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MONTE CARLO PARTICLE DISPERSION SIMULATION APPLICATION IN COAL FIRED FURNACES: COMPARISON WITH EXPERIMENTAL DATA

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ABSTRACT

Several important industrial processes involve particles or liquid droplets suspended in a turbulent flow. These particles/droplets do not follow the mean trajectories of the fluid and disperse quickly due to interactions with the turbulent velocity fluctuations. This process of dispersion due to turbulent velocity fluctuations has been an active area of research in recent years (Crowe et al., 1996). Models of turbulent particle dispersion find widespread use in the metallurgical, chemical process and power industry. In all such heterogeneous reacting flow systems, the reaction kinetics are controlled by the extent of mixing between the gas and the particulate phase and turbulent transport of particles governs the extent of mixing between the two phases. Therefore, the description of particle dispersion is central to the prediction of various properties such as the extent of reaction or temperature inside an industrial reactor.

A stochastic particle dispersion model is developed which accounts for anisotropy in the dispersion of particles in the three different coordinate directions. This new particle dispersion model, called the three-eddy interaction model captures the three particle effects that are deemed important to predict particle dispersion in turbulent flow. The stochastic dispersion model is tested against existing experimental data in grid generated turbulent and uniform homogeneous shear flow. In both the cases, the particle dispersion predictions when compared with experimental data yield reasonable results.

The three-eddy interaction model is implemented within a three-dimensional reacting flow framework and some existing coal combustion and reaction libraries are interfaced with the dispersion model. To demonstrate the predictive capability of the multiphase flow code, an International Flame Research Foundation (IFRF) furnace is numerically simulated. Computations are compared with experimental measurements and with predictions from the existing dispersion model available in the code (the cloud approach from Jain (1998)). Improved predictions of gas phase temperature profile are observed with the new particle dispersion model.

NOMENCLATURE

L_e Eddy length
L_f Lateral integral length scale
L_g Longitudinal integral length scale
$\dot{q}$ Particle number flow-rate
r_p Rate of change of particle mass
St Stokes number
S_p Particle source
t_c Crossing time
T_e Eddy lifetime
T_L Lagrangian integral time scale
T_{me} Moving Eulerian integral time scale
T_p Integral time scale of particle
u_e Instantaneous fluid velocity
$\overline{U}$ Mean fluid velocity
u' Fluctuating fluid velocity
$\vec{u}_r$ Relative velocity
X_p Particle position vector
X_f Fluid eddy position vector
α Mass fraction
η Mixture fraction of coal off-gas
τ_r Particle relaxation time

INTRODUCTION

A simple approach to obtain the instantaneous velocity of the fluid phase was first proposed by Hutchinson et. al. (1971) and subsequently developed by Gosman and Ionnides (1981). It is called the eddy interaction model. A complete description of the eddy interaction model in homogeneous isotropic stationary turbulent flows is given by Graham (1996b). In eddy interaction models, the instantaneous velocity of the fluid phase is obtained by adding to the mean fluid velocity a random fluctuating velocity that is sampled from an assumed pdf. The various moments of the assumed pdf are computed from a standard turbulence model. The particle moves through a succession of instantaneous fluid velocities. The interaction time of the particle with each instantaneous velocity can be prescribed from another assumed pdf of interaction times. In general the instantaneous particle velocity is not the same as the instantaneous fluid velocity.

Experimental investigations (Csanady, 1963) have demonstrated that for finite inertia particles, the following three effects are important and have to be accounted for to predict particle dispersion accurately.

1. The inertia effect (Wells and Stock, 1983; Reeks, 1977) predicts that the dispersion of solid particles might exceed the dispersion of the fluid particles in the absence of body forces.
2. The crossing trajectories effect (Yudine, 1959) predicts that in the presence of a drift velocity, a

finite inertia particle will disperse less than a fluid particle.
3. The continuity effect (Csanady, 1963), where the dispersion in the direction of the drift velocity exceeds the dispersion in the other two directions.

