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Eulerian–Eulerian multi-fluid methods for pulverized coal flames with nongray radiation

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ABSTRACT

A new Favre averaging method based on gas phase density applied to Eulerian–Eulerian simulations of turbulent multiphase reacting flows is proposed. The new Favre averaging method can reproduce turbulent dispersions of mass, momentum, heat and species of solid phases from their averaged transport equations. A new radiation model that can account for nongray gas–solid mixtures is developed for pulverized coal flames. The new models are validated against a pulverized coal ignition flame. Predictions of velocity, temperature and gas major species are found in good agreement with experiments. Pyrometer measurements of temperature are predicted by a radiation transport calculation. It is found that radiation cooling effects can lead to a 500 K temperature decline in solid phases. Radiation also has indirect influence on CO₂ predictions through the slow yet strongly temperature-dependent char reaction rates. The consideration of radiation improves predictions of both temperature and CO₂ concentrations. Effects of devolatilization model and number of phases are also discussed.

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1. Introduction

Pulverized coal combustion is commonly utilized in power boilers for electricity generation. The design of a pulverized coal boiler relies heavily on the understanding of the dynamics of pulverized coal combustion [1]. Numerical simulations are commonly used to predict flames in furnaces and to optimize furnace designs. The accuracy of a model set in a simulation is validated through the comparison of model predictions to experimental measurements. For example, the target flame of this study [2–4] investigated coal ignition processes in a methane pilot. An accurate simulation of coal flames demands a high-fidelity comprehensive approach to multiple physics, which include turbulence, multiphase flow, chemical reactions and heat transfer together with their interactions [1].

The treatment of multiphase flow depends on the target scale of simulation [5]. A multiphase flow model also decides available treatments of other physical processes. For the simulation of a coal–air flame at the laboratory scale, the carrier air flow is commonly modeled as a continuum medium in a Eulerian framework [1]. The dispersed coal particles may be modeled either in a

Lagrangian or Eulerian framework [1]. The former approach tracks discrete particles on a mesh in a Lagrangian fashion, while the latter treats particles as an inter-penetrating continuum governed by Eulerian transport equations. Both approaches have their intrinsic advantages. The Lagrangian approach has been adopted by several investigators [6–11] to investigate the same target flame as in this study. Simulations employing the Eulerian approach are less reported in the literature. The applications of Eulerian–Eulerian two-fluid methods in pulverized coal combustion, as pioneered by Zhou were summarized in [12] and citations therein. The two-fluid methods consider one carrier and one dispersed phase. One of the limitations is that a single dispersed phase cannot resolve the particle size distributions and size-dependent heterogeneous reaction rates. This leads to a multi-fluid approach employed in the current study. In multi-fluid methods, the carrier and dispersed phases do not have to be in kinetic and/or thermal equilibrium. The exchange of momentum, heat and mass may be accounted for through corresponding models. To the best of our knowledge, the target flame has not been simulated to date with any Eulerian–Eulerian multi-fluid method.

In order to obtain the Eulerian transport equations of the dispersed phases, a two step approach is employed [5]. In the first step, the dispersed particles are grouped into phases by their sizes and spatially averaged [13]. In the second step, the spatially averaged Eulerian governing equations are further averaged over

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Nomenclature

Roman symbols

a	stretching factor for full-spectrum k -distributions (–)
d_p	particle diameter (μm)
D_Y	species diffusivity (m^2/s)
f	k -distribution (cm)
G	incident radiation (W/m^2)
g	cumulative k -distribution (–)
I	radiation intensity (W/m^2)
k	reordered absorption coefficient (cm^{-1})
M	total number of solid phases
Nu	Nusselt number (–)
p	pressure (Pa)
p_{O_2}	O_2 partial pressure in the char oxidization model (atm as in the Harmor's model)
Pr	Prandtl number (–)
Nu	Reynolds number (–)
$\hat{s}$	unit vector into a given direction
S	source terms (units depend on equations)
ΔH	heat of reaction (W/m^3)
S_{rad}	radiative heat source (W/m^3)
T	temperature (K)
t	time (s)
u	velocity (m/s)
w	quadrature weight (–)
Y	species mass fraction (–)

Greek symbols

β	extinction coefficient (cm^{-1})
ϵ	wall emittance (–)
ε	volume fraction (–)
η	wavenumber (cm^{-1})

γ	weighted particle convective heat transfer coefficient ($\text{W}/(\text{m}^3 \text{K})$)
κ	absorption coefficient (cm^{-1})
κ	thermal conductivity ($\text{W}/(\text{m K})$)
μ	viscosity ($\text{kg}/(\text{m s})$)
Φ	scattering phase function (–)
ρ	density (kg/m^3)
σ_s	scattering coefficient (cm^{-1})
τ_p	particle response time scale (s)
τ_{ij}	shear stress (N/s^2)

Subscripts

b	black body emission
η	wavenumber
g	gas phase
j	spatial coordinate index
m	dispersed phase index
P	Planck mean

Superscripts

0	reference state for full-spectrum k -distributions
ρ	source term in continuity equation
u	source term in momentum equation
Y	source term in species mass fraction equation

Operators

$\langle \cdot \rangle$	ensemble average
$\langle \cdot \rangle_F$	Favre average
$\bar{\cdot}$	ensemble average
$\tilde{\cdot}$	Favre average

unresolved turbulent scales to obtain Reynolds-averaged transport equations. Ensemble averages for all phases have been adopted in previous studies. However, taking a Favre average is a common practice in gaseous turbulent combustion because it requires fewer modeled terms [14]. The corresponding dispersed phases are usually averaged differently. For example, in [15] a Favre average based on dispersed phase density leads to different types of continuity equations as found from an ensemble average. This may introduce a set of inconsistent equations, for example, missing turbulent dispersion of the dispersed phase in its continuity equations [15].

Radiative heat transfer is an important heat transfer mode in pulverized coal flames due to large amounts of radiatively participating gases and particulates at high temperature [1,16,17]. Traditional treatments employ bulk emissivity and a simple radiative transfer equation (RTE) solver for absorption [17]. A recent comprehensive comparison of different spectral models and RTE solvers revealed that spectral models that can account for nongray gas spectral variations are more important than RTE solvers in gaseous flames with not-so-small optical thickness [18]. The k -distribution methods, which can achieve line-by-line spectral accuracy with much less computational costs, were found to be superior in gaseous flames [16,18]. The k -distribution methods were recently applied to gas–solid mixtures [19]. The new model accounts accurately for nongray gas and solid emission and absorption, in contrast to references [7–9,11], which account for radiation in very primitive fashion.

