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DEVELOPING MULTIPHASE AND REACTING TURBULENCE MODELS

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ABSTRACT

To simulate turbulent dispersed multiphase flows and combustion using two-fluid approaches, second-order moment two-phase turbulence models and second-order turbulence-chemistry models were proposed by the present author. These models are used to simulate turbulent gas-particle flows, bubble-liquid flows, turbulent diffusion combustion, turbulent premixed combustion and NOx formation. The development of these models and their application are reported in this paper

Key Words: multiphase flows, combustion, modeling

NOMENCLATURE

B Pre-exponential factor
c Empirical constants
D Diffusion term
E Activation energy
G Source term
k Turbulent kinetic energy/ Subgrid scale kinetic energy
k Reaction-rate coefficient
N Time-averaged particle number density
n Number density fluctuation
P Production term
p Pressure
R Correlation term/ Universal gas constant
T Temperature
t Time
V Time-averaged velocity
v Fluctuation velocity
w Reaction rate
Y Mass fraction

Greek Alphabets

α Volume fraction
β Inverse relaxation time
Γ Transport coefficients
δ Kronic-Delta unit tensor
Δ Filtered space scale
ε Dissipation term
μ Dynamic viscosity
ν Kinematic viscosity
Π Pressure-strain term
σ Prandtl number
Θ Particle pseudo-temperature
ρ Density
τ Stress/characteristic time

Subscripts-

c Chemical reaction
e Effective
i,j,k,l Coordinates directions
g Gas
l Laminar
p Particle
pg Two-phase correlation
r Relaxation
s/sgs Subgrid scale
T Turbulent

INTRODUCTION

Dispersed multiphase flows, including gas-particle/droplet flows or liquid-particle/bubble flows, are widely encountered in engineering facilities. It is well known that for simulating dispersed multiphase flows there are two approaches to treat the dispersed phase: trajectory or Lagrangian approach and pseudo-fluid approach. Hence we have Eulerian-Lagrangian (E-L) simulation and Eulerian-Eulerian (E-E) simulation. The latter is frequently called two-fluid modeling. Many engineering applications, including the commercial computer codes, adopt E-L models, but E-E models have their specific features. The advantage of the two-fluid modeling is that the algorithm developed for the fluid phase can be easily modified for the dispersed phase. Also the storage and computational time are not as excessive as it is for the trajectory models. The key problem of two-fluid modeling is the closure models of particle turbulence (particle turbulent fluctuation), leading to particle diffusion/dispersion. Early closure models for the particle turbulence are based on the idea of Hinze-Tchen's particle-tracking-fluid theory of particle fluctuation, originally proposed by Tchen (1947), and finally developed by Hinze (1975). According to Hinze-Tchen's model, particle fluctuation should be always weaker than the fluid fluctuation and the larger the particle size, the weaker the particle fluctuation. Hence larger particles should diffuse slower than smaller particles. However, in the experiments of enclosed gas-particle jets it was found that larger particles diffuse faster than smaller particles, and the particle RMS fluctuation velocity is larger than the gas RMS fluctuation velocity in enclosed gas-particle jets. Therefore, a transport equation theory of particle turbulence was proposed by the author, and a k-ε-kp two-phase turbulence model against the k-ε-Ap model was proposed and used to simulate a gas-particle jet. Subsequently, for anisotropic gas-particle flows, a unified second-order moment (USM) or two-phase Reynolds stress equation model was proposed by the author.

For simulating gas and two-phase (pulverized-coal-air or liquid-spray-air) combustion and NOx formation the turbulence-chemistry model is of vital importance. Most investigators and commercial software developers adopt the eddy break-up (EBU) and presumed PDF models. Experimental validation indicates that these models frequently give the prediction results not in agreement

with experiments. On the other hand, the more advanced PDF equation model requires very large computation cost and is difficult to be used in practical large-size furnaces. The laminar-flamelet and conditional moment closure models may be encouraging, but it still needs to solve many problems in the present stage of development before its application in engineering. In recent years, a second-order moment (SOM) turbulence-chemistry model is proposed by the present author and is used for both RANS and large-eddy simulation (LES) of turbulent combustion. In RANS modeling of swirling diffusion combustion, experimental validation shows that the SOM model is much better than the EBU and presumed PDF models, and its computation requirement is not much larger than the EBU and presumed PDF models. The SOM-LES modeling statistical results are even better than the RANS-SOM results. In this paper we will briefly summarize these research results.

THE USM AND k-ε-kp TWO-PHASE TURBULENCE MODELS

The particle turbulent fluctuation in dilute gas-particle flows is a dominant factor leading to particle dispersion. In the framework of two-fluid models, Tchen (1947) first considered the single-particle fluctuating motion in a fluid eddy, and afterwards Hinze (1975) used the Taylor's statistical theory of turbulence to obtain the Hinze-Tchen's model for the ratio of the particle viscosity over the gas viscosity as

$$\nu_p / \nu_f = (k_p / k_f)^2 = (1 + \tau_{r1} / \tau_T)^{-1} \qquad (1)$$

where $\tau_{r1} = \rho_s d_p^2 / (18\mu), \quad \tau_T = k / \varepsilon$

ν is the kinematic viscosity, D is the diffusion coefficient, k is the turbulent kinetic energy, τ_{r1} is the Stokes' particle relaxation time, τ_T is the gas turbulence time scale, ρ_s is particle material density, μ is gas dynamic viscosity and ε is the dissipation rate of gas turbulent kinetic energy. The subscripts p and f denote particle and fluid respectively. This model can simply be denoted as an "Ap model"(algebraic particle turbulence model). It is used together with the gas turbulence k-ε model, constituting a k-ε-Ap two-phase turbulence model, and even nowadays is widely adopted as particle dispersion models in two-fluid models in many commercial codes. As above indicated, according to Eq.(1), the particle fluctuation should be always smaller than the gas fluctuation and the larger the particle size, the smaller the particle fluctuation. However, in contrast to what predicted by the Ap model, the LDV and PDPA measurements show that the particle turbulence intensity is larger than the gas one in the whole flow field of confined gas-particle jets and in the reverse flow zones of recirculating and swirling gas-particle flows, and the particle turbulence intensity increases with the increase of the particle size in a certain size range.