The aim of the present work is to develop a three-eddy interaction model that can account for all of the above effects and can predict particle dispersion in a homogeneous turbulent shear flow. In order to aid the development of the model, Stoke's law is assumed to be applicable in the particle equation of motion. All forces on the particle except drag and gravity will be neglected (Maxey and Riley, 1983). Throughout the development of the model a homogeneous isotropic turbulence field will be assumed.

MODEL DESCRIPTION

At the start of the particle/fluid interaction (t=0), the particle is assumed to be sitting at the center of the eddy. Within an eddy the instantaneous fluid velocity is assumed to be a constant. This assumption is the basis of the discrete Monte Carlo simulation. At any point and at any given time, a fluid velocity is measured by any observer is fluctuating with time. This occurs because turbulent flow is random in nature. In a Monte Carlo simulation each eddy represents a constant velocity fluid element. A simulated eddy velocity is represented by

$$u_e = \overline{U} + u' \quad (1)$$

This velocity comprises of a mean velocity and a fluctuating velocity. In a homogeneous turbulence field, the mean velocity can be safely assumed to be zero. The fluctuating velocity is sampled from an assumed pdf with a zero mean and a variance equal to the root mean square velocity. Throughout the duration of an eddy, the instantaneous eddy velocity remains a constant in space and time as long as the non-fluid particle remains in that eddy. At some later time ($t \neq 0$), both the eddy and the non-fluid particle must have moved in space. The eddy gets convected with its instantaneous fluid velocity while the non-fluid particle movement is governed by the particle equation of motion. The non-fluid particle remains under the influence of that eddy until the interaction time exceeds the eddy lifetime (T_e) or the separation of the non-fluid particle and the center of the eddy exceeds the eddy length (L_e). The choice of the pdf for sampling the length scales and time scales is described in Graham and James (1996) and Wang and Stock (1992).

In the three-eddy interaction model, the interaction time of a particle with a one-dimensional eddy is governed by length and time scale in that direction. In homogeneous isotropic stationary turbulence an eddy lifetime is generated from the same pdf in each direction. The components of the instantaneous velocity of the fluid remain a constant for the eddy lifetime generated in that particular direction. Thus, the final position of a fluid particle will depend upon the fluctuating velocity in each direction. In addition, the time over which a fluctuating velocity persists will be different in the three coordinate directions. This makes the interaction time of a fluid particle with a non-fluid particle different in each coordinate direction. Similarly, the length scales seen by a fluid particle will be different in the three directions. Eddies in a three-eddy interaction model can be visualized as one-dimensional that together constitute a three-dimensional eddy of any arbitrary shape. A non-fluid particle may escape the effect of that eddy in one direction, but it may still be under the effect of the same eddy in the other two directions. This model differs from a spherical eddy interaction model in the correlation of eddy lifetimes in the different coordinate directions. This model prescribes complete de-correlation of the eddy lifetime in each coordinate direction, while an eddy interaction model results in a complete correlation of the eddy lifetimes in all three directions.

Particle effects

The next task is to ascertain the values of eddy lifetime and eddy length from the turbulent time scales available in the turbulence model. Also the effect of gravity has to be accounted for in the particle dispersion simulation.

Wang and Stock (1993), using random Fourier modes, have shown that the integral time scale of the fluid element following a particle lies somewhere between the Lagrangian integral time scale (T_L) and the moving Eulerian integral time scale (T_{me}). Wang and Stock also suggest that the fluid element time scale is a function of the turbulence structure parameter defined as $\beta = u'(T_{me}/L_f)$ and the Stokes number defined as $St = \tau_r / T_{me}$ Assuming $\beta = 1$ and using numerical simulation in homogeneous, isotropic, turbulence, Wang and Stock (1993) suggest the following empirical relation between the three time scales,

$$T_{pi} = T_{mei}\left(1 - \frac{1 - T_{Li}/T_{mei}}{(1 + St_i)^{0.4(1+0.01St_i)}}\right) \quad (2)$$