The current research is built upon the open-source multiphase flow solver Multiphase Flow with Interphase eXchanges (MFIx) [20]. MFIx is a general-purpose CFD packages developed at the

National Energy Technology Laboratory (NETL) for fluid–solid systems with heat transfer and chemical reactions. It utilizes multi-fluid methods to simulate dense fluid–solid reacting flows encountered in fluidized beds. Momentum exchanges in these dense fluid–solid systems are dominated by collisions between solid particles. However, in dilute systems like pulverized coal combustion, momentum exchanges are dominated by gas turbulence and drag forces. Particle collisions are negligible. Therefore, special treatments are required to extend the multi-fluid equations from dense collision-dominated systems to dilute drag-dominated systems.

The purpose of this study comprises two parts. First, a new averaging method for turbulent multiphase reacting flows is proposed. In this new approach, both carrier and dispersed phases are modeled as Eulerian continua. Their governing equations are Favre averaged using the same gas phase bulk density as a weight. This approach offers three advantages: (1) it retains the advantage of Favre averages in gaseous flames that requires fewer terms to be modeled in the carrier phase equations. Turbulence and combustion models studied comprehensively in gaseous combustion can be applied directly without significant changes; (2) turbulent dispersions of volume, temperature and composition, as a result of their correlation with velocity are recovered; and (3) averaged two-way couplings are consistent. With these advantages, a set of consistent averaged equations for the dispersed phases are derived. Secondly, a recently developed radiation model that accounts for the nongray nature of both carrier and dispersed phase is applied. Temperature predictions are compared between experiments and simulations with radiation feedback. The effects of radiation are demonstrated by comparing cases with and without radiation. In particular, solving radiation transport gives a

straightforward interpretation of particle temperature measurements from two-color pyrometers.

In this study, we present both a new Favre averaging method as well as a new nongray radiation model simultaneously. A Favre average is different from the ensemble average only when density varies. This variation is accompanied by temperature variations in combustion, in which case the radiative heat transfer becomes important as well. Therefore, it is difficult to find a combustion example that has only one effect. The rest of the paper is organized as follows. In Section 2, the theoretical models are presented. In this section, a new Favre averaging method is presented in Section 2.2, a combustion model in Section 2.4, and a radiation model in Section 2.5. Details of the target flame and numerical configurations are provided in Section 3. Simulation results are compared to experiments in Section 4.

2. Theoretical models

2.1. Eulerian–Eulerian governing equations

In this study, the gas and solid phase governing equations are first spatially averaged to obtain their Eulerian governing equations [13]. The solid particles with different sizes are grouped into multiple solid phases because their distinct responses to momentum and heat transfer. Each phase has a nominal size. The spatially averaged governing equations are based on MFIX equations with simplifications. In particular, particle–particle direct interactions are removed to reflect the negligible collisions. The spatially averaged governing equations of the gas and solid phases are summarized here for completeness. For the Eulerian–Eulerian governing equations with four-way couplings, the readers are referred to the MFIX user manuals [20]. Further turbulence averaging is presented in the next section.

2.1.1. Gas phase governing equations

The spatially averaged Eulerian carrier phase governing equation for the conservation of mass is

$$\frac{\partial}{\partial t}(\rho_g) + \frac{\partial}{\partial x_j}(\rho_g u_{gj}) = \sum_{m=1}^M S_{gm}^{\rho} \quad (1)$$

where ρ_g , u_g and S_{gm}^{ρ} are the gas phase bulk density, velocity and source term due to mass transfer from solid phase m . The momentum equation of the gas phase reads

$$\begin{aligned} \frac{\partial \rho_g u_{gi}}{\partial t} + \frac{\partial}{\partial x_j}(\rho_g u_{gj} u_{gi}) = & -\varepsilon_g \frac{\partial p_g}{\partial x_i} + \varepsilon_g \frac{\tau_{ij}}{\partial x_j} + \rho_g g_i + \sum_m S_{gmi}^{ud} \\ & + \sum_m S_{gmi}^{u\rho} \end{aligned} \quad (2)$$

where ε_g , p_g , τ_{ij} and g are the gas volume fraction, gas phase pressure, shear stress and gravitational acceleration constant, respectively. The fourth term on the right hand side

$$S_{gmi}^{ud} = \frac{\rho_m}{\tau_{pm}}(u_{mi} - u_{gi}) \quad (3)$$

accounts for the drag force between the gas phase and the solid phase m , which has a bulk density of ρ_m , and a velocity of u_m . The momentum response time τ_{pm} is a particle property relative to gas and is a function of particle diameter d_{pm} and material density ρ_m^0 as $\tau_{pm} = \rho_m^0 d_{pm}^2 / 18\mu_g$. The last term $S_{gmi}^{u\rho}$ represents momentum exchange accompanied by mass transfer between gas and solid phase m . Although the gas volume fraction ε_g is close to unity in pulverized flames, we retain it in our formulations because the Favre averaging introduced here is not limited to dilute flows.

The gas phase energy equation in terms of gas phase temperature T_g is

$$\rho_g c_{pg} \left(\frac{\partial T_g}{\partial t} + u_{gj} \frac{\partial T_g}{\partial x_j} \right) = \frac{\partial}{\partial x_j} \left(k_g \frac{\partial T_g}{\partial x_j} \right) + \sum_{m=1}^M \gamma_{gm} (T_m - T_g) + S_{rad,g} + \Delta H_g \quad (4)$$

where c_{pg} , k_g , $S_{rad,g}$ and ΔH_g are specific heat, thermal conductivity, radiative heat source and heat of reaction, respectively. The weighted particle convective heat transfer coefficient $\gamma_{gm} = hA_p/V_p = 6Nu_mk_g/d_m^2$ is related to the particle Reynolds number Re_m through $Nu_m = 2 + 0.6Re_m^{1/2}Pr^{1/3}$ for small particles. The gas temperature is related to its pressure and density through ideal gas law, i.e., $\varepsilon_g p = \rho_g \bar{R}T_g$. Note that ρ_g is the bulk density here.

The conservation equation for species mass fraction Y_{gn} of species n in the gas phase is

$$\frac{\partial \rho_g Y_{gn}}{\partial t} + \frac{\partial}{\partial x_j}(\rho_g u_{gj} Y_{gn}) = \frac{\partial}{\partial x_j} \left(D_{yn} \frac{\partial Y_{gn}}{\partial x_j} \right) + S_{gn}^Y \quad (5)$$

where D_{yn} and S_{gn}^Y are the diffusivity and source term due to chemical reactions.