Based on the concept of particle turbulence transport, starting from two-phase instantaneous momentum equations, using Reynolds expansion and time averaging, an energy equation model (kp model) of particle turbulence was derived and closed (Zhou & Huang, 1987; Zhou & Huang, 1990) and subsequently a two-phase Reynolds stress transport equation model, i.e. a time-averaged unified second-order moment (USM) two-phase turbulence model was proposed (Zhou & Soo, 1991; Zhou, Liao & Chen, 1994). The gas and particle Reynolds stress equations in their closed form are obtained as

$$\frac{\partial}{\partial t}(\rho\overline{v_i v_j}) + \frac{\partial}{\partial x_k}(\rho V_k \overline{v_i v_j}) = D_{ij} + P_{ij} + G_{p_{ij}} + \Pi_{ij} - \varepsilon_{ij} \qquad (2)$$

$$\frac{\partial}{\partial t}(N_p\overline{v_{pi} v_{pj}}) + \frac{\partial}{\partial x_k}(N_p V_{pk}\overline{v_{pi} v_{pj}}) = D_{p,ij} + P_{p,ij} + \varepsilon_{p,ij} \qquad (3)$$

where D_{ij}, P_{ij}, Π_{ij}, ε_{ij} are terms having the same meanings and are closed using the same methods as those well known in single-phase fluid Reynolds stress equations. The new source term for two-phase flows

$$G_{p,ij} = \sum_p \frac{\rho_p}{\tau_{rp}}(\overline{v_{pi} v_j} + \overline{v_{pj} v_i} - 2\overline{v_i v_j})$$

is a phase interaction term expressing the fluid Reynolds stress production/destruction due to fluid-particle interaction. The transport equation of dissipation rate of fluid turbulent kinetic energy for two-phase flows is:

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_k}(\rho V_k \varepsilon) = \frac{\partial}{\partial x}(c_\varepsilon \frac{k}{\varepsilon}\overline{v_k v_l}\frac{\partial \varepsilon}{\partial x_l}) + \frac{\varepsilon}{k}[c_{\varepsilon 1}(G + G_p) - c_{\varepsilon 2}\rho\varepsilon] \qquad (4)$$

where the new source term is

$$G_p = \sum_p \frac{\rho_p}{\tau_{rp}}(\overline{v_{pi} v_i} - \overline{v_i v_i}).$$

For a closed system, beside Eqs. (2), (3) and (4), the transport equations of $\overline{n_p v_{pi}}$, $\overline{n_p v_{pj}}$, $\overline{n_p n_p}, \overline{v_{pi} v_j}, \overline{v_{pj} v_i}$ also should be used. For example, the transport equations of $\overline{v_{pi} v_j}$ and particle turbulent kinetic energy are derived based on the fluid and particle momentum equations and closed as:

$$\frac{\partial}{\partial t}(\overline{v_{pi} v_j}) + (V_k + V_{pk})\frac{\partial}{\partial x_k}(\overline{v_{pi} v_j}) = \frac{\partial}{\partial x_k}[(\nu_e + \nu_p)\frac{\partial}{\partial x_k}(\overline{v_{pi} v_j})] + \frac{1}{\rho\tau_{rp}}[\rho\overline{v_{pi} v_{pj}} + \rho\overline{v_i v_j} - (\rho + \rho_p)\overline{v_{pi} v_j}] - (\overline{v_{pk} v_j}\frac{\partial V_{pi}}{\partial x_k} + \overline{v_k v_{pi}}\frac{\partial V_j}{\partial x_k}) - \frac{\varepsilon}{k}\overline{v_{pi} v_i}\delta_{ij} \qquad (5)$$

$$\frac{\partial}{\partial t}(N_p k_p)+\frac{\partial}{\partial x_k}(N_p V_{pk} k_p)=$$
$$\frac{\partial}{\partial x_k}(N_p c_p^s \frac{k_p}{\varepsilon_p}\overline{v_{pk}v_{pl}}\frac{\partial k_p}{\partial x_l})+P_p-N_p\varepsilon_p \quad (6)$$

where the last term on the right-hand side of Eq.(5) is closed by assuming that the dissipation of two-phase velocity correlation is proportional to the dissipation rate of the fluid turbulent kinetic energy.
and

$$\varepsilon_p=-\frac{1}{\tau_{rp}}[\overline{v_{pi}v_i}-\overline{v_{pi}v_{pi}}+\frac{1}{N_p}(V_i-V_{pi})\overline{n_p v_{pi}}]$$

Equations (2)-(6) constitute the unified second-order moment two-phase turbulence model. It is found that the k-ε-kp model is a reduced form of the USM model in case of nearly isotropic turbulent flows, which consists of the following expressions and equations

$$\overline{v_i v_j}=\frac{2}{3}k\delta_{ij}-\nu_t(\frac{\partial V_i}{\partial x_j}+\frac{\partial V_j}{\partial x_i});$$

$$\overline{v_{pi}v_{pj}}=\frac{2}{3}k_p\delta_{ij}-\nu_p(\frac{\partial V_{pi}}{\partial x_j}+\frac{\partial V_{pj}}{\partial x_i}) \quad (7)$$

$$\overline{n_p v_{pi}}=-\frac{\nu_p}{\sigma_p}\frac{\partial N_p}{\partial x_i}\quad,\quad \overline{n_p v_{pj}}=-\frac{\nu_p}{\sigma_p}\frac{\partial N_p}{\partial x_j} \quad (8)$$