When the particle has small inertia, it sees the Lagrangian integral time scale. Very heavy particles that follow the mean path of the fluid see the Eulerian integral time scale. How the time scale changes with Stokes number is described by the above expression
Eddy lifetime and eddy length in each direction is computed from the following expressions

$$T_{ei} = 2T_{pi} \quad (3)$$

and

$$L_{ei} = 2L_i \quad (4)$$

Where L_i is equal to L_f if the gravity is acting in that direction or it is equal to the Eulerian lateral integral length scale (L_g) if it is the other two directions. As seen from (4), the single-eddy interaction time will be different in each direction if the integral time scales vary with the coordinate axis. Similarly, (see (5)) the length scales will be different in each coordinate direction. Thus, the model is capable of simulating the continuity effect.

Graham (1996b) discusses the effect of gravity on the crossing trajectory effect. He states that neglecting gravity leads to over-predicted dispersion coefficients, even though gravity is accounted for in the particle equation of motion. Chen and Crowe (1982) report similar findings. Putting directional dependence on the eddy length and eddy lifetime modifies equation for the crossing time in a three-eddy interaction model. The following is obtained for the crossing time

$$\left| \vec{X}_p(t + t_{ci}) - \vec{X}_f(t + t_{ci}) \right| = L_{ei} \quad (5)$$

For the limiting case of $t_{ci} / \tau_r = 0$, (5) with the help of the particle equation of motion can be reduced to

$$t_{ci} = \frac{L_{ei}}{|\vec{u}_r|} \quad (6)$$

Equation (4) assumes that the fluid and non-fluid particles are coincident at the start of the interaction. The drift velocity or the free fall velocity acting on a particle reduces the crossing time in all three directions. This effect is important in predicting heavy particle dispersion accurately.

The crossing trajectory effect can be simulated in each direction by setting the interaction time to be the smallest of (T_{ei}, t_{ci}). Values of both will have directional influence; therefore, the three-eddy interaction model is capable of simulating particle dispersion in complex turbulent flows with different scales in each direction.

Gas and Particle Phase Description

The particle dispersion model discussed in the last sub-section is implemented within the framework of ARCHES, a computer software package intended for modeling three-dimensional reacting and non-reacting multiphase flow in complex Cartesian geometry and developed at the University of Utah. A description of the turbulence mixing process applied to coal combustion is discussed in Smoot and Smith (1985).

The interaction between the gas and the particle-phase is accomplished through the accumulation of the Eulerian source terms. This procedure is equivalent to the particle source in cell technique (Crowe et al., 1977) for Lagrangian methods. Individual particles are tracked through a flow field by solving the ordinary differential equation (ODE) governing particle motion. The fluid properties required to solve the ODE are obtained by three-dimensional linear interpolation at the particle location. Along with the solution of the particle motion equation, a number of ODE's of the form

$$\frac{d\alpha_j}{dt} = rate_j \quad (7)$$

are solved for each mass fraction of the coal particle (Smoot and Smith, 1985). The rate in (10) is the rate of depletion of that particular mass fraction of coal. Two major reactions occur during the combustion history of the coal particle. The first reaction called devolatization occurs during the early stages of coal burnout. A number of models have been proposed in the literature to account for the amount of volatiles and its rate of evolution from the coal particle (Baxter, 1989). Details of the devolatization modeling can be found elsewhere (Smoot and Smith, 1985). The second major reaction that occurs at a later stage of coal burnout is the char oxidation reaction. The char reaction occurs due to the diffusion of gaseous species from the bulk gases (e.g. CO_2, O_2 etc.) to the surface of the coal particle. The char oxidation reactions are considered diffusion controlled or kinetic controlled depending on the temperature of the particle. The reaction kinetics is modeled by the nth order global reaction rate with an oxidation mechanism, details of which can be found in Smoot and Smith (1985).

Finally the particle energy equation must also be solved to obtain the particle temperature. A predictor-corrector method along with a first-order Euler's integration method is used to solve the ODE's. The time steps for integration are variable and are calculated based on limiting ODE for stiffness. Thus, the particle properties at each time steps are computed.

