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A MONTE-CARLO METHOD FOR CALCULATING TURBULENT REACTING DISPERSED FLOW

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ABSTRACT--- This paper deals with Monte-Carlo calculations of turbulent reacting dispersed flow in which the dispersed phase (liquid or solid) is very small sized and distributed uniformly. A hybrid probability density function (pdf) for modelling turbulent reacting dispersed flow is introduced. Its transport equation is derived from the governing equations for describing the evolution of the hybrid pdf. A numerical method for solution of this kind of transport equation is developed in terms of a combined Monte-Carlo method. No turbulence model is needed for the effects of convection, reaction and interaction between the both phases in the transport equation of the hybrid pdf. Therefore the gradient-diffusion assumptions for both phases from the conventional moment method can be avoided. The simulation results are in good agreement with published experimental data.

NOTATION

C_u	constant for particle interaction model
C_Φ	constant for particle interaction model
C_n	constant for particle interaction model
d_d	particle diameter
f	probability function
f_i	force
F	distribution function
F_i	specifical force
I	random variable
J	molecular mass transport
p	mass density function
P	pressure
S_d	mass transfer between both phases
S_i	mass transfer through chemical reaction
t	time
u	velocity fluctuation
U	velocity vectory
V	volume
V_d	particle-volume
$X_{i\ or\ j}$	coordinate

grecch symbol

α	random variable	Φ	symbol for scalar variable
γ	loading ratio	μ	dynamical viscosity
θ	volumetric ratio	ρ	density
ρ_d	density of disperse phase		
σ	conzentration of disperse phase		
τ	Newton´s shear stress tensor		
Ω^*	turbulence frequence modulated by disperse phase		

Indices

c	carrier phase	d	disperse phase
	statistical mean valu	"	fluctuation
'	mass weighted mean	< >	arithmetrical mean

INTRODUCTION

The turbulence effects are significant in the most industrial applications. There are generall two methods to describe turbulence effects, the conventional moment method and the pdf (probability density function) method. The description of turbulent reacting dispersed two-phase flow by the pdf method overcome the most turbulent closure problems. Hereby the gradient-diffusion assumptions can be avoided which are commonly used for both phases with the conventional moment method and lead inevitable to an illimitable complexity for modelling turbulent reacting dispersed flow (Elghobashi and Abou-Arab, 1983; Besnard and Harlow, 1988; Chen, 1986).

Shang and Schecker (1990) introduced a hybrid joint pdf to lay hold of flow field parameters for both phases. The flow field parameters can be treated as stochastical functions of space and time coordinate. From the conservation equation set a transport equation of the hybrid joint pdf can be deduced which afford not only the hydrodynamical information but also stochastical information about the turbulent flow field. This transport equation is used for pursuing the evolution of the hybrid joint pdf rather than preassuming its form. Unfortunately, it is impossible to date to solve this kind of equations with the conventional finite difference algorithm because of the high dimensionality of the hybrid joint pdf.

Pope (1981) introduced a Monte-Carlo method to solve a transport equation of the joint pdf for turbulent reacting single phase flow. For the statistical description of the movement of dispersed particles in turbulent flow field a Monte-Carlo simulation is commenly used (Shuen, 1983; Durst, 1984) From the both procedures a hybrid Monte-Carlo method was combined (Shang,1991). In this paper the combined Monte-Carlo method is shown for solving the transport equation of the hybrid joint pdf for the turbulent reacting dispersed flow. A particle laden round jet and a dust explosion in a vessel are numerically simulated. The simulation results show good agreement with the published experimental data.