2.1.2. Solid phase governing equations

After the solid particles are grouped into phases according to their particle sizes, the conservation equations for the solid phase m among all M phases are given as follows. The conservation of mass reads,

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_m u_{mi}}{\partial x_i} = -S_{gm}^{\rho} \quad (6)$$

where ρ_m and u_m are the bulk density and velocity of solid phase m , respectively. S_{gm}^{ρ} is the mass transfer from solid phase m to gas phase as it appeared in the gas phase continuity equation (Eq. (1)). Mass transfer between different solid phases is neglected.

For a dilute gas–solid flow dominated by drag, such as in the pulverized coal flame considered in this study, only two-way couplings between the carrier and dispersed phases are considered. Direct interactions between two particles, such as collisions, are neglected. Therefore, solid pressure and stress, both derived from normal and frictional stresses during particle collisions, are not considered in solid phase momentum equations. The resulting momentum equation of solid phase m reads

$$\frac{\partial \rho_m u_{mi}}{\partial t} + \frac{\partial}{\partial x_j}(\rho_m u_{mj} u_{mi}) = -\varepsilon_m \frac{\partial p_g}{\partial x_i} + \rho_m g_i - S_{gmi}^{ud} - S_{gmi}^{u\rho} \quad (7)$$

The last two terms represent momentum exchange by drag or accompanied mass transfer from solid phase m to gas. Their signs are due to their positive signs in the gas phase momentum equation.

The energy equation of solid phase m in terms of its phase temperature T_m is

$$\rho_m c_{pm} \left(\frac{\partial T_m}{\partial t} + u_{mj} \frac{\partial T_m}{\partial x_j} \right) = -\gamma_{gm} (T_m - T_g) + S_{rad,m} + \Delta H_m \quad (8)$$

where c_{pm} , $S_{rad,m}$ and ΔH_m are specific heat, radiative heat source and heat of reaction, respectively. The specific heat of a solid phase depends on its composition using Merrick's model [21]. Because particles do not collide with each other, there is no heat diffusion within solid phases, i.e., no contact heat conduction between two spatially separated solid particles. However, an apparent heat diffusion in turbulent gas–solid flows due to the random motions of particles, will be recovered in the second step of averaging for turbulent flows. Also note that because there are no solid pressures, the solid phase does not require an additional equation of state as the gas phase. Similarly, the conservation equation for species mass fraction Y_{mn} of species n in the solid phase m is

$$\frac{\partial \rho_m Y_{mn}}{\partial t} + \frac{\partial}{\partial x_j}(\rho_m u_{mj} Y_{mn}) = S_{mn}^Y \quad (9)$$

where S_{mn}^V is source term due to chemical reactions and transport. These terms account for species mass transfer due to both homogeneous and heterogeneous reactions. After adding all contributions from chemical reactions, the all-inclusive source terms are used in conservation equations. Note that the diffusion term does not appear for the same reason as in the energy equations.

2.2. Favre averaged Eulerian–Eulerian equations

2.2.1. Favre average using gas phase bulk density

In turbulent flows with density variations such as combustion, a Favre average is superior to an ensemble average for the gas phase, because it leads to fewer higher order unclosed terms [14]. The Favre averaged value of a quantity x of either the gas or dispersed phase is $\tilde{x} = \langle \rho_g x \rangle / \langle \rho_g \rangle$. It should be noted that here only the gas phase bulk density ρ_g is used as the Favre weight for both gas and dispersed phases.

For the dispersed phase m ($m = 1, \dots, M$) with a spatially averaged bulk density ρ_m , the density ratio $\phi_m = \rho_m / \rho_g$ is used to recover the gas phase density in all conservation equations. The Favre averaged density ratio is

$$\tilde{\phi}_m = \frac{\langle \rho_g \frac{\rho_m}{\rho_g} \rangle}{\langle \rho_g \rangle} = \frac{\bar{\rho}_m}{\bar{\rho}_g} \quad (10)$$

where $\bar{\rho}$ is the ensemble average of the density.

For any quantity x of the solid phase m ,

$$\begin{aligned} \langle \rho_m x \rangle &= \left\langle \rho_g \frac{\rho_m}{\rho_g} x \right\rangle = \bar{\rho}_g \tilde{\phi}_m \tilde{x} = \bar{\rho}_g \langle (\tilde{\phi}_m + \phi_m'')(\tilde{x} + x'') \rangle_F \\ &= \bar{\rho}_g \tilde{\phi}_m \tilde{x} + \bar{\rho}_g \phi_m'' x'' = \bar{\rho}_m \tilde{x} + \bar{\rho}_g \phi_m'' x'' \end{aligned} \quad (11)$$

where $\langle \cdot \rangle_F$ is the Favre average when the term is longer than an over-line tilde.

In particular, if $x = u_{mi}$, the i th velocity component of solid phase m

$$\begin{aligned} \langle \rho_m u_{mi} \rangle &= \left\langle \rho_g \frac{\rho_m}{\rho_g} u_{mi} \right\rangle = \bar{\rho}_g \tilde{\phi}_m \tilde{u}_{mi} \\ &= \bar{\rho}_g \langle (\tilde{\phi}_m + \phi_m'')(\tilde{u}_{mi} + u_{mi}'') \rangle_F \\ &= \bar{\rho}_g \tilde{\phi}_m \tilde{u}_{mi} + \bar{\rho}_g \phi_m'' u_{mi}'' = \bar{\rho}_m \tilde{u}_{mi} + \bar{\rho}_g \phi_m'' u_{mi}'' \end{aligned} \quad (12)$$

The Favre fluctuation correlation term $\bar{\rho}_g \phi_m'' u_{mi}''$ is modeled according to the Bossinesq assumption similar to that of the gas phase, i.e.,

$$\bar{\rho}_g \phi_m'' u_{mi}'' = -\frac{v_t}{Sc_t} \frac{(\partial \bar{\rho}_g \tilde{\phi}_m)}{\partial x_i} = -\frac{v_t}{Sc_t} \frac{\partial \bar{\rho}_m}{\partial x_i} \quad (13)$$

This term gives the turbulent dispersion of solid phases in continuity equations. After taking a Reynolds average, the spatially averaged solid continuity equation (Eq. (6)) becomes

$$\left\langle \frac{\partial}{\partial t} (\rho_m) \right\rangle + \left\langle \frac{\partial}{\partial x_j} (\rho_m u_{mj}) \right\rangle = -\langle S_{gm}^p \rangle \quad (14)$$