Since the individual particles are followed in a Lagrangian reference frame, the Eulerian gas-phase equations are coupled to the Lagrangian particle equations via particle source terms. The particle mass source to the gas phase is the change in mass of all the particles that traverse a particular cell of interest. For a particular cell, the mass source is calculated from

$$S_p = \iint_{n,V} \dot{q} r_p dV dt \quad (8)$$

Similar expressions can be written for the sources of momentum and enthalpy. Thus, the overall effect of the particles is captured into the Eulerian gas-phase computation.

RESULTS AND DISCUSSION

Particle dispersion model validation

In this section, the numerical simulation results of the three-eddy interaction model and the eddy interaction model are compared with the data of Snyder and Lumley (1971). For convenience the eddy interaction model of Graham (1996a) will be referred to as a single-eddy interaction model. Using a grid system Snyder and Lumley (1971) collected a comprehensive set of particle dispersion data in a nearly isotropic decaying turbulent flow field. They used particles ranging from very light, that behave like fluid particles and do not experience inertia and crossing trajectory effect, to heavy particles, that experience both inertia and crossing trajectory effects. In all of the following figures, lines represent the numerical simulation results, while symbols are experimental data. Figure 1 compares the predicted and experimental transverse particle dispersions using the single-eddy interaction model of Graham (1996b). The comparison in Figure 1 is in fair agreement with experimental data. Figure 2 compares the predicted and experimental dispersion of particles in the transverse direction using a three-eddy interaction model. Within the statistical noise between the single and the three-eddy interaction model, reasonable agreement is observed when comparing Figure 1 and Figure 2. In both the models, the same Eulerian length scale and Lagrangian integral time scale are used. Figure 3 compares the predictions of the single-eddy and the three-eddy interaction model in the gravity direction. The single-eddy interaction model of Graham (1996b) is not able to predict a higher dispersion in the longitudinal direction compared to the transverse displacement (Figure 1). As predicted by previous studies (Reeks (1977) and Lu et al. (1993)) the three-eddy interaction model predicts that particles disperse quickly in the direction of gravity due to the continuity effect.

Huang and Stock (1997) made measurements of particle dispersion in a homogeneous uniform shear flow. In the experimental setup, a constant mean velocity is present only in a direction perpendicular to the mean flow and the

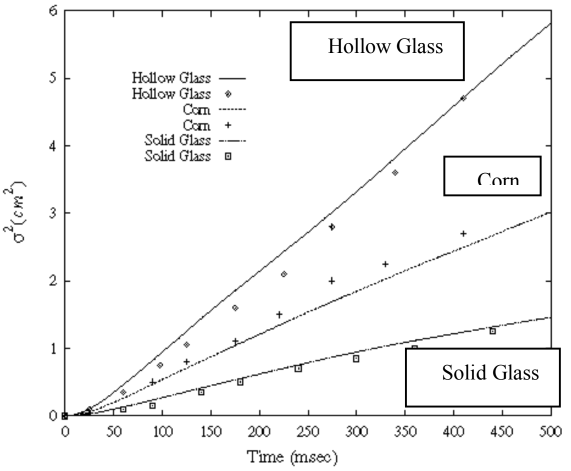

Figure 1: Comparison of single-eddy interaction model predictions with experimental data of Snyder and Lumley (1971)

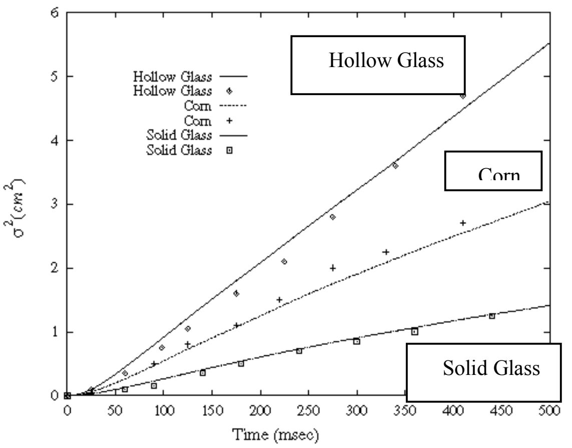

Figure 2: Comparison of three-eddy interaction model predictions with experimental data of Snyder and Lumley (1971).

