained by assuming a constant diffusion coefficient. This assumption is inherent in the Markovian autocorrelation function. Hence, the STP model reproduces those results exactly. However, this does not mean that data from real systems will be as accurately predicted, since assumptions inherent in the diffusion equation with a constant diffusion coefficient neglect many important issues in turbulent transport of particles [Baxter, 1989]. Agreement with data derived from a paper by Kalinske and Pien [1944] is satisfactory. Baxter points out though, that the Markovian correlation function is just a stochastic method of obtaining turbulence parameters, and cannot be trusted to be accurate for all turbulent flows.

The relationships used for calculating the particle turbulence characteristics, i.e., (EQ 20) and (EQ 23) are not fundamental. The Markovian assumption particularly, is a major weakness in the STP model. The gross features of the autocorrelation function measured from actual turbulence flows are similar to the exponential function which characterizes the statistical properties of Markovian processes (EQ 23). However, the latter lacks some well established properties of turbulent autocorrelation functions [Baxter, 1989]. Consequently, many important physical effects in turbulent particle dispersion are lost by making the Markovian assumption.

$R_{ij}^p(\tau)$ and $\langle v^2 \rangle$ determine the variance of the pdf for particle position (EQ 14), which in turn describes the dispersion of the particles. Incorporation of a more accurate and realistic description of these particle turbulence statistics would be a distinct improvement to the STP model. In the next section a method for obtaining $R_{ij}^p(\tau)$ and v^2 from Eulerian turbulence flow characteristics is discussed.

3.3 The Particle Velocity Correlation Function

3.3.1 Status

Obtaining Lagrangian properties from measurable Eulerian statistics is a fundamental problem in turbulent flow and diffusion. In the case of particle dispersion, things are further complicated by particle effects such as inertia and body forces. Inertial effects change the particles response time to turbulent fluctuations and body forces impart a drift velocity to the particle.

Analyses in the past have arrived at results by neglecting the difference between particles and fluid elements. However, analyses based on the above assumption, are useful only if the particle's inertia and drift velocity are very small. Friedlander [1957] studied the case of particles with large inertia and zero drift velocity. Meek and Jones [1973] attempted to extend this work to include finite inertia and drift velocity. However, they assumed the particle velocity correlation time was the same as the Lagrangian integral time scale, which is not true. Yudine [1959] and Csanady [1963] made significant studies for the case of zero inertia and large drift velocity. They realized that for this case the particle follows the fluid velocity fluctuations exactly so that v^2 is same as u^2 . Also the fluid element velocity correlation along a particle trajectory $\langle u_i(0)u_j(t) \rangle$ can be approximated by the Eulerian spatial velocity correlation $\langle u_i(0,0)u_j(v_{dt},0) \rangle$ where the fluid velocities are

with respect to a moving Eulerian reference frame and v_d is the particle drift velocity. Csanady [1963] has assumed exponential Eulerian spatial and Lagrangian fluid point correlations and arrived at results for the dispersion coefficient, which are useful for atmospheric flows. However, in industrial flows particles have finite inertia, and consequently, their behavior is different from that of a fluid element with drift velocity. Reeks [1977], and Pismen and Nir [1978] have provided a comprehensive analyses incorporating the effects of particle inertia and drift velocity. The former used Phythian's second order iteration approximation, and the latter used the independence hypothesis to obtain Lagrangian fluid element velocities from Eulerian flow velocities. Consequently, their final results were either integral equations [Reeks] or integro-differential equations [Pismen and Nir]. Wang [1990], in a recent study, has arrived at mathematically simple but physically realistic relationships for $R_{ij}^p(\tau)$ and v_d^2 . These relationships are proposed to be implemented in the STP model and will be discussed in some detail here.

3.3.2 An Accurate Relationship for $R_{ij}^p(\tau)$

The results presented in this section have been derived by Wang [1990] and further details can be found in his analysis.

A relationship for the particle Lagrangian autocorrelation function in terms of the available Eulerian flow parameters is needed. Wang derives this in two steps. First the particle velocity correlation is related to that of a fluid element moving along the particle trajectory. The correlation function for this fluid element is then related to fluid Eulerian velocity correlations. Combining the above two relations the particle velocity correlation is found in terms of three dimensionless Eulerian turbulence parameters; the Stokes number, the drift parameter, and the turbulence structure parameter.

Most analyses in the past have not distinguished between the particle and fluid element correlations, and thus, the first step of the derivation itself, is a big improvement. Reeks [1977], and Pismen and Nir [1978] have taken this into account. However, their complex analysis of the relation between fluid Lagrangian and Eulerian velocities has made their final results mathematically unwieldy. Wang has avoided this by using an approach similar to Csanady's, while including inertial effects at the same time.

Since the fluctuating components of the velocities are of interest here, the analysis is done in a frame of reference moving with the mean fluid velocity (moving Eulerian frame).

When the particle density is much larger than the fluid density, the BBO (Basset-Boussinesq-Oseen) equation of motion reduces to the following form [Maxey and Riley, 1985]

$$\frac{dV_i(t)}{dt} = \frac{(U_i(x(t), t) - V_i(t))}{\tau_a} + g_i \quad (\text{EQ 25})$$

$$\frac{dx_i}{dt} = V_i(t) \quad (\text{EQ 26})$$

where τ_a is the aerodynamic response time for a particle, defined as

$$\tau_a = \frac{\rho_p d_p^2}{18\mu_g} \quad (\text{EQ 27})$$

In the first step of the derivation the particle velocity correlation tensor

$$R_{ij}^p(\tau) = \langle v_i(t) v_j(t + \tau) \rangle \quad (\text{EQ 28})$$

is related to the fluid velocity correlation tensor along the particle trajectory, namely

$$R_{ij}^f(\tau) = \langle u_i^p(0) u_j^p(\tau) \rangle = \langle u_i(x(0), 0) u_j(x(\tau), \tau) \rangle \quad (\text{EQ 29})$$

(EQ 25) can be integrated [Reeks, 1977] to give the particle velocity

$$V_i(t) = \int_{-\infty}^t \frac{u_i(x(\tau), \tau)}{\tau_a} \exp\left(-\frac{\tau-t}{\tau_a}\right) d\tau + v_{d,i3} \quad (\text{EQ 30})$$

Maxey [1987] has shown that the mean velocity of a particle is slightly larger than v_d (by less than 3-5% in most cases). If this difference is neglected the instantaneous fluctuating velocity of the can be found as

$$v_i(t) = V_i(t) - \langle V_i(t) \rangle = V_i(t) - v_{d,i3} \quad (\text{EQ 31})$$

Combining (EQ 28), (EQ 29), (EQ 30), and (EQ 31)

$$R_{ij}^p(\tau) = \frac{1}{\tau_a^2} \int_{-\tau_a}^0 \int_{-\tau}^{\tau} R_{ij}'(\tau_1 - \tau_2) \exp\left(\frac{\tau_1 + \tau_2 - \tau}{\tau_a}\right) d\tau_1 d\tau_2 \quad (\text{EQ 32})$$

Partial integration of Equation 3.8 gives

$$R_{ij}^p(\tau) = \frac{1}{2\tau_a} \int_{-\tau_a}^{\tau} \exp\left(-\frac{|\zeta - \tau|}{\tau_a}\right) R_{ij}'(\zeta) d\zeta \quad (\text{EQ 33})$$

This relation shows the difference between the velocity correlation for a particle and a fluid element moving along the particle trajectory, due to particle inertia. Reeks [1977] has derived this same equation. It can be seen that Csanady's assumption of $RP = R'$ is good only if $\tau_a \rightarrow 0$, i.e., zero inertia particles.