After switching differential operator and averaging operator, it becomes

$$\frac{\partial}{\partial t} (\bar{\rho}_m) + \frac{\partial}{\partial x_j} (\bar{\rho}_m \tilde{u}_{mj}) + \frac{\partial}{\partial x_j} \bar{\rho}_g \phi_m'' u_{mj}'' = -\langle S_{gm}^p \rangle \quad (15)$$

Using Eq. (13) gives

$$\frac{\partial}{\partial t} (\bar{\rho}_m) + \frac{\partial}{\partial x_j} (\bar{\rho}_m \tilde{u}_{mj}) = \frac{\partial}{\partial x_j} \left(\frac{v_t}{Sc_t} \frac{\partial \bar{\rho}_m}{\partial x_i} \right) - \langle S_{gm}^p \rangle \quad (16)$$

This shows that the turbulent dispersion of particles can be recovered from modeling the correlation between fluctuations of particle bulk density and velocity. Particle bulk density does not correlate

with gas bulk density especially in reacting flows because the former is mostly affected by volume fraction and the latter is mostly altered by temperature and pressure. The capability of recovering the dispersion of solid particles in turbulent flows is crucial for the prediction of coal flames, because it has strong effects on the flame locations. The importance of this dispersion is demonstrated by a detailed numerical comparison between new and conventional Favre averaging method in Section 2.3.2.

Beside the solid phase continuity equation, the Favre averaged continuity equation for the gas phase has the same form as in single phase combustion, except that a bulk density replaces the material density, i.e.,

$$\frac{\partial}{\partial t} (\bar{\rho}_g) + \frac{\partial}{\partial x_j} (\bar{\rho}_g \tilde{u}_{gj}) = \sum_{m=1}^M S_{gm}^p \quad (17)$$

where $\bar{\rho}_g$ is the Reynolds-averaged bulk density, $\tilde{u}_g$ the Favre-averaged velocity based on gas phase bulk density, i.e., $\tilde{u}_g = \langle \rho_g u_g \rangle / \langle \rho_g \rangle$, and S_{gm}^p the net mass transfer from solid phase m to the gas phase. In this study we neglect statistical fluctuations of the source terms.

2.2.2. Momentum equations

The gas-phase bulk-density averaged momentum equation reads

$$\begin{aligned} \frac{\partial}{\partial t} (\bar{\rho}_g \tilde{u}_{gi}) + \frac{\partial}{\partial x_j} (\bar{\rho}_g \tilde{u}_{gi} \tilde{u}_{gj}) &= -\left\langle \varepsilon_g \frac{\partial p_g}{\partial x_j} \right\rangle + \left\langle \varepsilon_g \frac{\partial \tau_{ij}}{\partial x_j} \right\rangle \\ &\quad + \frac{\partial}{\partial x_j} (\bar{\rho}_g \tilde{u}_{gi}'' u_{gj}'') + \bar{\rho}_g g_i \\ &\quad + \sum_m S_{gmi}^{vd} + \sum_m S_{gmi}^{vp} \end{aligned} \quad (18)$$

All terms on the right hand side need modeling except the body force $\bar{\rho}_g g_i$. They are modeled as follows: The normal and shear stresses are assumed to be uncorrelated with gas volume fraction. Their averages are modeled as

$$\left\langle \varepsilon_g \frac{\partial p_g}{\partial x_j} \right\rangle \approx \bar{\varepsilon}_g \frac{\partial \bar{p}_g}{\partial x_j} \quad (19)$$

$$\left\langle \varepsilon_g \frac{\partial \tau_{ij}}{\partial x_j} \right\rangle \approx \frac{\partial}{\partial x_j} \left(\bar{\rho}_g \tilde{v} \frac{\partial \tilde{u}_i}{\partial x_j} \right) \quad (20)$$

Note that ρ_g is the bulk density, which scales with volume fraction ε_g . The Reynolds stress follows the turbulent viscosity assumption and becomes

$$\bar{\rho}_g \tilde{u}_{gi}'' u_{gj}'' = -\bar{\rho}_g v_t \left(\frac{\partial \tilde{u}_{gi}}{\partial x_j} + \frac{\partial \tilde{u}_{gj}}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \tilde{u}_{gk}}{\partial x_k} \right) \quad (21)$$

To model momentum transfer by drag forces $S_{gm}^{vd} = \left\langle \frac{\rho_m}{\tau_{pm}} (u_{mi} - u_{gi}) \right\rangle$, we start with the averaged drag forces with the statistical variation τ_{pm} neglected

$$\begin{aligned} \left\langle \frac{\rho_m}{\tau_{pm}} (u_{mi} - u_{gi}) \right\rangle &= \frac{\bar{\rho}_m}{\tau_{pm}} \langle (u_{mi} - u_{gi}) \rangle_F + \frac{\bar{\rho}_g}{\tau_{pm}} \langle \phi_m'' (u_{mi}'' - u_{gi}'') \rangle_F \\ &= \frac{\bar{\rho}_m}{\tau_{pm}} (\tilde{u}_{mi} - \tilde{u}_{gi}) + \frac{\bar{\rho}_g}{\tau_{pm}} \langle \phi_m'' (u_{mi}'' - u_{gi}'') \rangle_F \end{aligned} \quad (22)$$

Note that for the second equal sign to apply, the two linear operators, namely Favre average and minus sign, do not commute unless the same Favre weight is used in the Favre average, as employed in this study. This is one of the advantages provided by the new turbulent averaging method proposed in this work.