turbulence is stationary and homogeneous. Since the scale of the turbulence is distinctly less than the scale of the inhomogeneity, the turbulence and the rate of strain are assumed to be spatially uniform. Measurements by various researchers (Huang and Stock, 1997) show that in a reasonably homogeneous uniform shear, the turbulent velocity scale, length scale and time scale are different in all three directions. In this section, the numerical predictions from the single and three-eddy interaction model for fluid particles and non-fluid particles are compared with the experimental data of Huang and Stock (1997).

In the experiment the velocity scales, length scales and time scales are different in all three directions. The single-eddy interaction model is not capable of simulating such an experiment because it is based on only one length scale and time scale. Therefore, average time scales and length scales are used in this section to compare the results of the single-eddy interaction model with experimental data.

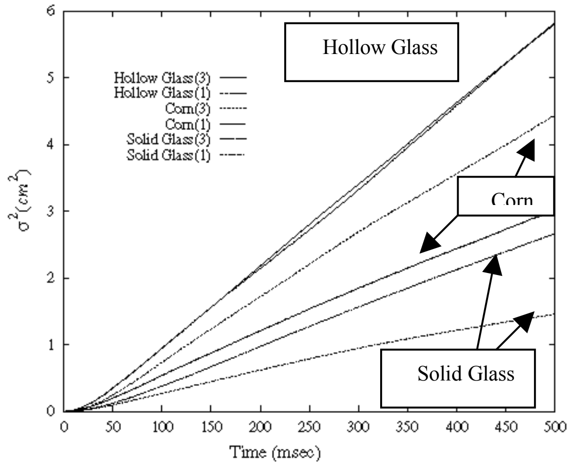

Figure 3: Comparison of three-eddy interaction model and single eddy interaction model predictions in the longitudinal direction.

Huang and Stock (1997) generated a uniform homogeneous shear flow using a shear generator. The objective of their study was to measure heavy particle dispersion in a simple shear flow. They first measured the Lagrangian scales of the fluid by measuring the dispersion of heat from a line source. Finally dispersion of two particle sizes was measured. The Lagrangian integral time scales in the *y* and *z* directions are computed from the diffusivity data of heat from a line source using the relation of Hinze (1975).

Figure 4 compares the numerical predictions of dispersion of fluid particles with experimental data. Good agreement with experimental data is observed.

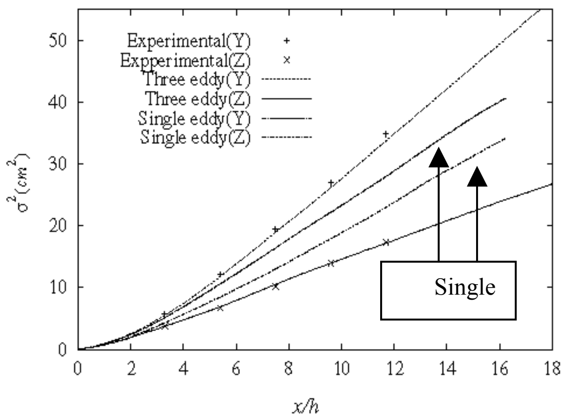

Figure 4: Comparison of single and three-eddy interaction model for fluid elements with experimental data of Huang and Stock (1997)

The three-eddy interaction model is able to capture the anisotropy due to the differences in time scales in the two directions. The single-eddy interaction model, which uses an average integral time scale, is only able to capture the anisotropy in the velocity scales. Figure 5 compares the particle dispersion predictions in the *z* directions obtained from the single and three-eddy interaction model with the experimental data of Huang and Stock (1997). Again the three-eddy interaction model gives improved predictions.