Next, to relate $R_{ij}^p(\tau)$ to available fluid turbulence statistics, Csanady's [1963] approach is used and modified to include the effects of inertia in the time scale. In this approach, the normalized velocity autocorrelations of the turbulent flow in the moving Eulerian frame are assumed to be exponential functions, namely,

$$D_L(\tau) = \exp\left(-\frac{|\tau|}{T_L}\right) \quad (\text{EQ 34})$$

$$D_{mE}(\tau) = \exp\left(-\frac{|\tau|}{T_{mE}}\right) \quad (\text{EQ 35})$$

$$f(r) = \exp\left(-\frac{|r|}{L_f}\right) \quad (\text{EQ 36})$$

$$g(r) = \left(1 - \frac{|r|}{2L_f}\right) \exp\left(-\frac{|r|}{L_f}\right) \quad (\text{EQ 37})$$

D_L is the fluid Lagrangian velocity correlation and D_{mE} is the one-point fluid Eulerian temporal velocity correlation. $f(r)$ and $g(r)$ are the longitudinal and transverse fluid spatial velocity correlations, respectively, and L_f is the fluid spatial integral length scale. Exponential correlations are commonly used, mainly because they fit experimental data [Hinze, 1975].

Now consider the fluid velocity correlation along the particle trajectory, with time delay τ . The mean spatial displacement of the particle in this time would be $v_d \tau$. Hence, a

spatial correlation should be included in $R_{ij}^p(\tau)$ to account for the relative displacement. In the limiting case of $v_d \rightarrow \infty$, the particle displacement is relatively large and the spatial correlation is dominant. Thus, we have $R'_{11} = R'_{22}(\tau) = g(v_d \tau)$ and $R'_{33}(\tau) = f(v_d \tau)$. In the other extreme, when $v_d \rightarrow 0$, $R_{ij}^p(\tau)$ is mainly a temporal correlation. The time scale T , for this correlation is a function of the particle inertia, and is not the same as T_L .

In general, when the effects of both inertia and drift velocity are present, there should be a smooth transition of $R_{ij}^p(\tau)$ from a fluid temporal velocity correlation to a fluid spatial velocity correlation, when the drift velocity increases from 0 to ∞ . This is done by using Csanady's hypothesis that $R'_{33}(\tau)$ is constant on the ellipses

$$\frac{\tau^2}{T^2} + \frac{v_d^2 \tau^2}{L_f^2} = \text{constant} \quad (\text{EQ 38})$$

Using the velocity correlations (EQ 34) - (EQ 38), $R_{ij}^p(\tau)$ is obtained as

$$R'_{11}(\tau) = R'_{22}(\tau) = u^2 \left(1 - \frac{v_d \tau}{2L_f}\right) \exp\left(-\frac{\tau}{T} \sqrt{1 + m_T^2 \gamma^2}\right) \quad (\text{EQ 39})$$

$$R'_{33}(\tau) = u^2 \exp\left(-\frac{\tau}{T} \sqrt{1 + m_T^2 \gamma^2}\right) \quad (\text{EQ 40})$$

where γ and m_T are the drift parameter and the turbulence structure parameter respectively.

$$\gamma = \frac{v_d}{u} = \frac{\tau_a q}{u} \quad (\text{EQ 41})$$

$$m_T = \frac{T u}{L_f} \quad (\text{EQ 42})$$

Substituting (EQ 39) or (EQ 40) into (EQ 33), the following relationship for the particle velocity correlation is obtained

$$R_{11}^p(\tau) = \left(\frac{u^2}{\theta} \right) \exp\left(-\frac{\tau}{\tau_a}\right) + \frac{u^2}{\theta} \exp\left(-\frac{\tau}{T} \sqrt{1+m_T^2 \gamma^2}\right) \left(-1 + \frac{m_T S_{iT} \gamma \sqrt{1+m_T^2 \gamma^2}}{\theta} + 0.5 m_T \gamma \frac{\tau}{T} \right) \quad (\text{EQ 43})$$

$$R_{33}^p(\tau) = \frac{u^2 S_{iT} \gamma \sqrt{1+m_T^2 \gamma^2}}{\theta} \exp\left(-\frac{\tau}{\tau_a}\right) - \frac{u^2}{\theta} \exp\left(-\frac{\tau}{T} \sqrt{1+m_T^2 \gamma^2}\right) \quad (\text{EQ 44})$$

where St is the Stokes number

$$St_T = \frac{\tau_a}{T} \quad (\text{EQ 45})$$

and

$$\theta = St_T^2 (1 + m_T^2 \gamma^2) - 1 \quad (\text{EQ 46})$$

The particle velocity scale is equal to $\sqrt{R_{ii}^p(0)}$ and the ratio of the particle to fluid mean square velocities is given by

$$\frac{v_1^2}{u^2} = \frac{v_2^2}{u^2} = \frac{1}{1 + St_T \gamma \sqrt{1+m_T^2 \gamma^2}} - \frac{0.5 m_T \gamma St_T}{(1 + St_T \gamma \sqrt{1+m_T^2 \gamma^2})^2} \quad (\text{EQ 47})$$

$$\frac{v_3^2}{u^2} = \frac{1}{1 + St_T \gamma \sqrt{1+m_T^2 \gamma^2}} \quad (\text{EQ 48})$$

The time scale T , which is physically the time scale for a fluid element travelling along the particle trajectory is needed. In the limit that $St \gg 1$, the particle's inertia is very large, so that the particle responds very slowly to fluctuations in fluid velocity. Consequently, the particle stays at one point for a time interval of the order of T_{mE} . Thus

$T \rightarrow T_{mE}$ when $St \gg 1$. On the other hand if $St \rightarrow 0$, the particle reduces to a fluid element and $T \rightarrow T_L$. In general T is a function of St and varies between T_L and T_{mE} . T_L is always less than T_{mE} [Wang and Stock, 1988] and $T_L = 0.3-0.6 T_{mE}$ [Sato and Yamamoto, 1987]. T_{mE} is a function of the parameter m .

Wang and Stock [1989] have done a numerical simulation using turbulence generated by Fourier modes and obtained the following curve fit for T as a function of the Stokes parameter

$$\frac{T(St)}{T_{mE}} = 1 - \frac{\text{constant}}{(1 + St)^{0.4(1 + 0.01 St)}} \quad (\text{EQ 49})$$

where the constant $\equiv 1 - T_L/T_{mE} = 0.644$, for $m = 1$.

To get the dimensionless parameters St_T and m_T , the parameters St and m based on Eulerian time scales are first calculated as

$$St = \frac{\tau_a}{T_{mE}} \quad (\text{EQ 50})$$

and

$$m = \frac{T_{mE} u}{L_f} \quad (\text{EQ 51})$$

(EQ 49) gives $T(St)$. St_T and m_T are then calculated as

$$St_T = St \cdot \frac{T_{mE}}{T(St)} \quad (\text{EQ 52})$$

and

$$m_T = m \cdot \frac{T(St)}{T_{mE}} \quad (\text{EQ 53})$$

This completes the description of a mathematically simple and more accurate method for obtaining $R_{ij}^p(\tau)$ and v^2 . This method is proposed to be implemented in the STP model.

It should be noted that the Markovian approximation used currently in the STP model, yields a form of the particle Lagrangian autocorrelation function (EQ 23), which is just the same as the exponential function assumed for the Lagrangian fluid velocity correlation (EQ 34). This gives

an idea of the important particle effects that are lost by using the Markovian approximation. Firstly, the difference between the particle and fluid velocity correlations, as shown by Wang in the first step of his derivation, is neglected. Secondly, the time scale used in the STP model is T_L , which is approximated by the maximum of T_g and β^{-1} (EQ 24). However T_{mE} is always greater than T_L , and the correct time scale for a particle velocity correlation is actually T , which takes values between T_L and T_{mE} , as explained in the second part of Wang's analysis. Also, (EQ 47) and (EQ 48) provide anisotropic relations for the rms particle velocity fluctuations.

Thus, using Wang's approach in the STP model should result in an improved turbulent particle dispersion model

3.4 New Model

It is proposed that the results presented in the previous section be incorporated in the STP model and the resulting model be evaluated by itself and within the framework of a comprehensive combustion code. A sensitivity analysis will be performed on the dispersion model.

3.4.1 The Particle Dispersion Model

The calculations involved in the particle dispersion model will be the same as described for the STP model in Section 3.2 on page 11, except that the particle turbulence characteristics, namely, $R_{ij}^p(\tau)$ and v^2 , will be determined by Wang's approach. The dimensionless parameters St , γ , and m can be calculated from available Eulerian flow characteristics. The time scale T , can be obtained using (EQ 49), where the constant, $1-T_L/T_{mE}$, is calculated appropriately for the particular flow. T_L is the most difficult to obtain experimentally, though some useful data have been obtained by Snyder and Lumley [1971], Shlien and Corrsin [1974], and Sato and Yamamoto [1987]. Alternatively, T_L can be calculated from measurable Eulerian characteristics, i.e., T_{mE} , L_f , and u , using approximate relations [Wang and Stock, 1988] or direct numerical simulations [Yeung, 1989].

