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3-D Turbulent Particle Dispersion Submodel Development

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Quarterly Progress Report #4

covering the period of 15 January to 15 April 1992

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DE-F622-901C 90094

to the Department of Energy
Pittsburgh Energy Technology Center
Pittsburgh, PA

Project Manager: James Hickerson

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

Graduate Students: S. Jain & S. Kumar

Phillp J. Smith
principal investigator

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1.0 Overview of Project

Many practical combustion processes which use solid particles, liquid droplets, or slurries as fuels introduce these fuels into turbulent environments. Examples include spray combustion, pulverized coal and coal slurry combustion, fluidized beds, sorbent injection, and hazardous waste incineration. The interactions of the condensed phases with turbulent environment have not been well described. Such a description is complicated by the difficulty of describing turbulence in general, even in the absence of particles or droplets. But the complications in describing the dispersion and reaction of the condensed phases in turbulent environments do not stem entirely or even primarily from the uncertainties in the description of the turbulence. Theoretical descriptions of the turbulent dispersion of particles and droplets are not well established, even when the characteristics of the turbulence are known. It is the purpose of this project to develop two different particle dispersion submodels (one for dilute phases and one for dense phases), and couple them with existing fluid-dynamics, heat transfer and reaction chemistry models to provide computational simulations capable of addressing industrial problems.

This report summarizes progress made on this project in the fourth quarter which includes preliminary results obtained from the particle dispersion submodel.

2.0 Dilute Particle Phase Dispersion Model Development

The approach we have developed to model particle dispersion in lightly loaded systems involves tracking particle clouds in a Lagrangian frame of reference. Lagrangian methods have the advantage of being able to account for time-temperature histories of reacting particles. This is important since particles arriving at any given spatial position in the system may have different histories and properties. However, Lagrangian methods developed in the past perform Monte-Carlo simulations of particle trajectories which require simulation of a large number of trajectories

to arrive at a numerically accurate and stable solution. The computational effort involved in predicting particle dispersion in industrial coal combustors by this method makes it inadvisable to use these models. We have developed a technique for computationally tracking clouds of particles, rather than individual particles, in which we calculate mean particle trajectories and the turbulent dispersion of the cloud about this mean position. The method deals with the reaction of coal particles and also coupling with the continuous phase using source terms for mass, momentum and energy exchanges. Details of the theory and implementation of this model for the stochastic transport of particles (STP) can be found in the first two quarterly reports (Smith 1991).

As indicated in the previous report (Smith 1992) preliminary results of the prediction of mean particle trajectories in a test case of non-reacting flow through a box seemed reasonable. Section 2.1 discusses work done in the last quarter involving implementation of source term calculations. Eulerian output calculations by the particle submodel are discussed in Section 2.2. Preliminary Eulerian output fields of particle properties obtained from particle submodel computations for a test case of turbulent flow through a box with reacting coal particles are presented in Section 2.3.

2.1 Particle Source Term Calculations

From the perspective of the Eulerian framework, the purpose of the particle model is to generate particle source terms for each variable in each computational cell. As discussed in Quarterly Progress Report #2 (Smith 1991) the source terms are calculated as

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

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

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

where lb and ub represent the lower and upper bounds of the cell, respectively.

Table 1 defines the specific variable substitutions for ϕ .

Table 1 Variable Substitutions to compute source terms

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

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

$W(x_i, t)$ is defined in terms of the pdf.

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

where

$$\int_{V(min-max)} P(x_i, t) dV \equiv \int_{x_{1,min}}^{x_{1,max}} \int_{x_{2,min}}^{x_{2,max}} \int_{x_{3,min}}^{x_{3,max}} P(x_i, t) dx_1 dx_2 dx_3 \quad (EQ 4)$$

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

$$\int_{V(min-max)} P(x_i, t) dV \equiv \frac{1}{A(t)} \quad (EQ 5)$$

Differences between $P(x_i, t)$ and $W(x_i, t)$ are trivial in a Cartesian reference frame. In this reference frame, W is used

to account for the finite limits of integration over P . Otherwise, the functions are identical.