THEORETICAL FOUNDAMENTS

All parameters of carrier and dispersed phase in a turbulent flow field are stochastical functions of space and time coordinate. It can be seized by a hybrid joint pdf $f_{u\Phi}$ (cd):

$$F_{u\Phi(cd)} = F_{u\Phi(cd)}(U_i, U_{di}, \Phi_n, \Phi_{dn}; X_i, t) \qquad (1)$$

$$f_{U\Phi(cd)} = \frac{\partial^4}{\partial U_i \partial U_{di} \partial \Phi_n \partial \Phi_{dn}} F_{U\Phi(cd)}(U_i, U_{di}, \Phi_n, \Phi_{dn}; X_i, t) \qquad (2)$$

The symbol Φ is for random scalar variables (concentrations, temperature or mixing grad ...) and the symbol U for random vectorial variables (velocities). The index n is the number of random scalar variables of carrier and dispersed phase. The mass weighted hybrid joint pdf $\widetilde{f_{u\Phi(cd)}}$ or hybrid joint mass density function $\widetilde{p_{u\Phi(cd)}}$ can be defined in order to consider the compressiblity of fluid due to the exotherm reaction or suppersonic flow:

$$\widetilde{f_{u\Phi(cd)}} = \int_{\rho_{\rho\sigma}} \rho_{\rho\sigma} f_{u\Phi(cd)} \, d\rho_{\rho\sigma} / \overline{\rho_{\rho\sigma}} \qquad (3)$$

$$\widetilde{p_{u\Phi(cd)}} = \widetilde{f_{u\Phi(cd)}} \, \overline{\rho_{\rho\sigma}} = \int_{\rho_{\rho\sigma}} \rho_{\rho\sigma} f_{u\Phi(cd)} \, d\rho_{\rho\sigma}$$

$$= \int_{\rho} \rho \, f_{u\Phi(cd)} \, d\rho + \int_{\sigma} \sigma \, f_{u\Phi(cd)} \, d\sigma \qquad (4)$$

The expectations, variances and covariances of the flow field parameters of carrier and dispersed phase can be determined with the aid of the hybrid joint pdf, if the mathematical formulation of this hybrid joint pdf $f_{u\Phi(cd)}$ is known for every space and time coordinate. In order to describe the evolution of the hybrid joint pdf in the turbulent flow field, a transport equation of the hybrid joint pdf can be deduced from the conversation equations of mass, momentum and energy for carrier and dispersed phase (Shang, 1991):

$$\frac{\partial \widetilde{p_{u\Phi(cd)}}}{\partial t} + U_i \frac{\partial \widetilde{p_{u\Phi(cd)}}}{\partial X_i} + \frac{\partial}{\partial U_i}\left[\frac{1}{\rho} \left\{ F_{ci} - \frac{\partial \bar{P}}{\partial X_i} \right\} \widetilde{p_{u\Phi(cd)}} \right]$$
$$+ \frac{\partial}{\partial U_{di}} \left[\frac{F_{di} \widetilde{p_{u\Phi(cd)}}}{\sigma} \right] + \frac{\partial}{\partial \Phi}\left[S \widetilde{p_{u\Phi(cd)}} \right] + \frac{\partial}{\partial \Phi_d}\left[S_d \widetilde{p_{u\Phi(cd)}} \right]$$
$$= -\frac{\partial}{\partial U_i}\left[\frac{1}{\rho} \left\langle \frac{\partial P''}{\partial X_i} - \frac{\partial \tau}{\partial X_i} \middle| (U\Phi)_{cd} \right\rangle \widetilde{p_{u\Phi(cd)}} \right]$$
$$+ \frac{\partial}{\partial \Phi}\left[\frac{1}{\rho} \left\langle \frac{\partial J}{\partial X_i} \middle| (U\Phi)_{cd} \right\rangle \widetilde{p_{u\Phi(cd)}} \right]. \qquad (5)$$

In this equation the effects of convection, reaction and interactions between the both phases are described exactly and therefor do not need the turbulence modelling. Unfortunately, this equation can not be solved by the conventional finite difference algorithm because of it´s high dimensionality. In this paper a combined Monte-Carlo-method is shown to solve this kind of transport equations of the hybrid joint pdf.