3.4.2 Evaluation of the Model

The model will first be compared to alternative accurate models like the SSF and STP model, under simplified conditions for which they have been calibrated. However, as pointed out before, because of the inherent assumptions in these cases, these comparisons not have much practical

significance. Hence, the emphasis of the evaluation will be on comparisons with experimental data.

The primary objective will be to make comparisons with data from setups that are similar to pulverized coal combustion applications. However, data with detailed particle dispersion characteristics is not very common, and other applications of particle dispersion like dense phase (fluidized bed) applications, liquid phase dispersion etc., will be explored for reliable data. Results from a proposed work by Prof. Klewicki of the Mechanical Engineering Department at the University of Utah, to make actual measurements of particle dispersion under conditions similar to pulverized coal combustion, might be used for evaluation of the model.

3.4.3 Evaluation of REMIF

The STP model has been incorporated as the particle description of a comprehensive coal combustion simulation called REMIF. This 2 dimensional code, like its predecessor PCGC-2, uses the $k-\epsilon$ method to predict the gas phase turbulence properties. The gas phase calculations are interlinked with the particle calculations through source terms. A flowchart for the overall code calculations and particle calculations is shown in Figure 9 and Figure 10 respectively. The improved STP model will be used likewise in the REMIF code.

Evaluation of the REMIF code in the past has been limited to comparison with PCGC-2. It is proposed evaluate REMIF more rigorously by comparison with the best available data.

3.4.4 Sensitivity Analysis

Inherent errors in input parameters and approximations in submodels used in the STP model produces errors in the simulation analogous to random and fixed errors in experimental measurements. A sensitivity analysis will provide an error analysis of the simulation.

The main goal of the sensitivity analysis is to simultaneously vary all parameters over all probable parameter combinations and to quantify the effects this variation has on a specific output. Various sensitivity techniques include one-at-a-time (brute force) methods, linear (sensitivity derivative) methods, and global non-linear methods. The first method, referred to as trend analysis, entails varying one parameter while holding the others constant and

Figure 9 Overall Flowcart for REMIF code

Figure 10 General Flowchart for Particle Calculations

observing the effect on a specific model prediction. This technique does not provide complete coverage of the probable parameter space. Linear methods vary a parameter between a high and low value and approximate the sensitivity derivative of the output with respect to that parameter linearly. Hence, this method is limited to small parameter ranges. Also, it neglects indirect effects. Finally, global non linear methods provide the most detailed sensitivity information. They can be applied over all probable parameter values and account for both direct and indirect parameter effects. However, the complexity of the computations involved in the turbulent particle dispersion simulation makes it inadvisable to perform a non linear sensitivity analysis considering all parameters.

The methodology proposed to be used is a two step technique developed by the principal investigator for performing a sensitivity analysis of the PCGC-2 simulation code. This methodology was developed specifically for large, complex computer codes requiring substantial computational time. It proceeds as follows. The first step employs a linear screening design to search the initial parameter set for those having primary effects. The second step incorporates the global non-linear FAST (Fourier Amplitude Sensitivity Test) sensitivity technique to examine those parameters identified by the screening design to be most important

A completely saturated screening design is capable of screening out real parameter effects and consists of $n+1$ simulations for n parameters. A "Plackett-Burman" design which is available from four to one hundred runs will be employed. A saturated design for the 10 parameters shown in Table 2 will require 11 converged simulations. The main objective of this step will be to identify those parameters exhibiting significant primary effects.

The second phase of the sensitivity analysis will be performed on the reduced set of significant parameters determined by the screening design. The global sensitivity analysis method proposed to be used (FAST) statistically varies all parameters simultaneously over the probable parameter space in a sinusoidal fashion with a specific frequency assigned to each parameter. Results from model predictions, corresponding to unique parameter sets, will be Fourier analyzed. The number of unique parameter sets, which corresponds to number of simulations (N), required to obtain the sensitivity information for n parameters is approximated as

$$N \approx n^{2.5} \quad (\text{EQ 54})$$

The average prediction, total deviation of the average prediction and the individual contribution to the total deviation caused by uncertainty in each parameter will be calculated.

Table 2 List of Input Parameters for Screening Design

Parameter	Description
1. $\langle U \rangle$	Local ensemble averaged gas velocity
2. β	Friction factor
3. $R_{ij}^p(\tau)$	Particle velocity correlation function
4. u	Fluctuating component of gas velocity
5. t_a	Aerodynamic response time of the particle
6. v_d	Drift velocity of the particle
7. L_f	Fluid integral length scale
8. T	Fluid time scale as seen by moving particle
9. T_L	Lagrangian fluid element time scale
10. T_{mE}	Fluid integral time scale in moving Eulerian reference frame

These sensitivity variables will be used to gain a physical insight into the turbulent particle dispersion process. Critical input parameters and modelling assumptions will be identified. This information will provide fundamental direction for future model development and focus attention on pertinent experimental work to better quantify critical input parameters.

4.0 Eulerian Turbulent Particle Phase Modeling Of Multiphase Mixtures

4.1 Introduction

Flows involving multiphase mixtures consisting of fluid and solid phases occur in a variety of industrial and real-life situations, such as flows in fluidized bed combustors, flows of grains through hoppers, flows in slurry pipelines, pneumatic transport, chute flows, rock falls, debris flows, subaqueous grain flows, snow avalanches, ice jams and drift of pack ice, sediment transport in rivers, dynamics of planetary rings, etc. The understanding and solution of such problems is dependent on an understanding of the mechanics of the flow of multiphase mixtures. In the present chapter an attempt is made to review the available literature on the analysis of problems concerning the flow

of multiphase mixtures in the cases of interest here, as mentioned in the above applications.

It is very essential at this stage to clarify the nature of the literature being reviewed herein. The important thing to realize is that in the flows considered here, the particles are not in such small quantities that we may treat the flow as consisting of several individual trajectories wherein particle-particle interactions may be neglected. On the other hand, in typical applications such as chute flows or fluidized beds, the solid fraction is close to the maximum possible solid fraction, i.e. the value of the average solid fraction may range from 0.3 - 0.6. In such a situation it would be an extremely tedious task to simulate the behavior of particles by considering individual trajectories and collisions, as one would do in a Lagrangian framework. Exhaustive treatments of such approaches are given elsewhere (Baxter, 1989). Hence, an alternative approach is preferred in the literature; that of treating the particles as a distributed continuum, or, in other words, as a "phase", and writing appropriate closed equations for the particle "phase", in an Eulerian framework.

Most of the applications listed above are concerned solely with the hydrodynamics of such flows, while some involve, additionally, the consideration of chemical reactions within the mixture (such as in fluidized bed combustors). But, even in such cases, one realizes that the study of the hydrodynamical aspects is a necessary prelude to any chemical balance calculations. This results from the fact that the equations are coupled.

The present chapter is a literature survey of the analysis of the hydrodynamics of the rapid flow of granular materials. Although a lot of work has been done in this area with respect to global and semi-empirical predictions for specific situations (especially true of fluidized beds, e.g. Grace and Matsen (1980), Kunii and Levenspiel (1991), etc.), the study of such flows at the more fundamental microscopic level is relatively new. Hence in this review we focus on the development of more general and widely applicable continuum and microstructural theories for rapid granular flows.

It must be mentioned here that most of the theories formulated to model rapid granular flow concern themselves solely with applications where the relative velocities between different phases is negligible, as is true in the case of flows like chute flows, slurry flows, and pneumatic con-

veying. One might be led to speculate that the models consequently suffer from a loss of generality, and that they may not be applicable to situations like those dealing with fluidized beds, where there are large relative velocities between the gas and solid phases. This is, however, not a problem, for the presence or absence of a relative velocity manifests itself in the governing equations used for the calculation of such flows, and the results obtained from the various theories are merely constitutive relations, and these by themselves are not affected by the governing equations. The presence of a significant relative velocity between phases can be readily accommodated by the inclusion of extra source and sink terms in the various equations.