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_j}(\rho V_j k)=\frac{\partial}{\partial x_j}(\frac{\mu_e}{\sigma_k}\frac{\partial k}{\partial x_j}) \quad (9)$$
$$+G+G_p-\rho\varepsilon$$

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\frac{\partial}{\partial x_j}(\rho V_j\varepsilon)=\frac{\partial}{\partial x_j}(\frac{\mu_e}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}) \quad (10)$$
$$+\frac{\varepsilon}{k}[c_{\varepsilon 1}(G+G_p)-c_{\varepsilon 2}\rho\varepsilon]$$

$$\frac{\partial(N_p k_p)}{\partial t}+\frac{\partial}{\partial x_k}(N_p k_p v_{pk})= \quad (11)$$
$$\frac{\partial}{\partial x_k}(\frac{N_p\nu_p}{\sigma_p}\frac{\partial k_p}{\partial x_k})+P_p-N_p\varepsilon_p$$

$$\frac{\partial}{\partial t}(k_{pg})+(V_k+V_{pk})\frac{\partial}{\partial x_k}(k_{pg})=$$
$$\frac{\partial}{\partial x_k}\left(\left(c_s\frac{k^2}{\varepsilon}+c_{kp}\frac{k_p^2}{\varepsilon_p}\right)\frac{\partial k_{pg}}{\partial x_k}\right)$$
$$+\frac{1}{\rho\tau_{rp}}(\rho_p k_p+\rho k-(\rho+\rho_p)k_{pg})$$
$$-\frac{1}{2}\left(\overline{v_i v_{pk}}\frac{\partial v_{pi}}{\partial x_k}+\overline{v_{pi}v_k}\frac{\partial v_i}{\partial x_k}\right)-\frac{1}{\tau_e}k_{pg} \quad (12)$$

Figure1 shows the simulation results of particle number density in wind-sand flows behind an obstacle, reported by Laslandes and Sacre (1998), using both k-ε-kp and k-ε-Ap models and their comparison with experiments. It is seen that the k-ε-kp model is much better than the k-ε-Ap model in predicting the particle dispersion.

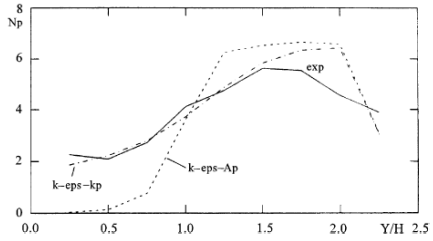

Figure 1 Particle Number Density

Alternatuvely, a mass-weighed averaged USM model was derived and closed (Yu, Zhou et al., 2003). In the time-averaged USM model the transport equations, relating to particle number density fluctuation, such as equations of particle diffusion mass fluxes and mean square values of particle number density fluctuation are introduced. So, the model includes too many equations and is rather complex. It will be more reasonable, if we use the mass-weighed averaging, like the Favre averaging for single-phase compressible turbulent flows, instead of time averaging. Moreover, the mass-weighed averaging will reduce the number of equations, because there is no number density fluctuation in the explicit form. The mass-weighed averaging for turbulent two-phase flows is an extension of the Favre averaging for single-phase compressible flows to two-phase flows. Both USM and MUSM models are used (Zhou & Chen, 2001;Yu, Zhou et al., 2003) to simulate swirling gas-particle flows with a swirl number of 0.47, measured by Sommerfeld and Qiu (1991) using PDPA. Figures 2 and 3 give the predicted particle tangential time-averaged and RMS fluctuating velocities respectively. It is seen that both models give the results in agreement with experimental results and there is only slight difference between the MUSM and USM predictions, but the MUSM model can save computational time than the USM model due to solving less equations.

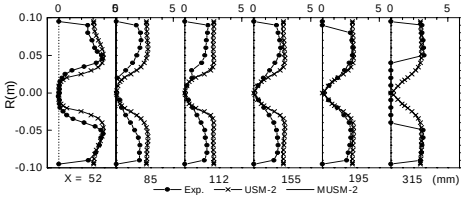

Figure 2 Particle Tangential Velocity

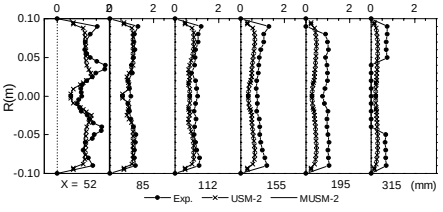

Figure 3 Particle Tangential Fluctuation Velocity

For simulating complex turbulent bubble-liquid-solid flows, a second-order moment three-phase turbulence model is proposed (Zhou, Yang et al., 2002). The derivation procedure is similar to that used for single-phase flows. This model was used to simulate bubble-liquid flows in a bubble column measured at the Ohio State University. Figures 4 and 5 are simulated bubble and liquid normal Reynolds stress in vertical direction respectively. It is seen that in the case studied the prediction results are in very good agreement with the PIV measurement results, and the bubble turbulence is much stronger than the liquid turbulence. In other words, bubbles induce liquid turbulence.