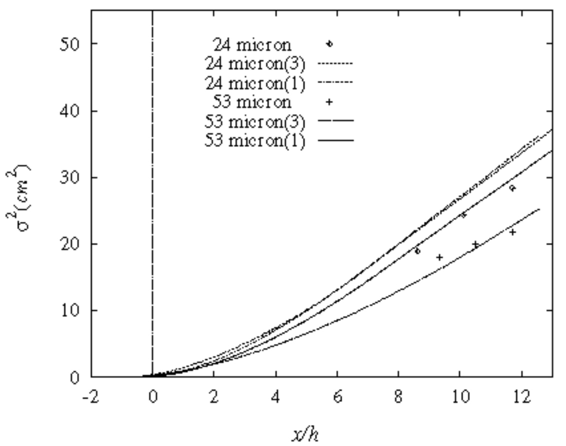

Figure 5: Comparison of particle dispersion prediction in the y-direction with the experimental data of Huang and Stock (1997) (1-single eddy model, 3-three-eddy model)

Combustion Modeling Validation

In the previous subsection, the particle dispersion model was evaluated against existing experimental data in simple non-reacting turbulent flows. The case study presented in this section is a verification of the implementation of the particle dispersion model in a reacting flow framework. The predictions from the multiphase reacting flow code are compared with experimental data obtained from a single burner coal-fired IFRF furnace. Michels and Payne (1980) have made detail measurements in a nearly square refractory tunnel furnace of approximate dimensions 2.0*2.0*6.2 m. The walls of the furnace were maintained at constant temperature by use of cooling pipes along the outside. The primary and secondary ducts were concentric and located at one end of the furnace. The furnace was horizontally fired and axisymmetric. Nevertheless, the simulation was performed on a full furnace to demonstrate its capability and to test the runtime of the simulation from start to convergence. Computation were performed on a 46*36*36 node mesh. Due to lack of particle velocity and distribution profile available at the inlet, a uniform profile was assumed.

Figure 6 compares the axial temperature predictions using the three-eddy interaction model and the cloud approach with available experimental data. Both models predict the trends remarkably well, except close to the burner where the stochastic approach predictions are much closer to experimental data than the cloud approach. This trend is attributed to the fact that the cloud approach produces smeared source terms that result in lower temperatures close to the burner. Also, a spike is observed in the simulated axial temperature profile from both the stochastic and the cloud approach. This spike is due to the devolatization reactions that emit volatiles that react to equilibrium as soon as they are mixed in the gas phase. This equilibrium assumption in the gas phase and the assumption of kinetic control in the particle-phase are approximations that might lead to a temperature spike close to the inlet. Also temperatures in the near burner region vary drastically within a short distance as we move away from the center of the flame. Also, when viewed with the visualization software, the stochastic approach appears to give an overall better flame shape than the cloud approach. Species concentration predictions along the centerline of the reactor do not compare very well with experimental data.

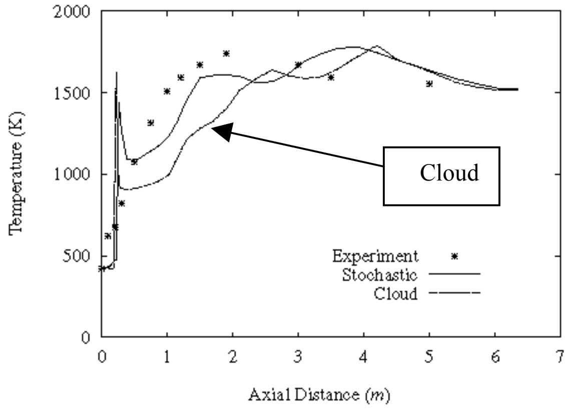

Figure 6: Axial temperature prediction comparison with experimental data.