The usual modeling approach used in the modeling of multiphase flows is to write equations separately for the different phases, and relate the separate equations by corresponding source and sink terms. Since several sources (e.g., Smoot and Pratt (1979), Smoot and Smith (1985)) document excellently the form of the equations to be used for the fluid phase, emphasis here is given only to the formulation of particle phase equations. In the following section we describe how the basic modeling equations for the particle phase are formulated.

4.2 Basic Modeling Equations And The Work Of Bagnold

Following Jenkins and Savage (1983) and Jackson (1986) we write down the basic equations governing the flow of the particle phase:

The equation of continuity for the granular phase may be written as follows:

$$D\rho/Dt + \rho \nabla \cdot \langle \mathbf{v} \rangle = 0 \quad (\text{EQ 55})$$

where ρ is the local mean (ensemble) bulk density of particles, $\mathbf{v}$ is the velocity vector, the D 's denote a material derivative, and the " $\langle \rangle$ " denote an ensemble average.

The basic equation of motion for the flow of granular material, in its ensemble averaged form, is:

$$D\langle \mathbf{v} \rangle / Dt = - \nabla \cdot \boldsymbol{\sigma} + \mathbf{f} \quad (\text{EQ 56})$$

where σ is the total shear stress tensor and f is the sum of all body forces per unit volume of the dispersed particulate phase.

If the individual grains (or particles) are incompressible, which is usually the case, then the bulk density ρ is given as

$$\rho = v\rho_p \quad (\text{EQ 57})$$

where ρ_p is the density of the particles themselves, and v is the local mean solid fraction. (EQ 55) and (EQ 56) reduce to:

Continuity:

$$Dv/Dt + v\nabla \cdot \langle v \rangle = 0 \quad (\text{EQ 58})$$

Momentum:

$$v(D\langle v \rangle/Dt) = -\nabla \cdot \sigma' + f' \quad (\text{EQ 59})$$

where

$$\sigma' = \sigma/\rho_p \text{ and } f' = f/\rho_p \quad (\text{EQ 60})$$

The body forces f constitute mainly of the weight. Other body forces such as electrostatic or electromagnetic forces also would need to be grouped in this term, if present, but our discussion in this review we shall not consider the presence of any such additional forces.

If there is a significant relative velocity between the fluid and solid phases, we modify (EQ 59) as follows:

$$v(D\langle v \rangle/Dt) = -\nabla \cdot \sigma' + f' + f_d' \quad (\text{EQ 61})$$

where f_d' is the drag force acting on the particles per unit volume, divided by the particle density. Typically this term may be calculated from Stokes' expression. This term appears in the gas-phase equation as well, but with the opposite sign.

The first quantity on the right side of (EQ 59), σ' , is the total shear stress tensor, consisting of both the pressure terms and the deviatoric shear stresses. It is interesting to note that the two terms, which normally are seen separately, in fluid mechanical analyses, are combined into a total shear stress. One needs a way to evaluate σ' from known properties such as mean velocities, mean velocity

gradients and solid fractions either in the form of direct relations or from the solution of supplementary equations for the fluctuation energy or some other such term, before one can solve the system of four equations represented by (EQ 58) and (EQ 59). In other words, one needs constitutive equations for the stress tensor.

Developing constitutive equations to accurately describe σ' in terms of primitive variables has been the main thrust of research in granular material flow in the past decade. The modeling of this term is quite complex, for there are several mechanisms which are responsible for this shear stress. These include energy loss by friction, collisions between particles, and viscous dissipation due to the turbulent fluctuations of the particles. In addition, one needs to account for the facts that the collisions may be inelastic, that real fluid-solid mixtures will not be monodisperse, and that real particles will, in general, be of irregular shape, among other things.

The pioneering work in the flow of granular materials was done by Bagnold (1954) who performed experiments on neutrally buoyant, uniformly sized spherical wax-lead beads suspended in Newtonian fluids (water and glycerine-water-alcohol mixtures) and sheared in an annular shear cell consisting of a stationary inner cylinder and a rotating outer cylinder. The outer cylinder was rotated at various speeds, corresponding to various shear rates, and the resulting torque on the inner cylinder was measured. The normal stress was also measured manometrically by using flexible rubber to form the inner cylinder, which was filled with water. Bagnold classified granular shear flows (with just one nonzero velocity gradient) into three regimes: *macroviscous*, *transitional*, and *grain inertia*, depending on the value of a dimensionless shear group [also known as the "Bagnold number" (Savage, 1984)],

$$N = \lambda^{1/2} \rho_f d^2 (v_{1,2}) / \mu \quad (\text{EQ 62})$$

(In the above notation, a comma followed by a subscript denotes a space derivative in the direction indicated by the subscript. e.g. $v_{i,j}$ is the derivative, in the j^{th} direction, of the velocity component in the i^{th} direction, or, in other words, $(\partial v_i) / (\partial x_j)$) Where ρ_f and μ are the mass density and viscosity of the interstitial fluid, d is the particle diameter, $v_{1,2}$ is the velocity gradient, and λ is known as the "linear concentration" of particles, defined by (Bagnold, 1954):

$$\lambda = d/s \quad (\text{EQ 63})$$

where s is the interparticle distance (see Figure 11). If the mean distance between particle centers is defined as bd and the resulting free distance is s (Figure 11), then we have:

$$b = s/d + 1 = 1/\lambda + 1 \quad (\text{EQ 64})$$

The solids fraction v may be expressed in terms of λ and the maximum possible solids concentration (which can be determined from the geometry of the particles; if the particles are all spherical then the densest packing would be the hexagonal packing) in the following way:

$$v = v_{\infty}/b^3 = v_{\infty}/(1/\lambda + 1)^3 \quad (\text{EQ 65})$$

Bagnold derived analytical expressions for the shear stress and the normal stress in both the macroviscous and the grain-inertia regimes. In the macroviscous regime, where viscosity is dominant, corresponding to small N , he found, from simple mean free path calculations, that the shear and normal stresses are linear functions of the velocity gradient $v_{1,2}$. In the grain-inertia regime, corresponding to large values of N , in which the fluid viscosity plays a minor role, and the major effects are due to particle-particle interactions, Bagnold supposed that the main mechanism for momentum transfer was the succession of glancing collisions as the grains of one layer overtake those of the adjacent slower layer (Figure 11). He found that both the change in momentum during a single collision and the rate at which collisions occur were proportional to the relative velocity between the two layers, and hence the stresses depended on the square of the shear rate. Assuming a scheme of rigid wall reflection, Bagnold (1954) deduced an expression for the normal shear stress in the 2-direction as:

$$\sigma_{22} = \rho_p \lambda f(\lambda) a^2 (v_{1,2})^2 \cos(\alpha_i) \quad (\text{EQ 66})$$

and that the grain shear stress was

$$\sigma_{12} = \sigma_{22} \tan(\alpha_i) \quad (\text{EQ 67})$$

where f is an unknown function of λ which determines the frequency of collisions, a is a constant, and α_i is an unknown dynamic friction angle dependent upon collision conditions.

From his experimental observations, Bagnold found that the dependence of the stresses on the velocity gradient agreed with his analysis for different values of the parameter N , and deduced the ranges of the three flow regimes: $N < 40$ corresponded to the macroviscous regime, $N > 450$ corresponded to the grain-inertia regime, and the remaining values of N were deemed to be in the transitional regime. For $\lambda < 12$, $f(\lambda)$ is proportional to λ , and for $\lambda > 12$, $f(\lambda)$ increases rapidly with λ . This is understandable since a large value of λ corresponds to a very small mean free path; thus when one keeps increasing λ there is more and more interference between adjacent layers of particles and, consequently, the shear stress corresponding to a particular shear rate keeps increasing with increasing λ , other things being held constant.

The angle α_i was found to be close to the angle of repose of the material, and not very dependent of the concentration. This and the presence of a considerable normal stress [somewhat similar to that exhibited by viscoelastic fluids (see Bird et al., 1987)] seem to suggest (Savage, 1984) that the behavior of the granular material follows a yield criterion similar to the Coulomb failure condition at limiting equilibrium [see Brown and Richards (1970)]:

$$|\sigma_{12}| = c + \sigma_{22} \tan(\phi) \quad (\text{EQ 68})$$

where c is the cohesion, and ϕ is the internal angle of friction of the bulk material. For dry, coarse materials, the cohesion c is negligible, and (EQ 68) takes on the form of (EQ 67).