The time integral is performed numerically. For constant $\dot{q}$ and $r_p^\dagger$, the volume integral need only address the spatial variation of W . This integral, for a Cartesian coordinate system, is given by

$$\int_V W(x_i, t) dV = A(t) \int_{x(lb)}^{x(ub)} \int_{y(lb)}^{y(ub)} \int_{z(lb)}^{z(ub)} P(x, y, z, t) dx dy dz \quad (EQ 6)$$

The designations lb and ub refer to the values of the variables at the lower and upper bounds, respectively. The limits correspond to individual Eulerian cell boundaries. One also has to limit the number of Eulerian cells included in the volume integration. That is, it is not practical to evaluate the source terms in all of the Eulerian cells over the limits $x, y, z = \pm\infty$. In practice, the integrals are carried out for a distance of at least $\pm$ three standard deviations in each coordinate direction. Cell boundaries do not generally fall at precisely $\pm$ three standard deviations from the mean position, therefore the integrals are carried out for more than three standard deviations and less than $\pm\infty$ in each direction.

Sometimes while calculating the source terms for three standard deviations from the mean position a wall is encountered in some direction. The complex interactions of particles with physical boundaries in combustors are approximated by assuming that the pdf elastically collides with the walls. This approximation is illustrated in two dimensions in Figure 1 for the case where there is a physical obstruction in the x - z plane

Figure 1 Reflection of pdf off a physical boundary in the x-z plane.

This type of reflection is continued until the reflected pdf hits another boundary. In that case the remaining area under the pdf in that direction is assigned a flat distribution. This treatment does not accurately describe the complex interactions of the particles with the walls. However, considerable additional research must be done before such descriptions can be made.

2.2 Eulerian Output Fields

While the Lagrangian reference frame is useful as a solution procedure, it is useful to be able to display particle properties in an Eulerian reference frame to get an idea of the spatial dependence of these properties.

The STP model can be used to describe particle properties (temperature, residence time, number density, etc.) at the node of each Eulerian computational cell in the flowfield in terms of moments of local probability density functions. The first moment, or mean, of each particle property is taken about zero and is defined as

$$\mu \equiv E\{\Psi\} = \begin{cases} \sum \Psi p(\Psi) & \text{if } \Psi \text{ is discrete} \\ \int_{-\infty}^{\infty} \Psi f(\Psi) d\Psi & \text{if } \Psi \text{ is continuous} \end{cases} \quad (\text{EQ 7})$$

Here, Ψ represents the random function and ψ represents individual realizations of this function. $E\{\}$ is the

expected value operator. The rest of the moments are taken with respect to this mean, and they are defined as

$$\mu_r \equiv E\{(\Psi - \mu)^r\} = \begin{cases} \sum (\Psi - \mu)^r p(\Psi) & \text{if } \Psi \text{ is discrete} \\ \int_{-\infty}^{\infty} (\Psi - \mu)^r f(\Psi) d\Psi & \text{if } \Psi \text{ is continuous} \end{cases} \quad (\text{EQ 8})$$

Essentially all particle properties are continuous but they are predicted by discretized mathematical equations. The function $p(x)$ is a probability function for the discrete variable and the function $f(x)$ is a probability density function for the continuous function. The first moment shows the central tendency of the variable, the second the degree of scatter around this tendency, the third the symmetry of the distribution, etc. An iterative process would be required if the calculations were to be performed as prescribed above, with the first iteration to calculate a mean and a second to calculate the remaining moments.

In practice, the discrete values of the particle properties at each time step i , in the calculation are used to calculate the moments of the local pdf in each Eulerian cell as follows

$$\mu = (\sum p_{i,j} \Psi_{i,j}) / (\sum p_{i,j}) \quad (\text{EQ 9})$$

$$\mu_2 = (\sum p_{i,j} \Psi_{i,j}^2) / (\sum p_{i,j}) - \mu^2 \quad (\text{EQ 10})$$

The factor $p_{i,j}$ represents the number of particles in each cell at each discrete time i and is calculated for each Eulerian cell as follows

$$p_{i,j} = \int_V g(t,i) P(\Psi_{i,j}, t, i) dV \quad (\text{EQ 11})$$

where the integral over V is over the volume of that computational cell. The function g is included to allow the results to be weighted with respect to other properties or products of other properties like number of particles, particle residence time, particle mass, etc.

The first moment of the distributions will be reported as indicated above. The principal root of the variance, or standard deviation, will be reported rather than the variance.