Figure 7 compares species concentration along the centerline of the reactor. The Oxygen profile predicts faster depletion of concentration from the model as compared to experimental data. Two reasons might contribute to the discrepancy. Firstly, the devolatization process, which is assumed to be kinetic limited, may be both kinetic as well as mixing limited. It has been observed (Smoot and Smith, 1985) that devolatization time scales range from 5 milliseconds to 200 milliseconds. The smaller of the two numbers is of similar order of magnitude as the mixing time scale. Thus, the volatiles coming out of the coal particles might be coming out too soon. Secondly, the chemistry in the gas phase is assumed to be in equilibrium at all times, i.e., the escaping volatiles react as soon as they are mixed. These two assumptions together might result in a lower oxygen concentration prediction from the two models. This might also result in the temperature spike observed in Figure 6. The plot in Figure 8 shows that both modeling approaches over-predict the CO mole fraction in the gas phase. Again this might be attributed to the equilibrium chemistry assumption in the gas phase.

CONCLUSION

A stochastic turbulent particle dispersion model has been developed which can account for anisotropy in the particle dispersion predictions in all three directions. Unlike past approaches, this approach is fundamentally more accurate because most turbulent flows are anisotropic in nature. The new particle dispersion model (three-eddy interaction model) captures all the three effects pertaining to particles in a turbulent flow field, namely, the inertia effect, the crossing trajectory effect and the continuity effect.

Comparing the predictions with two experimental data sets validates particle dispersion model. First, the model was tested against available grid generated turbulence data. This data set tests all three effects, namely the inertia, crossing trajectory and continuity effects in an isotropic flow field. Results presented in the previous section show that the particle dispersion model is capable of capturing all three effects accurately. Second, the model is tested against available experimental data in a homogeneous shear flow. This data set includes dispersion of particles as well as fluid elements in an anisotropic flow field. The new particle dispersion model is able to capture the anisotropy in a reasonable fashion for both particles and fluid elements. These two comparisons validate the capability of the model to accurately predict particle dispersion in an anisotropic flow field.

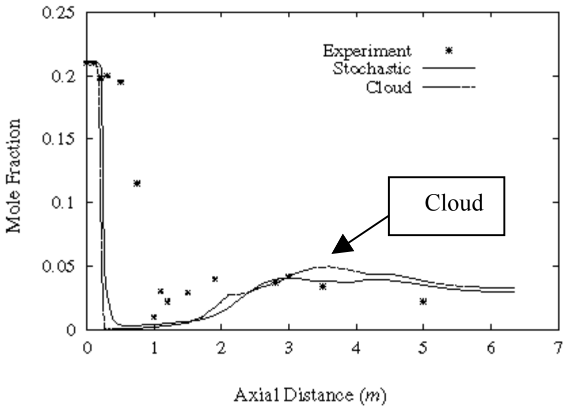

Figure 7: Comparison of Oxygen mole fraction along the centerline of the reactor

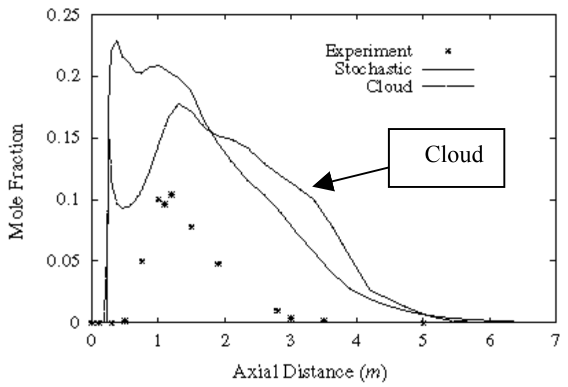

Figure 8: Comparison of CO model fraction along the centerline of the reactor

Additionally the overall capability of the three-eddy interaction model as implemented in a three-dimensional reacting flow framework was demonstrated by simulating the IFRF furnace. The predicted results were compared with those of the existing particle dispersion model predictions (cloud approach) as well as with in-flame experimental measurements. The simulation results for the gas-phase temperatures obtained from the stochastic approach were superior to the predictions obtained from the cloud approach.

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