This section was intended as a useful introduction to the various flow regimes present in granular flow and to the early attempts by Bagnold at analyzing granular flow behavior. Bagnold's work provided the basis for a lot of the approaches which have been attempted in the recent past (e.g. Kanatani (1979), Ogawa et al (1980), Ackermann and Shen (1982), Shen and Ackermann (1982), Pasquarell et al. (1988), to name a few). Furthermore, his highly accurate experimental data served as a sort of reference with which to compare the results of later analyses. In the next section we discuss more recent developments and outline the various theories that have been proposed for rapid granular flow.

Figure 11 Definition Sketch for Bagnold's Analysis

4.3 Theories For Rapid Granular Flows

In the previous section an introduction to various flow regimes was given. In the macro-viscous regime, the stresses are determined mainly by fluid viscosity effects. The grain inertia regime is so named because in this regime, the inertia associated with the individual grains determines the stresses. The transport of momentum and therefore the stresses in this regime occurs through inter-particle collisions and particle fluctuations. Additionally there is also a third mode of momentum transport, viz. momentum transport by friction and such other contact forces. This dominates in the so-called quasi-static regime and is important when particle concentrations are very high and the interstitial fluid is not very viscous. Although this is not very pertinent to this review (a discussion of quasi-static flows, also known as "slow flows" in contrast to the "rapid flows" in the grain inertia regime, would be more in place in a text on soil mechanics [e.g. Scott (1963), Schofield and Wroth (1968)]) it is mentioned here for completeness. It would be pertinent here to point out the fact that the most widely studied flow regime for granular flows has been the grain-inertia regime, and that there is scarce literature on other regimes.

The emphasis in the present section will be on modeling approaches to describe rapid granular flows in the grain-inertia regime. Theories for rapid granular flows may be grouped into two subsections; those which attempt to write constitutive equations for the granular material without looking at the microscopic scale of particulate motion, and attempt to relate the stress to the shear rate in some sort of semi-empirical way, not unlike the way constitutive equations are formulated in rheology; we shall refer to these as Continuum theories. In the other group of theories, the dynamics of individual particle collisions are analyzed, and the continuum properties are determined by averaging statistically over several particles. We shall refer to this second group of theories as Microstructural theories. In what follows, we shall examine both groups in detail and discuss the underlying principles behind each individual theory.

4.3.1 Continuum Theories

Goodman and Cowin's theory, and related theories

Goodman and Cowin (1972) developed a continuum theory intended for situations where interstitial fluid effects are negligible and where stress levels are low. The stress tensor was assumed to be composed of two parts: T^* , a

rate-independent part that was assumed to be related to the solids fraction v and its gradients, and T^* , a rate-dependent part that was assumed to behave as a Newtonian fluid. The latter assumption is clearly inappropriate as experiments (Bagnold, 1954) have shown otherwise. For cohesionless incompressible grains, the rate-independent part of the stress tensor was given by the proposed form:

The latter assumption is clearly inappropriate as experiments (Bagnold, 1954) have shown otherwise. For cohesionless incompressible grains, the rate-independent part of the stress tensor was given by the proposed form:

$$T^* = T_{ij}^* = -p\delta_{ij} - 2\alpha v_{,i}v_{,j} \quad (\text{EQ 69})$$

where p is the thermodynamic pressure and α depends upon v , p and v_c , the value of v corresponding to the critical voids ratio. Savage and Cowin (Savage, 1979) modified the theory of Goodman and Cowin (1972) so as to account for the nonlinear shear-rate effects evident in Bagnold's (1954) experiments. They assumed the stress tensor of cohesionless materials to be of the general form

$$T = a_0 I + a_1 D + a_2 M + a_3 (MD + DM) + a_4 D^2 + a_5 (MD^2 + D^2 M) \quad (\text{EQ 70})$$

where M is defined as the dyadic product tensor of the gradients of the solid fraction:

$$M = M_{ij} = v_{,i}v_{,j} \quad (\text{EQ 71})$$

and D is the rate of deformation tensor,

$$D = D_{ij} = \left(\frac{1}{2}\right)(v_{i,j} + v_{j,i}) \quad (\text{EQ 72})$$

and $a_0, a_1, \dots, a_5$ are functions of $v_0, v, \text{tr}M, \text{tr}D, \text{tr}D^2, \text{tr}MD$ and $\text{tr}MD^2$, where v_0 is a reference value of the solids fraction v , and tr stands for the trace of a matrix. Note that the first and third terms together comprise the rate-independent part of the tensor T^* , and the remaining terms constitute the rate-dependent part, T^* .

They then used a simplified form of (EQ 70), and used a different expression for the rate-dependent part, T^* , while keeping T^* of the same form as (EQ 69). Thus, for the case of isochoric flows, they simplified (EQ 70) to:

$$T^* = 4 \text{ }_0 I_2 I + 4 \text{ }_1 I_2^{0.5} D \quad (\text{EQ 73})$$

where

$$I_2 = (1/2)(\text{tr}^2 \mathbf{D} - \text{tr} \mathbf{D} \cdot \mathbf{D}) \quad (\text{EQ 74})$$

is the second principal invariant of the rate-of-deformation tensor. They assumed the coefficients β_0 and β_1 to be functions of the solid fraction, and, by comparing with experiments (Bagnold, 1954), deduced the following forms for β_0 and β_1 :

$$\beta_0 = \beta_0((v_m - v_0)/(v_m - v))^2 \quad (\text{EQ 75})$$

$$\beta_1 = \beta_1((v_m - v_0)/(v_m - v))^2 \quad (\text{EQ 76})$$

for $v_0 < v < v_m$,

where v_m is the maximum value of the solids fraction at which continued shearing can occur, v_0 is the solids fraction at which fluidity occurs (the concentration where the residual shear resistance at zero shear rate disappears), and β_0 and β_1 are constants. This theory predicts the existence of normal stress effects, a phenomenon which was observed by Bagnold (1954) and later also by Savage (1979).

Savage (1979) used the resulting constitutive equations (EQ 69), (EQ 73) - (EQ 76) to solve two simple problems: flow down an inclined chute and flow down a vertical channel, and found good agreement with experiment. However, their theory did not predict normal stresses when the simplified form, (EQ 73) was used. Savage (1984) gives a very good critical evaluation of Goodman and Cowin's (1972) theory and other related theories.

Fluid turbulence theories

The turbulent fluid approach was first formalized by Rabinowski (1978) who, in analogous manner to classical turbulence theory, decomposed all variables into mean and fluctuating parts, and derived balance equations by statistically averaging the equations so obtained. This approach was extended by Ahmadi and Shahinpoor (1983), Ahmadi (1985) and Ma and Ahmadi (1985). Rather than use a decomposition of the instantaneous variables in terms of ensemble mean variables, Ahmadi and Shahinpoor (1983) used a decomposition based on the Favre-averaged mean, i.e.

$$v = \bar{v} + v'' \quad (\text{EQ 77})$$

where $\bar{v}$ is the Favre average of variable v and is given by:

$$\bar{v} = \langle \rho v \rangle / \langle \rho \rangle \quad (\text{EQ 78})$$

Substituting these in their macroscopic balance laws for mass, momentum, angular momentum and energy, and ensemble averaging the resulting equations, and using the definition of the bulk density given in (EQ 57), Ahmadi and Shahinpoor (1983) obtained governing equations of the following form:

Continuity:

$$\left(\frac{\partial \bar{v}}{\partial t} \right) + (\bar{v} \bar{v})_k = 0 \quad (\text{EQ 79})$$

Momentum:

$$\rho_p v \frac{\partial \bar{v}_k}{\partial t} + \bar{v}_j (\bar{v}_k)_j = \langle t_{jk} \rangle - \langle \rho v_j v_k \rangle_j + \rho f_k \quad (\text{EQ 80})$$

Angular momentum:

$$\epsilon_{ijk} \langle t_{jk} \rangle = 0 \quad (\text{EQ 81})$$

Energy:

$$\rho \frac{\partial}{\partial t} (\bar{v}_k \bar{v}_j) + \rho \bar{v}_m (\bar{v}_k \bar{v}_j)_{,m} + \left(\frac{\partial}{\partial t} \right) \langle \rho v_j v_k \rangle + [\bar{v}_j \langle \rho v_k v_m \rangle + \bar{v}_k \langle \rho v_m v_j \rangle + \bar{v}_m \langle \rho v_j v_k \rangle + \langle \rho v_j v_k v_m \rangle]_{,m} = \bar{v}_j \langle t_{jk} \rangle_j + \bar{v}_k \langle t_{ij} \rangle_i + \langle v_j t_{ik,i} \rangle + \langle v_k t_{ij,i} \rangle + \rho \bar{v}_j f_k + \rho \bar{v}_k f_j \quad (\text{EQ 82})$$

where $\langle t_{jk} \rangle$ is the mean shear stress in the corresponding "laminar" case, i.e. which would correspond to the quasi-static state in granular material flow, and f_k refers to body forces.