2.3 Illustration of Predicted Results

Use of the equations discussed in the previous subsection yields information about particle behavior which has not been easily obtainable from combustion simulation codes in the past. In this section, particle properties will be illustrated using preliminary results obtained from particle submodel computations for a test case of pulverized coal combustion. For these computations the particle dispersion model was run in conjunction with a coal reaction submodel and converged gas phase properties were read into the particle submodel from a restart file written out by the three dimensional gas code.

Table 2 General characteristics of pulverized coal combustion test case used for predictions

Variables	Values
Combustor length, width, height	2.0, 0.2, 0.2 m
Primary, Secondary flowrate	.027, 4.1 g/s
Particle loading in primary	0.256
Initial particle size, density	50 μ m, 1340 kg/m ³
Primary, Secondary temp.	423, 763 K

Figures 2-4 depict Eulerian particle number densities, particle residence times and particle burnout respectively, predicted by the particle submodel. The general flow direction is along the length of the reactor from left to right. The flow rates used in this test case are very low and so the effect of gravity on particle trajectories is pronounced. Consequently particle number densities are higher in the lower half of the reactor as seen in Figure 2. In Figures 3,4 particle residence times and burnout are increasing along the length of the reactor as expected. Because of the low velocities particles take upto 7.5 seconds to exit the reactor. Particle burnout at the reactor exit is just 39 percent in this case because of two reasons. First, the air flow rates are very low and the fuel lean mixture does not have enough oxygen for complete burnout. Secondly, the particle and gas phases are not yet fully coupled, i.e., gas phase properties are not being updated to include the influence of reacting coal particles. Consequently temperatures and particle burnout are not as high as they would be in a fully converged case.

Other particle properties like temperature, mass, size etc., variances, and source terms were computed and they showed trends as expected. It should be noted that particle

clouds starting from just four different locations in the primary were tracked through the reactor to get these results unlike previous Lagrangian particle dispersion models which would involve simulation of hundreds of particle trajectories. This computational efficiency will play a key role in the success of this dispersion model within the framework of a comprehensive combustion simulation applicable to industrial situations.

3.0 Project Plans

This report has summarized the work accomplished in the fourth quarter of a project to develop a computationally accurate and efficient turbulent particle dispersion model for incorporation in computational fluid dynamical and combustion codes. Computer coding of a stand alone particle dispersion model for lightly loaded systems has been completed. Preliminary results obtained from this model are encouraging.

This model will be incorporated in the three dimensional combustion code allowing full coupling between the gas and particle phase calculations. This will involve inclusion of source terms in the gas phase transport equations and development of algorithms to run the gas and particle phase computations in series and parallel. The comprehensive simulation will then be evaluated by comparison with available data.

Figure 2 Computed Eulerian field for particle number density.

7.7355e+07

0.00

Figure 3 Eulerian representation of particle residence times in the reactor.

7.351

0.00 sec.

Figure 4 Particle burnout in an Eulerian reference frame.

0.3965

0.00

4.0 Nomenclature

Symbol	Units	Definition
a	varies	weighting function
A	varies	weighting function
A_p	m^2	projected area of particle normal to fluid velocity
b	-	constant
$\bar{k}$	$\frac{m^2}{s^2}$	mass-averaged turbulent kinetic energy
N	-	normal distribution
P	varies	probability density function
$\dot{q}$	#/s	particle number flowrate
r_j	$\frac{kg}{m^3 \cdot s}$	rate of mass production per unit volume of j^{th} component of solid phase
S_g^m	$\frac{kg}{m^3 \cdot s}$	gas phase mass source term for particle continuity equation
S_p^m	$\frac{kg}{m^3 \cdot s}$	particle mass source term for gas phase continuity equation
S_g^u	$\frac{kg}{m^2 \cdot s^2}$	gas phase momentum source term for particle momentum equation
S_p^u	$\frac{kg}{m^2 \cdot s^2}$	particle momentum source term for gas phase momentum equation
V	m^3	volume
w	varies	weighting function
W	varies	weighting function
x	m	x-coordinate length
y	m	y-coordinate length
z	m	z-coordinate length

Greek

ϵ	$\frac{m^2}{s}$	dissipation rate of turbulent energy
η	-	coal gas mixture fraction
ϕ	varies	a general flow variable

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