SOLUTION ALGORITHM

The Monte-Carlo method is based on following hypothetical stochastical particles from both phases. Pope introduced a Monte-Carlo-method for solving the transport equation of the joint pdfs for the single phase reacting flow. The various simulation results (Givi, 1984; Nguyen, 1984 and Anand, 1987) verify this algorithm. It is generally used a Monte-Carlo simulation for the statistical description of the movement of dispersed particles in turbulent flow field. From the both procedures a hybrid Monte Carlo method is combined. Hereby, the hybrid pdf is represented by an ensemble of N hypothetical stochastical particles. The evoluation of the hybrid pdfs can be simulated by following the particles from both phases. The physical behaves of the fluid particles in turbulent flow field could be total different from that of the hypothetical stochastical particles, but if their hybrid pdfs are initialy indentical, they evoluate in the same way in time. Therefor, the combined Monte-Carlo method is an indirect method.

For the Monte-Carlo simulation the conditional expectations in the hybrid joint pdf transport equation must be formulated in discret form and can be simulated by the particle interaction models. The stochastical hybrid particles influence each ather in the turbulent flow field. The interactions between the hybrid stochastical particles can be classified in three kinds: A. Interactions between particles from carrier phase, B. Interactions between particles from dispersed phase and C. Interactions between particles from carrier and dispersed phase. A mixing and a momentum exchanging procedure takes place if particles from the one or both phases collide. These processes can be described by the particle interaction models.

A. Interactions between particles from carrier phase

The collision between particles from the carrier phase cause a mixing and a momentum exchanging procedure. These procedures are stochastical and therefor can be described statistiscally. Here two particles a and b are considered:

I. mixing:

$$\Phi^a_{[t+\Delta t]} = (1-\alpha)\,\Phi^a_{[t]} + \alpha\,\Phi_{m[t]} \qquad (6)$$

$$\Phi^b_{[t+\Delta t]} = (1-\alpha)\,\Phi^b_{[t]} + \alpha\,\Phi_{m[t]} \qquad (7)$$

$$\Phi_{m[t]} = \frac{1}{2}\left(\Phi^a_{[t]} + \Phi^b_{[t]} \right) \qquad (8)$$

$\Phi_{[t]}$ and $\Phi_{[t+\Delta t]}$ mean the parameter befor and after the mixing process. Because this mixing procedure can takes place only under realistic conditions, a random variable α (0,1) is introduced in oder to take nonideal mixing behaviour into account. It can be treated as a scale for mixing process.

II. momentum exchanging:

$$U^a_{i[t+\Delta t]} = (1-\alpha)\,U^a_{i[t]} + \alpha\,U_{mi[t]} \qquad (9)$$

$$U^b_{i[t+\Delta t]} = (1-\alpha)\,U^b_{i[t]} + \alpha\,U_{mi[t]} \qquad (10)$$

$$U_{mi[t]} = \frac{1}{2}\left(U^a_{i[t]} + U^b_{i[t]} \right) \qquad (11)$$

This model takes only the variation in velocity space but not the reorientation of velocities into consideration. It can be treated as follows:

$$U^a_{i[t+\Delta t]} = U_{mi[t]} + \frac{1}{2} I \, U_{di[t]} \qquad (12)$$

$$U^b_{i[t+\Delta t]} = U_{mi[t]} - \frac{1}{2} I \, U_{di[t]} \qquad (13)$$

$$U_{di[t]} = \left| U^a_{i[t]} - U^b_{i[t]} \right| \qquad (14)$$

I (-1, 1) and α (0,1) can be produced by a random generator. It is evident that these procedures occur stochastically. The selection of particles a and b can be taken by a life expectancy:

$$t_f^n = \frac{t_n^n \Omega^*}{c_j} \qquad (15)$$

Ω^* is the turbulence frequence modulated by dispersed phase, c_j constant for various models, e.g. c_f = 1,5 (mixing), c_u = 0,75 (momentum exchanging) or c_n = 0,375 (reorientation) and t_n^n (0, ∞) a random variable, whose distribution can be taken from the Kosaly´s model (Kosaly, 1983). The value of c_j based on the consideration of turbulent dispersed flow (Chen, 1986, Spalding, 1971, Lin, 1973, and Warhaft, 1981). Exact descriptions of these three models can be taken from the work (Pope, 1985 and Shang, 1991).