To model the second term on the right-hand side of Eq. (22) involving correlations, we assume that the particles in pulverized coal flames are so small that they trace all turbulent eddy motions. Then solid velocity resembles the gas phase velocity and decouples from solid bulk density. Therefore, all correlations between solid velocity and density ratios are negligible. If these correlations are

not negligible, then the transport equation of $\bar{\rho}_g \phi_m'' u_{mi}''$ may be used to remove some of the cross-correlation terms. Nevertheless, small differences between solid and gas velocities are permitted as required by the drag model. The momentum transfer from solid phase m to the gas phase by drag is

$$S_{gmi}^{vd} = \left\langle \frac{\rho_m}{\tau_{pm}} (u_{mi} - u_{gi}) \right\rangle \approx \frac{\bar{\rho}_m}{\tau_{pm}} (\tilde{u}_{mi} - \tilde{u}_{gi}) \quad (23)$$

The next term $S_{gmi}^{v\rho}$ accounts for the momentum transfer accompanied by mass transfer, i.e.,

$$S_{gmi}^{v\rho} = \begin{cases} S_{gm}^\rho \tilde{u}_{mi} & \text{if } S_{gm}^\rho > 0; \\ S_{gm}^\rho \tilde{u}_{gi} & \text{otherwise.} \end{cases} \quad (24)$$

Similar to the gas momentum equation, the bulk-density averaged momentum equation of solid phase m reads

$$\frac{\partial \langle \rho_m u_{mi} \rangle}{\partial t} + \frac{\partial \langle \rho_m u_{mj} u_{mi} \rangle}{\partial x_j} = - \left\langle \varepsilon_m \frac{\partial p_g}{\partial x_j} \right\rangle + \bar{\rho}_m g_i - S_{gmi}^{vd} - S_{gmi}^{v\rho} \quad (25)$$

In order to average the convection term, note that

$$\begin{aligned} \langle \rho_m u_{mj} u_{mi} \rangle &= \langle \rho_g \phi_m u_{mj} u_{mi} \rangle = \bar{\rho}_g \langle \phi_m u_{mj} u_{mi} \rangle_F \\ &= \bar{\rho}_g \langle (\tilde{\phi}_m + \phi_m'') (\tilde{u}_{mj} + u_{mj}'') (\tilde{u}_{mi} + u_{mi}'') \rangle_F \\ &= \bar{\rho}_g \left[\tilde{\phi}_m \tilde{u}_{mj} \tilde{u}_{mi} + \tilde{\phi}_m \widetilde{u_{mj} u_{mi}''} + \tilde{u}_{mj} \phi_m'' u_{mi}'' + \tilde{u}_{mi} \phi_m'' u_{mj}'' + \langle \phi_m'' u_{mj}'' u_{mi}'' \rangle_F \right] \\ &= \bar{\rho}_m \tilde{u}_{mj} \tilde{u}_{mi} + \bar{\rho}_m \widetilde{u_{mj} u_{mi}''} + \bar{\rho}_g \tilde{u}_{mj} \phi_m'' u_{mi}'' + \bar{\rho}_g \tilde{u}_{mi} \phi_m'' u_{mj}'' \\ &\quad + \bar{\rho}_g \langle \phi_m'' u_{mj}'' u_{mi}'' \rangle_F \end{aligned} \quad (26)$$

However, only the first two terms are retained, because each term (temporal derivative, convection and diffusion) in the momentum equations involves the correlation between the density ratio (ϕ'') and the solid velocity (u''). Their collective effects are that a transport equation for this correlation is embedded in the momentum equation. This embedded equation is set to zero here for convenience. Therefore, the resulting convection term is

$$\frac{\partial}{\partial x_j} \langle \rho_m u_{mj} u_{mi} \rangle \approx \frac{\partial}{\partial x_j} (\bar{\rho}_m \tilde{u}_{mj} \tilde{u}_{mi}) + \frac{\partial}{\partial x_j} (\bar{\rho}_m \widetilde{u_{mj} u_{mi}''}) \quad (27)$$

The turbulent dispersion of the dispersed phase is recovered through solid phase velocity correlations analogous to the carrier phase.

$$\bar{\rho}_m \widetilde{u_{mi}'' u_{mj}''} = -\bar{\rho}_m v_t \left(\frac{\partial \tilde{u}_{mi}}{\partial x_j} + \frac{\partial \tilde{u}_{mj}}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \tilde{u}_{mk}}{\partial x_k} \right) \quad (28)$$

The effects from gas stresses are

$$\left\langle \varepsilon_m \frac{\partial p_g}{\partial x_j} \right\rangle \approx \bar{\varepsilon}_m \frac{\partial \bar{p}_g}{\partial x_j} \quad (29)$$

The resulting solid phase momentum equations are

$$\begin{aligned} \frac{\partial}{\partial t} (\bar{\rho}_g \tilde{u}_{gi}) + \frac{\partial}{\partial x_j} (\bar{\rho}_g \tilde{u}_{gi} \tilde{u}_{gj}) &= - \frac{\partial}{\partial x_j} \left(\bar{\rho}_m v_t \left(\frac{\partial \tilde{u}_{mi}}{\partial x_j} + \frac{\partial \tilde{u}_{mj}}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial \tilde{u}_{mk}}{\partial x_k} \right) \right) \\ &\quad - \bar{\varepsilon}_m \frac{\partial \bar{p}_g}{\partial x_j} + \bar{\rho}_m g_i - S_{gmi}^{vd} - S_{gmi}^{v\rho} \end{aligned} \quad (30)$$

2.2.3. Energy equations

The gas phase bulk-density averaged energy equation in terms of T_g is

$$\begin{aligned} \bar{\rho}_g c_{pg} \left(\frac{\partial \tilde{T}_g}{\partial t} + \tilde{u}_{gj} \frac{\partial \tilde{T}_g}{\partial x_j} \right) &= \frac{\partial}{\partial x_j} \left(k_{g,\text{eff}} \frac{\partial \tilde{T}_g}{\partial x_j} \right) + \sum_{m=1}^M \gamma_{gm} (\tilde{T}_m - \tilde{T}_g) \\ &\quad + S_{\text{rad},g} + \Delta H_g \end{aligned} \quad (31)$$

where the effective conductivity accounts for molecular and turbulent thermal diffusion

$$k_{g,\text{eff}} = k_g + \bar{\rho}_g c_{pg} \frac{v_t}{\text{Pr}_t} \quad (32)$$

The Favre averaged energy equations of solid phases are

$$\begin{aligned} \bar{\rho}_m c_{pm} \left(\frac{\partial \tilde{T}_m}{\partial t} + \tilde{u}_{mj} \frac{\partial \tilde{T}_m}{\partial x_j} \right) &= \frac{\partial}{\partial x_j} \left(\bar{\rho}_m c_{pm} D_{Tm,\text{eff}} \frac{\partial \tilde{T}_m}{\partial x_j} \right) \\ &\quad - \gamma_{gm} (\tilde{T}_m - \tilde{T}_g) + S_{\text{rad},m} + \Delta H_m \end{aligned} \quad (33)$$

where the effective diffusivity is due to turbulent diffusion

$$D_{Tm,\text{eff}} = \frac{v_t}{\text{Pr}_t} \quad (34)$$

$\text{Pr}_t = 1.0$ is assumed in this study. The recovered turbulent thermal diffusivity is similar to that in the continuity and momentum equations. Also note that the derivation of interface heat transfer relies on commutation between the Favre average and linear operators, which is the unique advantage of the current averaging method.