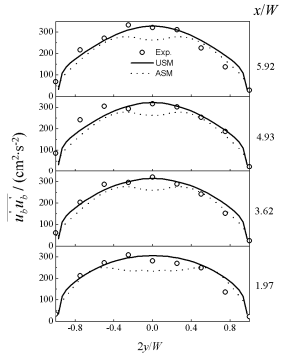

Figure 4 The Bubble Normal Reynolds Stress in Vertical Direction

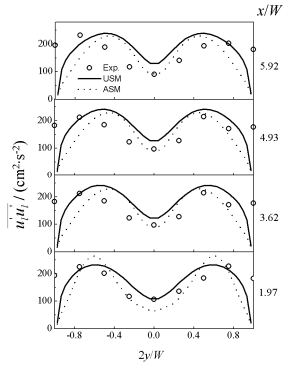

Figure 5 The Liquid Normal Reynolds Stress in Vertical Direction

THE USM-Θ TWO-PHASE TURBULENCE MODEL FOR DENSE GAS-PARTICLE FLOWS

Dense gas-particle flows are encountered in fluidized combustors and pneumatic conveying. In dense gas-particle flows there are both large-scale particle fluctuations due to particle turbulence and small-scale particle fluctuations due to inter-particle collisions. A USM-Θ two-phase turbulence model for dense gas-particle flows was proposed (Yu & Zhou et al., 2005). In this model the gas turbulence and particle large-scale fluctuation are predicted using the USM two-phase turbulence model, and the particle small-scale fluctuation due to inter-particle collisions is predicted using the particle pseudo-temperature equation--Θ equation, given by Gidaspow's kinetic theory (Gidaspow, 1994). This is not a simple superposition, since there are interaction terms in the particle Reynolds stress equations and the Θ equation. Some of the closed USM-Θ model equations are:

The gas Reynolds stress equation

$$\frac{\partial\left(\overline{\alpha_g}\rho_{gm}\overline{u_{gi}u_{gj}}\right)}{\partial t}+\frac{\partial\left(\overline{\alpha_g}\rho_{gm}U_{gk}\overline{u_{gi}u_{gj}}\right)}{\partial x_k}$$
$$=D_{g,ij}+P_{g,ij}+\Pi_{g,ij}-\varepsilon_{g,ij}+G_{g,gp,ij} \quad (13)$$
where $G_{g,gp,ij}=\beta\left(\overline{u_{pi}u_{gj}}+\overline{u_{gi}u_{pj}}-2\overline{u_{gi}u_{gj}}\right)$

The particle Reynolds stress equation

$$\frac{\partial\left(\overline{\alpha_p}\rho_{pm}\overline{u_{pi}u_{pj}}\right)}{\partial t}+\frac{\partial\left(\overline{\alpha_p}\rho_{pm}U_{pk}\overline{u_{pi}u_{pj}}\right)}{\partial x_k}$$
$$=D_{p,ij}+P_{p,ij}+\Pi_{p,ij}-\varepsilon_{p,ij}+G_{p,gp,ij} \quad (14)$$
where $G_{p,gp,ij}=\beta\left(\overline{u_{pi}u_{gj}}+\overline{u_{pj}u_{gi}}-2\overline{u_{pi}u_{pj}}\right)$

The equations of dissipation rate of turbulent kinetic energy for gas and particle phases:

$$\frac{\partial\left(\overline{\alpha_g}\rho_{gm}\varepsilon_g\right)}{\partial t}+\frac{\partial\left(\overline{\alpha_g}\rho_{gm}U_{gk}\varepsilon_g\right)}{\partial x_k}$$
$$=\frac{\partial}{\partial x_k}\left(C_g\overline{\alpha_g}\rho_{gm}\frac{k_g}{\varepsilon_g}\overline{u_{gk}u_{gl}}\frac{\partial\varepsilon_g}{\partial x_l}\right)$$
$$+\frac{\varepsilon_g}{k_g}\left[c_{\varepsilon 1}\left(P_g+G_{g,gp}\right)-c_{\varepsilon 2}\overline{\alpha_g}\rho_{gm}\varepsilon_g\right] \quad (15)$$
where $G_{g,gp}=2\beta\left(k_{gp}-k_g\right),\ c_{\varepsilon 3}=1.8$

$$\frac{\partial\left(\overline{\alpha_p}\rho_{pm}\varepsilon_p\right)}{\partial t}+\frac{\partial\left(\overline{\alpha_p}\rho_{pm}U_{pk}\varepsilon_p\right)}{\partial x_k}$$
$$=\frac{\partial}{\partial x_k}\left(\overline{\alpha_p}\rho_{pm}C_p^d\frac{k_p}{\varepsilon_p}\overline{u_{pk}u_{pl}}\frac{\partial\varepsilon_p}{\partial x_l}\right)$$
$$+\frac{\varepsilon_p}{k_p}\left[C_{\varepsilon p,1}\left(P_p+G_{p,gp}\right)-C_{\varepsilon p,2}\overline{\alpha_p}\rho_{pm}\varepsilon_p\right] \quad (16)$$

where β is the inverse relaxation time,
$G_{p,gp}=2\beta\left(k_{pg}-k_p\right)$

The two-phase velocity correlation equation:

$$\frac{\partial\overline{u_{pi}u_{gj}}}{\partial t}+\left(U_{gk}+U_{pk}\right)\frac{\partial\overline{u_{pi}u_{gj}}}{\partial x_k}$$
$$=D_{g,p,ij}+P_{g,p,ij}+\Pi_{g,p,ij}-\varepsilon_{g,p,ij}+T_{g,p,ij} \quad (17)$$