B. Interactions between particles from dispersed phase

An another life expectancy is used as "collision expectancy" to select particles for collision of solid dispersed particles:

$$t_s^n = \frac{t_n^n \Omega^*}{c_j}(1 - \theta) \qquad (16)$$

$$\theta = \frac{V_c}{V_c + V_d} \qquad (17)$$

The collision frequency of particles is direct proportional to volumetric ratio θ. The procedures are similar:

$$U^a_{di[t+\Delta t]} = (1 - \alpha) U^a_{di[t]} + \alpha U_{dmi[t]} \qquad (18)$$

$$U^b_{di[t+\Delta t]} = (1 - \alpha) U^b_{di[t]} + \alpha U_{dmi[t]} \qquad (19)$$

$$U_{dmi[t]} = \frac{1}{2}\left(U^a_{di[t]} + U^b_{di[t]} \right) \qquad (20)$$

$$U^a_{di[t+\Delta t]} = U_{dmi[t]} + \frac{1}{2} I\, U_{ddi[t]} \qquad (21)$$

$$U^b_{di[t+\Delta t]} = U_{dmi[t]} - \frac{1}{2} I\, U_{ddi[t]} \qquad (22)$$

$$U_{ddi[t]} = \left| U^a_{di[t]} + U^b_{di[t]} \right| \qquad (23)$$

The specifical terms must be formulated in the conversation equations and hence in the transport equation of the hybrid joint pdf if disintegration or coalescence process of disperse particles occur. The same procedures can be utilized (Shang, 1991).

C. Interactions between particles from carrier and dispersed phase

These effects are formulated by the "source term" in the conversation equations and the transport equation for hybrid joint pdf. They can be treated as determinativ because all disperse particles occur similar:

$$U^n_{i[t+\Delta t]} = U^n_{i[t]} + \frac{F^n_{ci}}{\rho_n} \Delta t \qquad (24)$$

$$U^n_{di[t+\Delta t]} = U^n_{di[t]} + \frac{F^n_{di}}{\sigma_n} \Delta t \qquad (25)$$

$$\Phi^n_{[t+\Delta t]} = \Phi^n_{[t]} + S^n \Delta t \qquad (26)$$

$$\Phi^n_{d[t+\Delta t]} = \Phi^n_{d[t]} + S^n_d \Delta t \qquad (27)$$

For the momentum exchanging process the following forces can be considered. drag force, virtual mass force and Basset force ect:

$$F^n_d = \frac{12 \rho^n C^n_d}{\rho_d d^{nd}_d}\left(U^{nc}_{[t]} - U^{nd}_{d[t]} \right)^2 \Delta t + \frac{\rho^n}{2 \rho_d} \Delta\left[U^{nc}_{[t]} - U^{nd}_{d[t]} \right] + \frac{9 \sqrt{\pi \rho^n \mu}}{d^{nd}_d \rho_d} \Delta\left[U^{nc}_{[t]} - U^{nd}_{d[t]} \right] \sqrt{\Delta t} \qquad (28)$$

This procedure carries out statistically because of the stochastical distribution of velocities of both phases. It influencs not only the form of the hybrid pdf but also the evolution of the hybrid pdf.

SIMULATION RESULTS

The Monte-Carlo simulation is carried out for turbulent dispersed flow with and without chemical reactions: a particle laden round jet and a dustexplosion in a vessel.

I. particle laden round jet

The initial and boundary conditions are the same from the Hardalupas´s experimental work (Hardalupas, Taylor and Whitelaw, 1989). In Fig. 1 and Fig. 2 the mean centreline velocitiy distribution in x direction (axial direction) is shown. The results of the Monte Carlo simulation are compared with the experimental data. Here is a the mass loading ratio $\{\gamma = \dot{m}_d/\dot{m}_c\}$. The glass bead diameter is 40 µm in Fig. 1 and 80 µm in Fig. 2 The mean centreline velocity decreases with increasing mass loading ratio. In Fig. 2 the mean centreline velocity of the carrier phase is carried. It is evident that the experimental data represent the mean values in some kind of way. Fig. 2 shows that the interactions between the both phases are significant. The velocities of carrier phase fall off stronger then that of dispersed phase. It is based on the fact that the dispersed phase diminishes slowly due to the inertia.