2.2.4. Species equations

Similarly to the energy equations, the transport equation of bulk-density averaged gas species mass fraction (Y_{gn}) of species n reads

$$\bar{\rho}_g \tilde{Y}_{gn} \frac{\partial}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho}_g \tilde{u}_{gj} \tilde{Y}_n) = \frac{\partial}{\partial x_j} \left(\bar{\rho}_g D_{Yn,\text{eff}} \frac{\partial \tilde{Y}_n}{\partial x_j} \right) + S_{Yn}^g \quad (35)$$

where

$$D_{Yn,\text{eff}} = D_m + \frac{v_t}{\text{Sc}_t} \quad (36)$$

Similarly the transport equation of solid species mass fraction (Y_{mn}) of species n in solid phase m reads

$$\bar{\rho}_m Y_{mn} \frac{\partial}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho}_m \tilde{u}_{mj} Y_n) = \frac{\partial}{\partial x_j} \left(\bar{\rho}_m D_{Ymn,\text{eff}} \frac{\partial Y_n}{\partial x_j} \right) + S_{Yn}^m \quad (37)$$

where

$$D_{Ymn,\text{eff}} = \frac{v_t}{\text{Sc}_t} \quad (38)$$

$\text{Sc}_t = 1.0$ is assumed in this study.

2.3. Turbulence models

2.3.1. $k-\epsilon$ model

The standard $k-\epsilon$ model is used [22]

$$\frac{\partial}{\partial t} (\bar{\rho}_g k) + \frac{\partial}{\partial x_j} (\bar{\rho}_g \tilde{u}_{gj} k) = \frac{\partial}{\partial x_j} \left(\bar{\rho}_g \left(\nu + \frac{v_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right) + P_k - \bar{\rho}_g \epsilon \quad (39)$$

$$\frac{\partial}{\partial t} (\bar{\rho}_g \epsilon) + \frac{\partial}{\partial x_j} (\bar{\rho}_g \tilde{u}_{gj} \epsilon) = \frac{\partial}{\partial x_j} \left(\bar{\rho}_g \left(\nu + \frac{v_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right) + C_{\epsilon 1} \frac{\epsilon}{k} P_k - C_{\epsilon 2} \bar{\rho}_g \frac{\epsilon^2}{k} \quad (40)$$

where the source term P_k is given by

$$P_k = -\bar{\rho}_g \widetilde{u_{gi}'' u_{gj}''} \frac{\partial \tilde{u}_{gi}}{\partial x_j} \quad (41)$$

and turbulent viscosity is given by

$$\nu_t = C_\mu \frac{k^2}{\epsilon} \quad (42)$$

The model constants are

$$C_\mu = 0.09; \quad \sigma_k = 1.0; \quad \sigma_\epsilon = 1.3; \quad C_{\epsilon 1} = 1.6; \quad C_{\epsilon 2} = 1.92 \quad (43)$$

2.3.2. Effects of turbulent particle dispersion

In order to demonstrate the differences between the conventional and the proposed Favre averaging methods, a nonreactive nonradiative simplification of the target flame is considered here by arbitrarily disabling reactions and radiative heat transfer in the numerical simulation. Detailed description of numerical configurations are presented in Section 3.2. The primary focus here is to compare the prediction of solid phase bulk density (equivalent to particle volume fraction when particle material density is fixed). The spatial distribution of particle bulk density is crucial to all solid phase transport equations. In particular, it has profound effects on the flame location.

The conventional Favre averaging method averages conservation equations using solid bulk density. Only the continuity equation is derived here, assuming that the other equations are identical between the two Favre averaging methods. This change alone is sufficient to demonstrate the subtle differences between the two Favre averaging methods. After being averaged by the conventional Favre averaging method based on solid phase bulk density, the continuity Eq. (6) becomes

$$\frac{\partial}{\partial t}(\bar{\rho}_m) + \frac{\partial}{\partial x_j}(\bar{\rho}_m \tilde{u}_{mj}) = -\langle S_{gm}^p \rangle \quad (44)$$

where the Favre averaged solid phase velocity is $\tilde{u}_{mj} = \langle \rho_m u_{mj} \rangle / \langle \rho_m \rangle$.

In this work, the new Favre averaged continuity Eq. (16) is

$$\frac{\partial}{\partial t}(\bar{\rho}_m) + \frac{\partial}{\partial x_j}(\bar{\rho}_m \tilde{u}_{mj}) = \frac{\partial}{\partial x_j} \left(\frac{v_t}{Sc_t} \frac{\partial \bar{\rho}_m}{\partial x_i} \right) - \langle S_{gm}^p \rangle \quad (45)$$

in which the Favre averaged velocity is defined as $\tilde{u}_{mj} = \langle \rho_g u_{mj} \rangle / \langle \rho_g \rangle$.

The different partial differential equations lead to distinct spatial distributions of the solid density, shown in Fig. 1. In this figure, the predicted solid bulk density at different downstream locations is compared as obtained with the two Favre averaging methods. Only the smallest solid particles are shown in this figure, because solid particles of other sizes have identical trends. It can be seen

Fig. 1. Predicted bulk density of solid phase of size 16.6 μm. The thin lines are predictions from conventional Favre averaging based on solid phase bulk density. The conventional Favre averaged conservation equation of mass does not contain diffusion terms. The thick lines are predictions from the new Favre averaging method based on gas phase bulk density. The averaged conservation equation of mass contains a turbulent diffusion term. Radial profiles of solid bulk density solved by two averaged equations are compared at 4 downstream locations, namely 1, 5, 10 and 20 cm above the jet nozzle.

that Eq. (45) predicts radial dispersion of solid particles as seen by the radially broadened profiles at downstream locations. On the other hand, Eq. (44) allows for almost no radial dispersion. Instead, the solid bulk density accumulates at downstream locations because of reduced velocity.

2.4. Combustion models

The Eddy Dissipation Concept (EDC) model [23] is employed for gaseous turbulent combustion. The EDC model assumes that the local mass fraction of each species decays toward its chemical equilibrium composition. The decay rate is related to turbulent flow fields through two variables

$$\tau = C_\tau \left(\frac{v}{\epsilon} \right)^{1/2} \quad \text{with } C_\tau = 0.4082 \quad (46)$$

$$\xi = C_\xi \left(\frac{v\epsilon}{k^2} \right)^{1/4} \quad \text{with } C_\xi = 2.1377 \quad (47)$$

The mass change rate of gas species i due to turbulent reaction is

$$S_{gi}^Y = \frac{\rho}{\tau} \cdot \frac{\xi^2}{1 - \xi^3} \cdot (Y_i^* - Y_i) \quad (48)$$

where Y_i^* is chemical equilibrium composition. This composition is calculated from CEQ [24], a Fortran library to compute equilibrium compositions using Gibbs function continuation. The EDC model employed in this work does not require a gaseous reaction kinetic mechanism.