The particle pseudo-temperature transport equation:

$$\frac{3}{2}\left[\frac{\partial\left(\overline{\alpha_p}\rho_{pm}\Theta\right)}{\partial t}+\frac{\partial\left(\overline{\alpha_p}\rho_{pm}U_{pk}\widetilde{u}_{pk}\Theta\right)}{\partial x_k}\right]$$

$$= -\frac{\partial}{\partial x_k}\left(\frac{3}{2}\overline{\alpha_p \rho_{pm} u_{pk}\theta} + \Gamma_\Theta \frac{\partial \Theta}{\partial x_k}\right)$$
$$+ \mu_p\left(\frac{\partial U_{pk}}{\partial x_i} + \frac{\partial U_{pi}}{\partial x_k}\right)\frac{\partial U_{pi}}{\partial x_k} + \mu_p \varepsilon_p$$
$$- P_p \frac{\partial U_{pl}}{\partial x_l} + \left(\xi_p - \frac{2}{3}\mu_p\right)\left(\frac{\partial U_{pl}}{\partial x_l}\right)^2 - \overline{\gamma} \quad (18)$$

where the notations in Eq,(18) are the same as that given by Gidaspow. The interaction between the large-scale and small-scale particle fluctuations is the third term on the right-hand-side of Eq.(18), expressing the effect of the dissipation rate of particle turbulent kinetic energy on the particle pseudo-temperature. Simulation results for dense gas-particle flows in a downer measured by Wang, Bai and Jin (1992) indicate that for predicting the particle volume fraction (Fig.6) and particle velocity (Fig.7) the USM-Θ model is much better than the DSM-Θ model, not accounting for particle turbulence, the USM model, not accounting for inter-particle collision and the k-ε-k_p-Θ model, not accounting for the anisotropy of turbulence. Figure 8 shows the predicted particle horizontal RMS fluctuation velocity for horizontal gas-particle pipe flows measured By Kussin and Sommerfeld (2002). It is seen that the USM-Θ model can more reasonably predict particle RMS fluctuation velocities than other models.

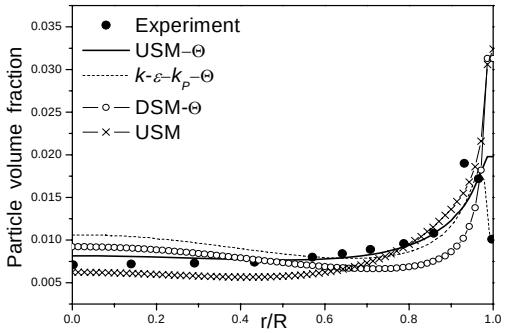

Figure 6 Particle Volume Fraction

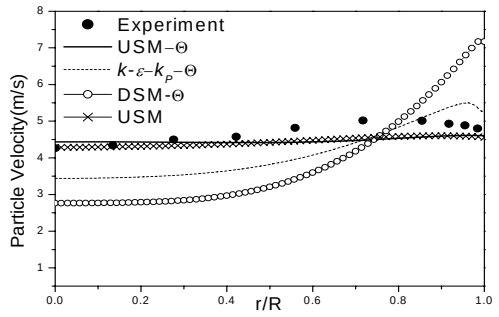

Figure 7 Particle Time-Averaged Velocity

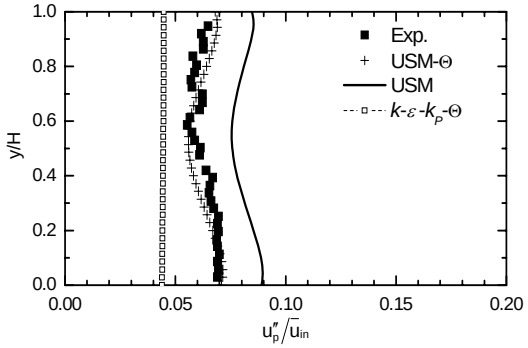

Figure 8 Particle Horizontal RMS Fluctuation Velocity

USM AND k-kp TWO-PHASE SUBGRID-SCALE STRESS MODELS FOR LARGE-EDDY SIMULATION

Most Eulerian-Lagrangian and Eulerian-Eulerian (two-fluid) large-eddy simulation (LES) of gas-particle flows are based on single-phase subgrid scale (SGS) stress models. The interaction between two-phase SGS stresses is not fully taken into account. Two kinds of two-phase SGS stress models are proposed by the present author for two-fluid LES of gas-particle flows: a unified second-order moment (USM) two-phase SGS stress model and a two-phase SGS energy (k-kp) stress model, in which the interaction between two-phase SGS stresses is fully taken into account. For the USM SGS model, the gas and particle SGS stresses are given by :

$$\tau_{gs,ij} = -\rho_g R_{gs,ij} = -\rho_g(\overline{u_{gi}u_{gj}} - \overline{u_{gi}}\,\overline{u_{gj}}) \quad (19)$$

$$\tau_{ps,ij} = -\rho_p R_{ps.ij} = -\rho_p(\overline{u_{pi}u_{pj}} - \overline{u_{pi}}\,\overline{u_{pj}}) \quad (20)$$

$$\frac{\partial}{\partial t}(\alpha_g \rho_g R_{gs,ij}) + \frac{\partial}{\partial x_k}(\alpha_g \rho_g \overline{u}_{gk} R_{gs,ij}) =$$
$$D_g^{sgs} + P_g^{sgs} + G_{pg}^{sgs} + \Pi_g^{sgs} - \varepsilon_g^{sgs} \quad (21)$$

$$\frac{\partial}{\partial t}(\alpha_p \rho_p R_{ps,ij}) + \frac{\partial}{\partial x_k}(\alpha_p \rho_p \overline{u}_{pk} R_{ps,ij}) =$$
$$D_p^{sgs} + P_p^{sgs} + \varepsilon_p^{sgs} \quad (22)$$