It can be easily seen that the momentum equation is similar to the equation of motion of turbulent compressible fluids. This comparison was further elucidated by Ahmadi and Shahinpoor (1983) by defining

$$\theta_{jk} = \langle \rho v_j v_k \rangle \quad (\text{EQ 83})$$

whereupon (EQ 80) reduces to

$$\rho_p v \left(\frac{\partial}{\partial t} \right) \bar{v}_k + \bar{v}_j (\bar{v}_k)_j = \theta_{jk} + \rho_p v f_k \quad (\text{EQ 84})$$

Here they neglect t_{jk} in comparison with θ_{jk} (a good assumption when one is dealing with the grain-inertia regime).

They then proceeded, in analogy with classical turbulence theories, to close (EQ 79), (EQ 81) - (EQ 84) by writing constitutive equations for θ_{jk} . Ahmadi and Shahinpoor (1983) used a simple form analogous to the mixing length model of Prandtl and obtained the necessary constants for the case of simple shear flow by comparison with the data of Bagnold (1954). For the case of simple shear flow, they obtained the following equations for θ_{jk} :

$$\theta_{21} = \eta \rho_p d^2 (v^{(1/3)} / (v_m - v)^2) \left(\frac{\partial}{\partial y} \langle v_1 \rangle \right) \left(\frac{\partial}{\partial y} \langle v_1 \rangle \right) \quad (\text{EQ 85})$$

and

$$\theta_{11} = -\gamma_1 \rho_p d^2 (v^{(1/3)} / (v_m - v)^2) \left(\frac{\partial}{\partial y} \langle v_1 \rangle \right)^2 \quad (\text{EQ 86})$$

$$\theta_{22} = -\gamma_2 \rho_p d^2 (v^{(1/3)} / (v_m - v)^2) \left(\frac{\partial}{\partial y} \langle v_1 \rangle \right)^2 \quad (\text{EQ 87})$$

where η , γ_1 and γ_2 are constants. By comparison with the experimental data of Bagnold (1954), they obtained

$$\eta = 0.0503 \text{ for } v_m = 0.63 \quad (\text{EQ 88})$$

Ahmadi and Shahinpoor (1983) also found that γ_1 and γ_2 were about 3η for a reasonable agreement with the data of Bagnold (1954). It can be seen that the ratio θ_{12} to θ_{22} is a constant, in agreement with the analysis and data of Bagnold (1954).

In later approaches (Ahmadi, 1985; Ma and Ahmadi, 1985) the gradient diffusion assumption was dropped, and the authors attempted to write a transport equation for the fluctuation kinetic energy, and relate the stresses to the mean velocities, velocity gradients and the kinetic energy k . They then assumed that the system was at equilibrium, and equated the production to the dissipation, and eliminated the triple velocity correlations. This is similar to the k - ϵ model except for the fact that, in granular flow, one does not need to write an equation for the dissipation; the particle diameter, d , and the interparticle separation, s , are appropriate choices for a length scale description.

4.3.2 Microstructural Theories

In contrast to the continuum approaches, microstructural approaches analyze particle motions and interactions at the microscopic level, and employ statistical averages to obtain continuum properties. There are two schools of thought here; in one, the granular medium is thought of to be analogous to a dense fluid, and the kinetic theory of dense gases (Chapman and Cowling, 1970) is used to arrive at the final continuum properties. In the other school, simple mean free path theories, similar to Bagnold's (1954) approach, are utilized. We shall consider both approaches in detail below.

Simple mean free path theories

The first theory of this kind was the one by Bagnold (1954) which has earlier been described. Ackermann and Shen (1982) and Shen and Ackermann (1982) endeavored to improve on this approach by considering the fluctuations of the particles and writing a kinetic energy balance to obtain the frequency of collisions. Thus they did not need to use an unknown function such as the $f(\lambda)$ used by Bagnold (1954). The approach of Shen and Ackermann (1982) is described below.

Shen and Ackermann (1982) used an expression for the shear stress similar to Bagnold's:

$$T_{ij} = p_i f M_j \quad (\text{EQ 89})$$

where p_i is the number of particles per unit area of a plane of constant i , M_j is the momentum transferred in the j th direction due to collision between two particles in the i th plane, and f is the frequency of collisions. They determined p_i from geometric considerations as follows:

$$p_i = (6v_m / d^2) (\lambda / (\lambda + 1))^3 \quad (\text{EQ 90})$$

where λ is given by (EQ 63). The momentum exchange due to collision in the j th direction was found by elementary methods of mechanics, based upon a constant coefficient of restitution and frictionless collisions. Shen and Ackermann (1982) assumed that the fluctuation of the velocity was isotropic. The frequency of collisions was obtained from an energy balance in which the fluctuation energy of the particles was equated to the loss by collisions and the loss due to viscous dissipation by drag. They thus accounted for the effects of the interstitial fluid on the dissipation of energy. Shen and Ackermann (1982) thus

arrived at the final form of the equation for the shear stress:

$$\sigma_{21} = \left(\frac{v_{\infty}}{2}\right) \lambda \rho_p d^2 \left(\frac{\lambda}{1+\lambda}\right)^{3/2} \left(\frac{\partial v_1}{\partial x_2}\right)^2$$

$$\left[\frac{((1+e)^3 (0.05 + 0.08\mu))}{\left(1.5C_d \frac{\rho_f}{\lambda \rho_p} + \frac{(1-e^2)}{8} + \mu \frac{(1+e)}{2\pi} - \mu^2 \frac{(1+e^2)}{8}\right)} \right]^{0.5} \quad (\text{EQ 91})$$

and the normal stress:

$$\sigma_{22} = \left(\frac{v_{\infty}}{2}\right) \lambda \rho_p d^2 \left(\frac{\lambda}{1+\lambda}\right)^{3/2} \left(\frac{\partial v_1}{\partial x_2}\right)^2$$

$$\left\{ \frac{[(1+e)^3 (0.05 + 0.08)]}{1.5C_d \frac{\rho_f}{\lambda \rho_p} + \frac{(1-e^2)}{8} + \mu \frac{(1+e)}{2\pi} - \mu^2 \frac{(1+e^2)}{8}} \right\} \quad (\text{EQ 92})$$

where λ is the coefficient of friction between the particles, e is the coefficient of restitution for impact between two particles, and C_d is the drag coefficient for flow of fluid around a single sphere.

One can see that Shen and Ackermann (1982) and Ackermann and Shen (1982) also obtained the square dependence of the shear stress on the shear rate. It is also evident upon inspection that the ratio of the normal to the shear stresses is a constant. However, they found that their predictions for the shear stresses were about one order of magnitude less than what was obtained experimentally by Bagnold (1954). To account for this, Shen and Ackermann suggested that groups of more than two particles may be colliding with each other for some of the time. To incorporate this in their analysis, they replaced the diameter of the particle d in (EQ 91) and (EQ 92) by an effective diameter, αd . By comparing their expressions with experimental data they found that the best fit to the experimental data was obtained if the value of α was 3.16.

This theory has been used and extended by several workers, notably Shahinpoor and Siah (1981), Raymond and Shen (1986), Pasquarell et al. (1988), Shen and Hopkins (1988) and Babic and Shen (1989).