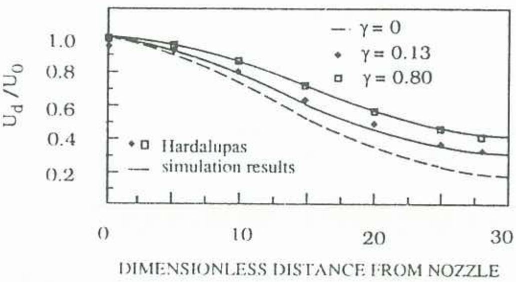

Fig. 1: The axial mean centrelinie velocity of dispersed phase (d_d = 40 µm)

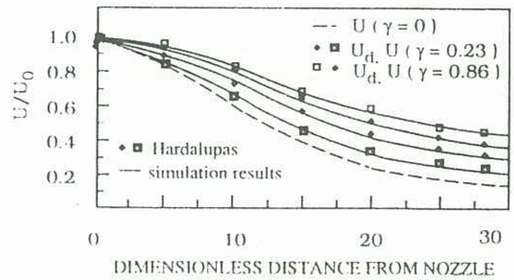

Fig. 2: The axial mean centrelinie velocity of carrier and dispersed phase (d_d = 80 µm)

II dust explosion in a vessel

In the Fig. 3 the simulation result for a dust explosion in a vessel is illustrated. It should be noted that the turbulence plays an important role on the dust explosion process. For a high turbulence intensity (high fluctuations in velocity) the dust flame might be strongly accelerated so that the maximum of explosion pressure is higher than that with a lower turbulence intensity. The simulation results are compared with the experimental data of Kauffman, Srinath et. al. 1984

Fig. 4 shows the effect of turbulence intensity and dust concentration on the maximum rate of pressure rise. It is to observe that the high turbulence intensity leads to increased rates of combustion and therefore the rate of pressure rise.

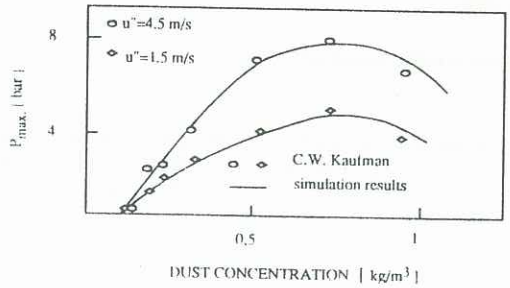

Fig. 3: Effect of turbulence intensity and dust concentration on P_{max}

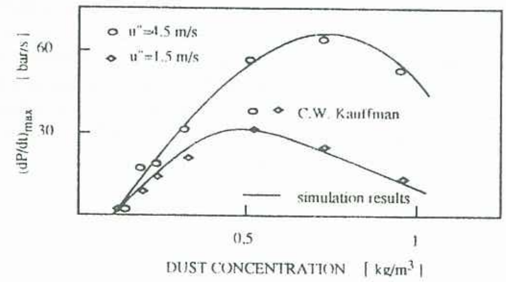

Fig. 4: Effect of turbulence intensity and dust concentration on $(dP/dt)_{max}$

5. CONCLUDING REMARKS

A combined Monte-Carlo method is used for solving the hybrid pdf transport equation because the conventional finite difference algorithm is not suitable for the solution of this kind of transport equations. The great benedict of this indirect Monte-Carlo simulation is that the expenditure of computer capacity groves linear with the number of the variables, whiles that of the conventional finite difference methods increases expotentially. It is hence better suitable for the complicated calculations with many variables.

Particle interaction models are introduced for simulating the turbulent effects between the both phases in turbulent dispersed flow. The nimerical simulation is carried out for turbulent flow with or without chemical reactions. The simulation results agree well with the experimental data.

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