The mass loss rate of the coal particles from devolatilization is determined from Ubhayakar's two rates model [25] and Kobayashi's model [26]. Both models define two competing devolatilization rates of the Arrhenius form. The total rate of devolatilization is the sum of two, i.e.,

$$\frac{dm_{\text{vol}}}{dt} = -[\alpha_1 B_1 \exp(-E_1/RT_p) + \alpha_2 B_2 \exp(-E_2/RT_p)] m_{\text{coal}} \quad (49)$$

The model parameters are identical to the original reference, i.e., for Ubhayakar's model

$$\alpha_1 = 0.39, \quad B_1 = 3.7 \times 10^5 \text{ s}^{-1}, \quad E_1 = 7.37 \times 10^4 \text{ J/mol}$$

$$\alpha_2 = 0.8, \quad B_2 = 1.46 \times 10^{13} \text{ s}^{-1}, \quad E_2 = 2.51 \times 10^5 \text{ J/mol}$$

and for Kobayashi's model,

$$\alpha_1 = 0.3, \quad B_1 = 2.0 \times 10^5 \text{ s}^{-1}, \quad E_1 = 1.046 \times 10^5 \text{ J/mol}$$

$$\alpha_2 = 1.0, \quad B_2 = 1.3 \times 10^7 \text{ s}^{-1}, \quad E_2 = 1.67 \times 10^5 \text{ J/mol}$$

In this study, Ubhayakar's model is used as reference, while Kobayashi's model is included for comparison.

The oxidation of fixed carbon in char is modeled from a single step heterogeneous reaction with O_2 in gas phase, i.e.,

A half order reaction rate proposed by Harmor [27] is used for char mass loss rate

$$\frac{dm_{C(s)}}{dt} = 9.3 \exp\left(\frac{8152}{T_m}\right) p_{O_2}^{1/2} \quad [\text{g/s}] \quad (51)$$

where p_{O_2} is the oxygen partial pressure in atm, T_m is the particle temperature of phase m in Kelvin.

2.5. Radiation models

In this section, a new radiation model is introduced. It is based on the k -distribution approach, which is extended here to nongray gas–solid mixtures. The k -distribution methods are a relatively new spectral model family that can treat nongray effects

accurately. They possess several advantages for combustion simulations: (1) k -distributions utilized in this work are derived from gas and particle spectroscopic databases. They can achieve almost identical accuracy as would be obtained from the original spectroscopic line structure (known as line-by-line accuracy) but at a much lower computational cost. (2) It does not require knowledge of the specific problem at hand to specify model “tuning” parameters. The same programs and databases are employed for all optical thicknesses. Furthermore, it was shown that k -distributions preserve total emission, which is a crucial property when the flame becomes optically thin, such as the target laboratory flame investigated here. Total emissivity models or Planck-mean gray models may employ outdated databases. (3) Despite the attractive properties k -distributions possess, they are rarely used outside the radiation community. In particular, they have not been applied to pulverized coal flames to date, in which radiation is known to be important.

2.5.1. Particle radiative properties

The complex refractive indices of coal composition employed in this study are listed in Table 1. The values are identical to Ref. [16,28], except that the complex refractive index of volatile matter not provided therein is assumed to be that of coal.

The complex refractive index of the m th solid phase is assumed to be linear with its composition, i.e.

$$\mathbf{m}_m = \sum_n \mathbf{m}_{mn} Y_{mn} \quad (52)$$

where $\mathbf{m}_{mn}$ and Y_{mn} are the complex refractive index and mass fraction of the n th composition, respectively.

The complex refractive indices of solid phases are used to calculate bulk spectral radiative properties (absorption, scattering and extinction coefficients) of the solid phase through the Buckius–Hwang correlations [29]. It should be noted that due to the dependency of size ratio on wavelength (i.e. $\pi d_p/\lambda$), a gray complex refractive index does not guarantee a gray absorption (or scattering) coefficient. Furthermore, the optical properties of solid phases are unlikely to be constant across the spectrum. Therefore, it is useful to consider nongray particle radiative properties in general. The nongray treatment of solid phases is combined with that of nongray gases through k -distribution methods.

2.5.2. k -distribution methods for nongray radiatively participating gas–solid mixtures

The k -distribution of a gas mixture is a reordered gas spectrum according to its absorption coefficient [16]. The reordering process and the resulting k -distributions are exact for homogeneous mixtures. For nonhomogeneous mixtures, a correlated or scaled absorption coefficient assumption is needed to decouple dependency of absorption coefficient on spectral variables from thermodynamic variables [16,30]. However, the radiative properties of solid phases have distinct spectral dependency from that of gases, which severely challenges the validity of correlated or scaled absorption coefficient assumption.

Besides, the Eulerian–Eulerian approach to gas–solid reacting flows demands accounting for different temperatures of each phase and splitting radiative heat sources across energy equations

of each phase. To address the above challenges when applying the k -distribution methods to multiphase reacting flows, a new k -distribution method was proposed to partially relax the correlated- k assumption for solid particles [19]. The theory is briefly reviewed here.

2.5.3. Regression-based full-spectrum k -distributions

A full spectrum k -distribution is a reordered spectral absorption coefficient defined as [30]

$$f(k) = \frac{1}{I_b} \int_{\eta} \delta(k - \kappa_{\eta}) I_{b\eta} d\eta \quad (53)$$

where η is the wavenumber, κ_{η} the spectral absorption coefficient, and $I_{b\eta}$ the Planck function. The cumulative k -distribution

$$g(k) = \int_0^k f(k') dk' \quad (54)$$

is a dimensionless spectral variable. An integration over g corresponds to an integration over wavenumbers. The inverse function of Eq. (54), $k(g)$, is the reordered absorption coefficient in a full-spectrum k -distribution calculation. Since g is bounded between 0 and 1, the numerical integration is performed using a quadrature scheme [30].