Shahinpoor and Siah (1981) endeavored to account for the effect of rotation of particles and include not just $\langle v^2 \rangle$ but

also $\langle \omega^2 \rangle$ in the energy balance, ω being the angular velocity of the particle. Raymond and Shen (1986) tried to incorporate an anisotropic velocity fluctuation distribution in the theory, and Shen and Hopkins (1988) tried to extend the theory from monodisperse grains to polydisperse mixtures. Assuming a log normal distribution of sizes, they solved for the stresses in a simple shear flow of spheres and showed that the shear stresses decreased with increasing standard deviation. Babic and Shen (1989) gave an alternative explanation for the discrepancies in Ackermann and Shen's (1982) predictions, viz. that the stresses were falling one order of magnitude short of measured values. Babic and Shen (1989) partitioned the total shear stress into a collisional part and a kinetic part, and stated that the reason for the failure of the previous mean free path models was that they did not take into account kinetic stresses, and thus computed the stresses due to the collisions alone. Babic and Shen (1989) also performed calculations based on their derived expressions and obtained close agreement with experimental data.

Kinetic Theories

The first attempt at modeling the collisional behavior of a granular mixture in analogy to the mathematical modeling of the behavior of dense gases (Chapman and Cowling, 1970) was made by Savage and Jeffrey (1981) and extended by Jenkins and Savage (1983). In what follows, we give a brief description of the Jenkins and Savage (1983) method of determining constitutive equations for the particle phase.

Jenkins and Savage (1983) wrote down the balance laws for a granular medium in the following form:

$$\frac{\partial}{\partial t} \langle n\psi \rangle = n \langle D\psi \rangle - \nabla \cdot \langle n c \psi \rangle + C(\psi) \quad (\text{EQ 93})$$

where

$$D\psi = (dc/dt) \cdot \left(\frac{\partial \psi}{\partial c}\right) \quad (\text{EQ 94})$$

where ψ is any property of a particle, c is the velocity of an individual particle, n is the average number density of the particles, and $C(\psi)$ is the mean collisional rate of change of ψ per unit volume. The ensemble average of any quantity ψ can be given as

$$\langle \psi \rangle = (1/n) \int \psi(c) f^{(1)}(c, r) dc \quad (\text{EQ 95})$$

where $f^{(1)}(c, r)$ is the single particle velocity distribution function [i.e. $f^{(1)}(c, r) dr_1 dc_1$ is the probability of a single particle having a velocity c which lies within a range of dc_1 of c_1 and a position vector r which lies within a range of dr_1 of r_1 . [For convenience, the time dependence of all variables is assumed implicitly and is not explicitly mentioned]

The collisional mean rate of change of ψ is given by (assuming purely binary collisions):

$$C(\psi) = -\nabla \cdot \Theta(\psi) + \chi(\psi) \quad (\text{EQ 96})$$

where $\Theta(\psi)$ and $\chi(\psi)$ are given by:

$$\Theta(\psi) = -(1/2) d \int_{(c_{12} \cdot k > 0)} \int k(\psi_1' - \psi_1) f^{(2)}(c_1, r_1, c_2, r_2) d^2(c_{12} \cdot k) dk dc_1 dc_2 \quad (\text{EQ 97})$$

$$\chi(\psi) = (1/2) \iint \int_{c_{12} \cdot k > 0} (\psi_1' + \psi_2' - \psi_1 - \psi_2) f^{(2)}(c_1, r_1, c_2, r_2) d^2(c_{12} \cdot k) dk dc_1 dc_2 \quad (\text{EQ 98})$$

in which ψ_1 is the initial value of quantity ψ of particle 1, ψ_2 is the initial value of ψ of particle 2, and ψ_1' and ψ_2' are the corresponding final values [i.e. their values after the collision] and k is the unit vector in the direction of the line connecting the centers of the two particles (i.e., $r_2 - r_1 = dk$), and $f^{(2)}(c_1, r_1, c_2, r_2)$ is the joint pair distribution function, i.e. $f^{(2)}(c_1, r_1, c_2, r_2) dc_1 dr_1 dc_2 dr_2$ is the probable number of pairs of particles, such that one is situated at position vector r which is within a range dr_1 of r_1 , and moving with a velocity c which is within a range dc_1 of c_1 , the other at position r' such that it is within a range dr_2 of r_2 , and moving with velocity c , such that it is within a range dc_2 of c_2 (In the above integrals, $r_2 = r_1 + dk$).

Substituting (EQ 94) - (EQ 98) in (EQ 93), taking ψ to be mass, momentum, and fluctuation energy, and simplifying, assuming, among other things, that momentum transport is negligible compared to collisional transfer, Jenkins and Savage (1983) obtained the following balance laws for the conservation of mass, momentum and fluctuation energy respectively:

$$(D\rho/Dt) = -\rho \nabla \cdot v \quad (\text{EQ 99})$$

$$\rho(Dv/Dt) = -\nabla \cdot \sigma + n f \quad (\text{EQ 100})$$

$$(3/2)\rho(DT/Dt) = -\nabla \cdot q - \text{tr}(\sigma \nabla v) - \gamma \quad (\text{EQ 101})$$

where σ is the collisional stress tensor, v is the ensemble averaged velocity, f denotes the body forces, and T is a fluctuation (or granular) temperature defined by

$$T = (1/3) \langle C^2 \rangle \quad (\text{EQ 102})$$

where C is the magnitude of the fluctuation velocity vector, C , defined by

$$C = c - v \quad (\text{EQ 103})$$

q is the flux of this fluctuation energy, and γ is the rate of dissipation of fluctuation energy. The expressions for σ , q and γ , i.e. the constitutive equations, depend upon the forms chosen for the various distribution functions.

Jenkins and Savage (1983) assumed that the pair distribution function could be expressed as the product of a normalized positional pair-distribution function $g^{(2)}(r_1, r_2)$ [i.e. the probability distribution that two particles 1 and 2 will be situated such at r and r' such that r is within a range dr_1 of r_1 and r' is within a range dr_2 of r_2] and the two single velocity distribution functions (i.e., $f^{(1)}(c_1, r_1)$ and $f^{(1)}(c_2, r_2)$):

$$f^{(2)}(c_1, r_1, c_2, r_2) = f^{(1)}(c_1, r_1) g^{(2)}(r_1, r_2) f^{(1)}(c_2, r_2) \quad (\text{EQ 104})$$

Jenkins and Savage (1983) also assumed that the single particle velocity distributions were Maxwellian about the mean velocity v , and that the normalized pair position distribution could be given by the expression:

$$g^{(2)}(r_1, r_2) = g_0(v) (1 - \alpha \cdot k \cdot v_{21} / (\pi T))^2 \quad (\text{EQ 105})$$

where $g_0(v)$ is given by:

$$g_0(v) = \frac{1}{1-v} + 3 \frac{v}{2(1-v)^2} + \frac{v^2}{2(1-v)^3} \quad (\text{EQ 106})$$

The anisotropy of the collisions is contained in the normalized pair distribution --- It would be necessary to account for this. For example, in a plane shear flow, one would expect that the collisions between pairs of particles in the direction of the mean flow would be much higher than in

the direction normal to the mean flow; hence an assumption of isotropy would be out of place.

With these assumptions, Jenkins and Savage (1983) obtain as constitutive equations:

$$\gamma = \kappa \frac{(1-e)}{2d^2} (12T - (3\pi + 4\alpha) d \left(\frac{T}{\kappa}\right) (\text{tr} D)) \quad (\text{EQ 107})$$

$$\kappa = 2\rho v g_0(v) d(1+e) \left(\frac{T}{\kappa}\right) \quad (\text{EQ 108})$$

$$\mathbf{q} = -\kappa \nabla T \quad (\text{EQ 109})$$

$$\boldsymbol{\sigma} = \pi^{1/2} \kappa d^{1/2} T^{1/2} \mathbf{I} - \left(\frac{1}{5}\right) \kappa (2 + \alpha) ((\text{tr} D) \mathbf{I} + 2D) \quad (\text{EQ 110})$$

where α is an arbitrary function of v .