For the k-kp SGS model they are given by:

$$\tau_{gs,ij} = -2\rho_g \cdot k_{gs,ij} =$$
$$-2\rho_g \cdot \frac{1}{2}\left(\overline{u_{gi}u_{gj}} - \overline{u_{gi}}\,\overline{u_{gj}}\right) \quad (23)$$

$$\tau_{ps,ij} = -2\rho_p \cdot k_{ps,ij} =$$
$$-2\rho_p \cdot \frac{1}{2}\left(\overline{v_{pi}v_{pj}} - \overline{v_{pi}}\,\overline{v_{pj}}\right) \quad (24)$$

$$\frac{\partial}{\partial t}\left(\rho_g k_{gs,ij}\right) + \frac{\partial}{\partial x_j}\left(\rho_g \overline{v_{gj}} k_{gs,ij}\right) =$$
$$\frac{\partial}{\partial x_j}\left(\frac{\mu_e}{\sigma_k}\frac{\partial k_{gs,ij}}{\partial x_j}\right) + G_{gk}^{sgs} + G_{pg,ij}^{sgs} - \rho_g \varepsilon_g \quad (25)$$

$$\frac{\partial}{\partial t}\left(\rho_p k_{ps,ij}\right)+\frac{\partial}{\partial x_j}\left(\rho_p \overline{v_{pj}} k_{ps,ij}\right)=$$
$$\frac{\partial}{\partial x_j}\left(\frac{\mu_p}{\sigma_p}\frac{\partial k_{ps,ij}}{\partial x_j}\right)+G_{pk}^{sgs}+\rho_p\varepsilon_p \quad (26)$$

The predicted particle RMS axial and tangential fluctuation velocities for swirling gas-particle flows measured by Sommerfeld and Qiu (1991) using the LES USM SGS model (Figs.9, 10) and for sudden-expansion gas-particle flows measured by Xu and Zhou (1999) using the LES k-kp SGS model (Fig.11) are better than the RANS modeling results using the USM two-phase turbuence model.

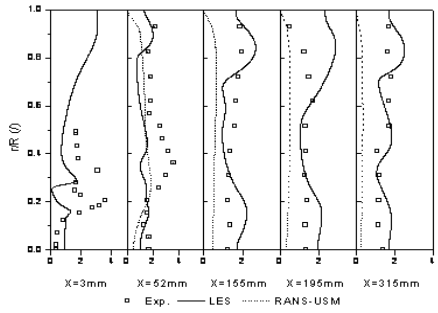

Figure 9 Particle RMS Axial Fluctuation Velocity

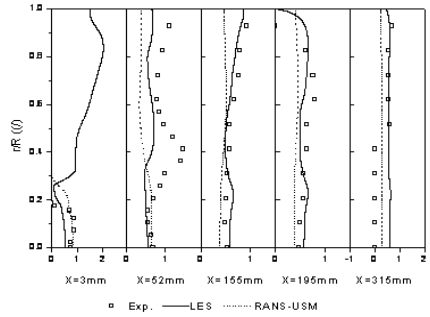

Figure 10 Particle RMS Tangential Fluctuation Velocity

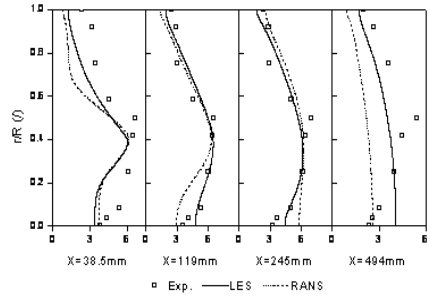

Figure 11 Particle RMS Axial Fluctuation Velocity

SECOND-ORDER MOMENT TURBULENCE-CHEMISTRY MODEL

To develop a reasonable and economical turbulence-chemistry model, a second-order moment (SOM) turbulence-chemistry model was proposed (Zhou, Qiao et al., 2002). For a two-component second-order reaction (global or elementary) the Arrhenius form of the instantaneous reaction rate can be given as

$$w_s = B\rho^2 Y_1 Y_2 \exp(-E/RT) \quad (27)$$

where B is the pre-exponential factor, Y and T are instantaneous species mass fraction and temperature respectively, E is the activation energy，R is the universal gas constant. By taking Reynolds expansion and time averaging, neglecting the third-order correlation, the time-averaged reaction rate is obtained as

$$\overline{w_s} = B\rho^2[(\overline{Y_1}\overline{Y_2}+\overline{Y_1'Y_2'})\bar{k}+ \overline{Y_1}\overline{k'Y_2'}+\overline{Y_1}\overline{k'Y_1'}] \quad (28)$$

where $k=\exp(-E/RT)$ is the reaction rate coefficient, a highly non-linear fuction of temperature, causing serious difficulty in turbulent combustion modeling. $\bar{k}=\int \exp(-E/RT)p(T)dT$ is the time-averaged value of k, p(T) is the probability density distribution function of temperature. The generalized form of the closed transport equations of the second-order moments can be obtained as

$$\frac{\partial}{\partial t}\left(\rho\overline{\phi'\psi'}\right)+\frac{\partial}{\partial x_j}\left(\rho v_j\overline{\phi'\psi'}\right)=$$
$$\frac{\partial}{\partial x_j}\left(\frac{\mu_e}{\sigma_g}\frac{\partial\overline{\phi'\psi'}}{\partial x_j}\right)+c_{g1}\mu_T\left(\frac{\partial\phi}{\partial x_j}\right)\left(\frac{\partial\psi}{\partial x_j}\right) \quad (29)$$
$$-c_{g2}\rho\left(\frac{a}{\tau_c}+\frac{b}{\tau_T}\right)\overline{\phi'\psi'}$$

where ϕ and ψ denote the mass fractions Y_1, Y_2 or the reaction-rate coefficient k, and c_{g1}, c_{g2} are empirical constants, τ_c, τ_T denote the reaction time scale and turbulence time scale, defined as

$$\tau_T = k/\varepsilon;\ ,$$
$$\tau_c = \left[B\rho\left(\overline{Y_2}+\beta\overline{Y_1}\right)\exp\left(-\frac{E}{R\bar{T}}\right)\right]^{-1}.$$

The SOM turbulence-chemistry model was used in Reynolds averaged N-S (RANS) modeling of methane-air swirling diffusion combustion (Zhou, Wang et al., 2003) and large-eddy simulation (LES) of methane-air swirling diffusion combustion (Hu, Zhou et al., 2006), methane-air jet combustion (Wang, Zhou et al., 2006) and propane-air premixed combustion (Wang, Zhou et al., 2008). For swirling diffusion combustion the RANS modeling predicted and measured temperature profiles are shown in Fig.12. Clearly, in most regions the SOM model predictions are in good agreement with the experimental results, while the predicted temperature profiles using the widely adopted EBU-Arrhenius (E-A) model show noticeable qualitative difference from the experimental results, particularly in the upstream region. The E-A model over-predicts the temperature. Since the E-A model exaggerates the turbulence effect and neglects or underestimates the kinetic effect; the reaction rate is over-predicted where the turbulent kinetic energy is high.