(EQ 99) - (EQ 101), along with (EQ 107) - (EQ 110) give a complete description of the motion of the particle phase. Using these Jenkins and Savage (1983) performed calculations for Couette flow and flow down chutes, and were able to get good agreement with experiment. The theory of Jenkins and Savage (1983) was also used by Hutter et al. (1986a, 1986b) to predict the flow of snow avalanches.

Their theory was subsequently improved upon by Lun (1984), Jenkins and Richman (1985a, 1985b), Pasquarell et al. (1988), and Pasquarell and Babic (1990) who attempted to include the effects of anisotropy into the single particle velocity distribution functions. Further, Lun and Savage (1986) showed that the assumption of a constant coefficient of restitution was not an appropriate one, and expanded the theory to include the effects of an impact velocity dependent coefficient of restitution on the shear stresses. Farrell et al. (1986) attempted to extend the theory to binary mixtures comprised of two sets of grains of different diameters. The approach was similar to the one outlined above, except that now one had to find an expression for the normalized joint probability function between particles of different sizes. Farrell et al. (1986) took the joint probability function g to be of the form:

$$g_{ij}(d_{ij}) = \frac{1}{\left(1 - \frac{v}{v_m}\right)} + \frac{(3d_i d_j)}{2d_{ij} \left(1 - \frac{v}{v_m}\right)^2} \left(\frac{v_i}{d_i} - \frac{v_j}{d_j}\right) \quad (\text{EQ 111})$$

where $d_{ij} = \left(\frac{1}{2}\right) (d_i + d_j)$ and v_m is the maximum solids fraction at closest random packing.

They also utilized the principle of equipartition of energy, which states that the fluctuation energy is equally divided among granules of all sizes, provided all the granules are made of the same material and hence possess the same coefficient of restitution. Farrell et al. (1986) therefore obtained the following condition:

$$\left(\frac{3}{2}\right) m_a T_a = \left(\frac{3}{2}\right) m_b T_b \quad (\text{EQ 112})$$

where m_a and m_b are the masses of each of the uniform sized particles from groups a and b respectively, and T_a and T_b refer to the fluctuation temperatures of the two different diameter sets. Thus knowing the fluctuation temperature of one of the two size fractions, the fluctuation temperature of the other could be determined.

Frictional and interstitial fluid effects were also incorporated into the kinetic theory by Abu-Zaid and Ahmadi (1990) and Ma and Ahmadi (1988) respectively.

Having introduced the various Continuum and Microstructural theories, we now proceed, in the next section, to discuss the various advantages and disadvantages of each.

4.4 Discussion And Conclusions

Of the various theories mentioned, the kinetic theory certainly seems to be most sound fundamentally. In addition, it is also capable of providing practical solutions, as has earlier been pointed out. Recent developments (Abu-Zaid and Ahmadi (1990) and Ma and Ahmadi (1988)) have also enabled us to include frictional and interstitial fluid effects, thus rendering the theory highly realistic. A lot of work has been done regarding inelastic effects and anisotropic distribution of velocity fluctuations. However, the problem in the application of the kinetic theory to practical problems arises in the application of appropriate boundary conditions, especially regarding the value of the fluctuation energy or its gradients at boundaries. Jenkins and Savage (1983) have pointed out this difficulty. However, this aspect has also been studied (e.g. Hui et al. (1984), Jenkins and Richman (1986)) and it appears that the values employed at the boundaries are strong functions of the coefficient of restitution in particle-wall interactions as well as the degree of roughness of the wall.

However, the simple mean free path theory also has its advantages. To begin with, the mean free path theories are conceptually very clear. Although they too analyze particle motions from a microscopic point of view, their method is less sophisticated and less rigorous than the kinetic methods. However, on closer inspection, one sees that there are several similarities in the two methods. In a recent paper, Pasquarelli et al. (1988) dwell on the similarities between the two approaches in terms of concepts as well as mathematical formulation. Moreover, the development of the mean free path theories seems to be slightly ahead of the kinetic theories in some respects. Most important among these is the fact that there does exist a method, among the mean free path theories (Shen and Hopkins, 1988), capable of predicting the flow of mixtures made up of multiple grain sizes (in fact a complete distribution of sizes), something which brings theoretical analysis very close to reality. So far, methods to handle such situations have not been developed in kinetic theories. As has been pointed out earlier, a technique has been developed, in the kinetic theory, which is capable of dealing with two grain sizes, but so far mixtures with multiple grain sizes haven't received too much attention.

There seems to be a slow abandonment of the older continuum theories, although a few papers have been published recently regarding these. It would seem that this is so due to the more empirical nature of such theories. A case in point is the theory of Ahmadi and Shahinpoor (1983), Ahmadi (1985) and Ma and Ahmadi (1985). In their theory, Ahmadi and Shahinpoor (1983) consider their granular equivalent of the Reynolds' stresses to be solely responsible for the stresses induced. However, we see from the more rigorous kinetic theory that the terms θ_{jk} ($= -\langle p v_j v_k \rangle$) correspond more to just the kinetic stress rather than the sum of the kinetic and collisional stresses. Hence it amounts to a large approximation to attribute all the collisional stress to the θ_{jk} in Ahmadi and Shahinpoor's (1983) theory. The mean free path theories too, until recently (see Babic and Shen, 1989) neglected the kinetic stress and attempted to attribute the stresses induced to purely collisional effects. As a result, the predicted results fell short of experimental predictions. But the kinetic theory, on its part, did not fully account for interstitial fluid effects. A complete theory, which includes all sources of energy loss, including inelastic collisions, frictional losses, momentum transfer by both rotational and translational means, interstitial fluid drag effects, and anisotropic velocity distributions, is still awaited.

Although, as mentioned in the first section, the theories are general in their nature and may be applied to situations where high relative velocities exist, it is conceivable that this may present problems. For example, the high velocity of the fluid stream certainly will affect the magnitude and nature of the particle velocity fluctuations, and it is not right now known whether the effect can or cannot be taken care of in compensating terms (it might change the form of the energy balance, for example). These considerations might be of concern to persons concerned with applications like fluidized bed reactors, etc.

5.0 Project Plans

This report has summarized the first 3 months 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 and outlined the theory for a proposed model that would include components for dealing with dilute systems as well as dense systems.

We have started to develop the computer algorithms to solve the outlined equations. This algorithmic development will continue over the next quarter. We will also begin the computer coding to incorporate this model into our three-dimensional combustion code. Evaluation will proceed from that point according to the tasks outlined in Section 1.

Figure 12 illustrates one of the objectives we are trying to accomplish by showing computed particle trajectories in a 3D simulation of a utility boiler. However at this point in our development these trajectories are following streamlines and thus do not yet include the desired turbulent dispersion effect.

Figure 12 Computed trajectories for representative particles in a corner fired boiler. The colored plane show the temperature field at a plane cutting through the furnace nose and through the three super-heater panels.

6.0 Nomenclature

Symbol	Definition
d_p	particle diameter
D_L	fluid Lagrangian velocity correlation
D_{mE}	fluid Eulerian temporal velocity correlation
$f(r)$	longitudinal fluid spatial velocity correlation
$f_{i,l}$	force acting on the particle
g	gravitational acceleration
$g(r)$	transverse fluid spatial velocity correlation
k	turbulent kinetic energy
L_f	fluid integral length scale
m_p	mass of particle
m_T	turbulence structure parameter
n	particle number density
$P(x_i, t)$	pdf for particle position
q	number of particles
$oac(q, \cdot)$	particle number flowrate
r	distance
R	velocity correlation function
St	Stoke's number
t	time
T	integral time scale
u	fluctuating component of fluid velocity
U	fluid velocity
v	fluctuating component of particle velocity

v_d	particle drift velocity
V	particle velocity
x	position (coordinate)
$\mathbf{x}$	vector position

Superscripts

f	fluid
p	particle
$\cdot$	arbitrary

Greek

b	friction factor
ϵ	dissipation rate of turbulent energy
g	drift parameter
m	mean (first moment of pdf)
μ_g	dynamic viscosity of gas
ρ_p	particle density
s	standard deviation
t	time
t_a	aerodynamic response time
z	arbitrary time

Subscripts

g	gas
i	coordinate direction, arbitrary
j	coordinate direction, arbitrary
l	arbitrary index
L	Lagrangian
mE	moving Eulerian
p	particle
T	pertaining to time scale T
l	arbitrary

7.0 References

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