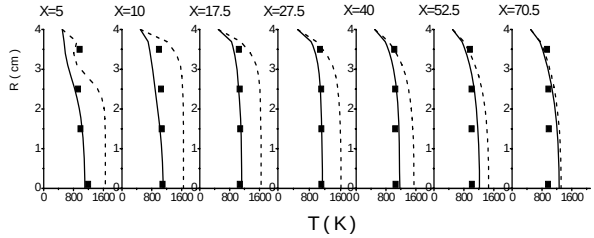

Figure 12 Temperature (■EXP —— SOM --- E-A)

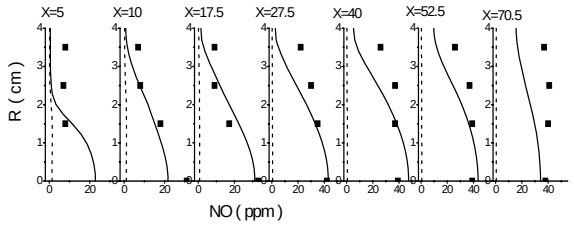

Figure 13 Thermal NO Concentration
(■ EXP —— SOM ---- E-A & PDF)

Figure 13 gives the RANS modeling predicted thermal NO profiles using the SOM model and the E-A+ simplified PDF model and their comparison with the measurement results. Generally speaking, the E-A+simplified PDF model seriously under-predicts the thermal NO formation and the predicted NO concentration is nearly one order of magnitude lower than that measured. As above indicated the simplified PDF model uses a product of two PDF's to approximate the joint PDF, hence under-predicts the reaction rate. Comparatively, the predictions using the SOM model are much better and are near to the experimental results. Figure 14 gives the LES obtained time-averaged temperature using both LES-SOM model (the algebraic SOM model) and LES-EBU model and also RANS-SOM modeling results in comparison with experimental results. It is seen that both LES-SOM and RANS-SOM results are in good agreement with the experimental results, and the LES-SOM results are better than the RANS-SOM results at the cross sections of x=5 and x=10. Obviously, in most regions the LES-SOM model is much better than the LES-EBU model, which remarkably over-predicts the temperature.

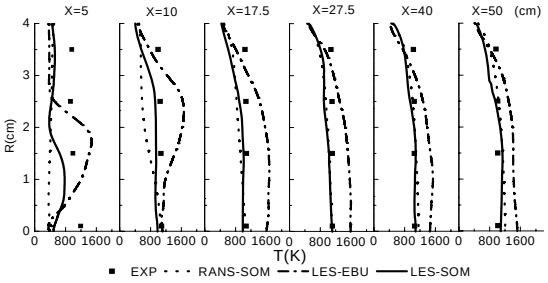

Figure 14 Time-Averaged Temperature

TWO-FLUID MODELING OF TWO-PHASE COMBUSTION

A full two-fluid model of coal combustion was proposed by the author, the time-averaged equations of turbulent reacting gas-particle flows are obtained by taking the decomposition of the instantaneous equations of two phases and then the Reynolds averaging and these equations can be found elsewhere (Zhou et al., 2000). For two-phase turbulence modeling, in case of isotropic turbulent flows, such as nonswirling and weakly swirling flows, a k-ε-kp model is used. For volatile and CO combustion in the comprehensive modeling of coal combustion, originally the conventional EBU-Arrhenius model is used. For radiative heat transfer a six-flux model is used. The NO formed in coal combustion consists of mainly thermal NO and fuel NO. For the reaction kinetics of thermal NO formation, the well-known Zeldovich mechanism is used

N2+O ⟶ NO + N

N+O2 ⟶ NO + O

N+OH ⟶ NO + H

The total reaction rate is determined by

$$W = 8.39\times10^{16}\rho^{1.5}T^{-0.5}Y_{N_2}Y_{O_2}{}^{0.5}$$

$$\times\exp(-564.4\times10^{3}/RT)$$

For the reaction kinetics of fuel NO formation, the DeSoete mechanism is used

HCN+O2 ⟶ NO

HCN+NO ⟶ N2

C+NO ⟶ N2

The special feature is the algebraic second-order moment (ASOM) turbulence-chemistry model for NO formation in turbulent combusting flows. The time-averaged reaction rate is

$$\overline{W_S} = B\rho^2[(\overline{Y_1}\overline{Y_2}+\overline{Y_1'Y_2'})\overline{K}+\overline{Y_1}\overline{K'Y_2'}+\overline{Y_2}\overline{K'Y_1'}]$$

(30)

$$K = \exp(-E/RT)$$

where, $\overline{K}=\int \exp(E/RT)p(T)dT$, *p(T)* is the PDF of temperature. Assuming a top-hat PDF gives

$$\overline{K} = \{\exp[-E/R(T+g_T^{1/2})]+\exp[-E/R(T-g_T^{1/2})]\}$$

$$g_T = \overline{T'^2} \qquad (31)$$

The correlations $\overline{K'Y_1'}$, $\overline{K'Y_2'}$, $\overline{Y_1'Y_2'}$ in Eq.(30) can be determined by the following algebraic expressions

$$\overline{Y_1'Y_2'} = C_1\frac{k^3}{\varepsilon^2}\frac{\partial\overline{Y_1}}{\partial x_j}\frac{\partial\overline{Y_2}}{\partial x_j};$$

$$\overline{K'Y_1'} = C_1\frac{k^3}{\varepsilon^2}\frac{\partial\overline{K}}{\partial x_j}\frac{\partial\overline{Y_1}}{\partial x_j};$$

$$\overline{Y_2'K'} = C_1\frac{k^3}{\varepsilon^2}\frac{\partial\overline{Y_2}}{\partial x_j}\frac{\partial\overline{K}}{\partial x_j} \qquad (32)$$

where k,ε are the turbulent kinetic energy and its dissipation rate.

Simulation of coal combustion and NO formation (Zhou and Zhang, 2003) was carried out in a swirl combustor measured by Abbas et al. (1991). The prediction results for cold flows are compared with the PDPA measurement results and for coal combustion are compared with the coal combustion experimental results.

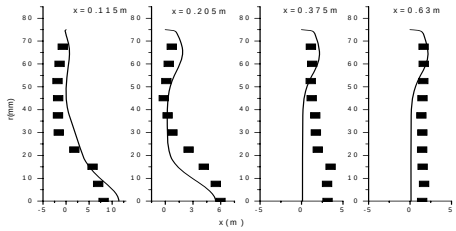

Figure 15 Gas Axial Velocity (—Pred ■ Exp)

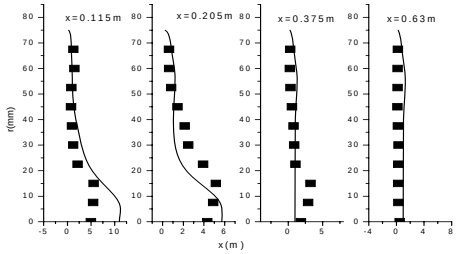

Figure 16 Turbulent Kinetic Energy (—Pred ■ Exp)

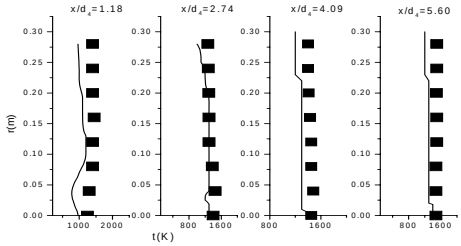

Figure 17 Temperature (— Pred. ■ Exp.)

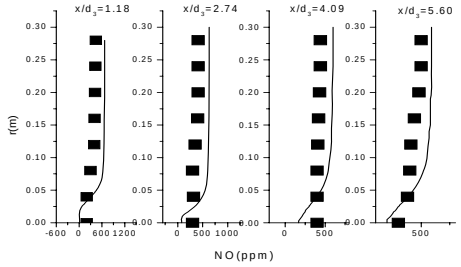

Figure 18 NO Concentration (— Pred. ■ Exp.)

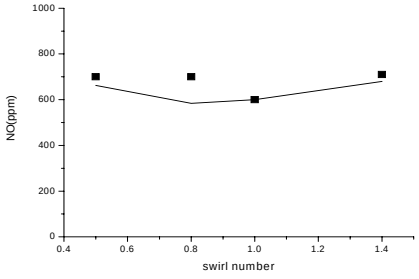

Figure 19 Averaged NO Concentration at the Exit

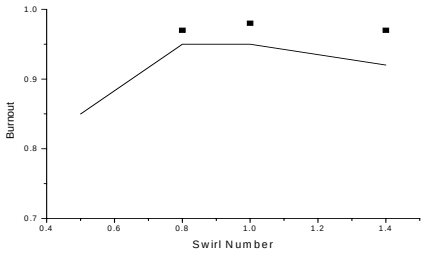

Figure 20 Coal Burn-Out Rate

Figures 15 and 16 show the predicted and measured gas velocity and turbulent kinetic energy for isothermal flows respectively. Figure 17 gives the predicted and measured temperature profiles. Good agreement between predictions and experiments are obtained. Figure 18 shows the predicted NO concentration profiles and their comparison with the experimental results. The agreement is also good. Figures 19 and 20 give the predicted averaged NO concentration at the exit and burnout rate vs. as the swirl number respectively and their comparison with experimental results. Both predictions and experiments show the common tendency: as the swirl number increases the NO concentration at first will decrease and then will increase, while the burnout rate at first will increase and then will decrease. There is a quantitative discrepancy between predictions and experiments. The predicted lowest NO emission and highest burnout rate occur at the swirl number of 0.8, but the measured ones occur at the swirl number of 1.0. This discrepancy may be caused by numerical errors and inaccuracies of the models. The overall NO formation in coal combustion should be determined by the temperature, coal concentration and turbulent fluctuation. With the increase of swirl number from 0.5 to 0.8, the temperature increases not so much, but the coal concentration in the inlet zone increases and the turbulent fluctuation decreases. Therefore, the NO formation decreases.

CONCLUSIONS

(1) For two-fluid modeling of gas-particle and bubble-liquid flows the USM and k-ε-kp two-phase turbulence models can more reasonably predict the particle/bubble turbulence than the traditional k-ε-Ap model.

(2) In dense gas-particle flows both particle large-scale fluctuation due to anisotropic particle turbulence and particle small-scale fluctuation due to inter-particle collision are important to particle dispersion.

(3) The SOM turbulence-chemistry model is much better than the widely used E-A and simplified PDF models, whereas it is much more economic than the PDF equation model

(4) The full two-fluid model of coal combustion together with an algebraic SOM turbulence-chemistry model can well simulate NO formation during coal combustion

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