The Radiative Transfer Equation (RTE) for a nonhomogeneous medium involving emission, absorption and scattering reads [19],

$$\begin{aligned} \frac{dI_{\eta}}{ds} = & \sum_{m=0}^M \kappa_{m\eta} I_{b\eta}(T_m) - \sum_{m=0}^M \kappa_{m\eta} I_{\eta} - \sum_{m=1}^M \sigma_{sm} I_{\eta} + \sum_{m=1}^M \frac{\sigma_{sm}}{4\pi} \\ & \times \int_{4\pi} I_{\eta}(\hat{s}') \Phi_m(\hat{s}, \hat{s}') d\hat{s}' \end{aligned} \quad (55)$$

where m is the phase number with 0 for gas and others for solid, M the total number of solid phases, $I_{\eta}(\hat{s})$ the spectral radiation intensity along direction $\hat{s}$, $\kappa_{m\eta}$ the spectral absorption coefficient, $I_{b\eta}$ the Planck function, T_m the temperature of the m th phase, σ_{sm} the spectral scattering coefficient and $\Phi_m(\hat{s}, \hat{s}')$ the scattering phase function between directions $\hat{s}$ and $\hat{s}'$.

Applying the reordering process of Eq. (53) to the above RTE, the reordered RTE becomes

$$\begin{aligned} \frac{dI_g}{ds} = & k_0^*(g) a(T_0, T^0, g) I_b(T_0) + \sum_{m=0}^M \hat{k}_m(g; T_m) a(T_m, T^0, g) I_b(T_m) \\ & - \left[k_0^*(g) + \sum_{m=1}^M \hat{k}_m(g; T_m) \right] I_g - \sum_{m=1}^M \sigma_{sm} I_g \\ & + \sum_{m=1}^M \left[\sigma_{sm} \frac{1}{4\pi} \int_{4\pi} \Phi_m(\hat{s}, \hat{s}') I_g(\hat{s}') d\Omega \right] \end{aligned} \quad (56)$$

where k_0^* are the correlated k values for the gas phase, $\hat{k}_m$ the effective solid absorption coefficient, T^0 the temperature at a reference state, and a the nongray stretching function.

Note that the spectral variable is converted from wavenumber η to the dimensionless reordered spectral variable g . The total radiative heat source is recovered by

$$S_{\text{rad}} = \int_0^1 k_g G_g dg - \sum_{m=0}^M 4\pi \kappa_{pm} I_b(T_m) \quad (57)$$

where $G_g = \int_{4\pi} I_g(s) ds$ is the incident radiation, k_g the total absorption coefficient from the k -distribution, and κ_{pm} the total Planck mean absorption coefficient of all phases.

As suggested by Eq. (57), a nongray calculation is essentially a series of gray calculations at different spectral variables g before numerical integration over g .

Table 1

Coal composition and their complex refractive indices.

Coal composition	$\mathbf{m}$
Fixed carbon	$2.2 - 1.12i$
Fly ash	$1.5 - 0.02i$
Volatile matter	$2.05 - 0.54i$

Fig. 2. Geometry and mesh. The left shows the geometry of computational domain. The mesh shows one of every 10 grid lines on both axial and radial directions. The right figure shows inlet geometry and all grid lines nearby.

2.5.4. Regression scheme for heat source splitting

While there is only a single radiation field in a gas–solid mixture with one gas phase and M solid phases, each phase demands a separate energy equation and radiative heat source. Proper splitting of the total radiative heat source across phases is a new challenge when applying the k -distribution method to gas–solid mixtures. The splitting is achieved by defining a new effective solid absorption coefficient in Eq. (56) through a regression [19]:

$$\hat{k}_m(k; T_m) = \frac{\int_{\eta} \kappa_{mn} I_{b\eta} \delta(k - \kappa_{\eta}^0) d\eta}{\int_{\eta} I_{b\eta} \delta(k - \kappa_{\eta}^0) d\eta} \quad (58)$$

The gas phase radiative heat source then becomes

$$S_0 = \int_0^1 k_0^*(g) G_g dg - 4\pi \kappa_{p0} I_b(T_0) \quad (59)$$

and the m th solid phase radiative heat source is

$$S_m = \int_0^1 \hat{k}_m(g) G_g dg - 4\pi \kappa_{pm} I_b(T_m) \quad (60)$$

The regression scheme utilizes a narrowband k -distribution database [31,32]. Three species (CO_2 , CO and H_2O) are considered for radiation calculations. CH_4 , although included in the database, is not considered because its absorption bands do not overlap with the emission bands of other species. Inclusion of CH_4 is likely to cause a false prediction of absorption [18]. After calculating the k -distribution of a narrowband from mixing the k -distribution of each individual gas component, a constant narrowband solid phase absorption coefficient is added. An “effective” solid phase absorption coefficient for the purpose of splitting radiative heat sources is determined from all narrowband values using regression [19].

Table 2

Thermophysical properties.

Parameter	Experimental value	Numerical value
Low heating value	28.1 MJ/kg	28.1 MJ/kg
<i>Proximate analysis (wt.%)</i>		
Fixed carbon	57.9%	57.9%
Ash	15.2%	15.2%
Volatile matter	26.9%	26.9%
<i>Ultimate analysis (wt.%)</i>		
Carbon	71.9%	71.9%
Hydrogen	4.4%	4.4%
Oxygen	6.53%	8.5%
Nitrogen	1.5%	0
Sulfur	0.44%	0

2.5.5. P_1 Radiative Transfer Equation (RTE) solver

Eq. (56) may be solved with the P_1 approximation. The P_1 RTE for an inhomogeneous gray medium with isotropic scattering is a Helmholtz equation:

$$\frac{\partial}{\partial x_i} \frac{1}{\beta} \frac{\partial}{\partial x_i} G - 3\beta(1 - \omega)G = -3\beta(1 - \omega)E \quad (61)$$

where G is the incident radiation, β the extinction coefficient and ω the scattering albedo. The extinction coefficient β is the sum of the absorption coefficient κ and the scattering coefficient σ_s . The scattering albedo is the ratio of the scattering coefficient σ_s and the extinction coefficient β . E represents the total effective emission from both gas and solid phases, as defined later when comparing the P_1 RTE with Eq. (56).

The nongray calculation is achieved by repeating gray calculation at different spectral locations. For example, for a given g value

in Eq. (56), the corresponding P_1 Eq. (61) may be solved for G_g with the emission and extinction coefficient as

$$E = \frac{1}{\beta_g} \left[k_0^*(g) a(T_0, T^0, g) I_b(T_0) + \sum_{m=1}^M k_m(g) a(T_m, T^0, g) I_b(T_m) \right] \quad (62)$$

and

$$\beta_g = k_0^*(g) + \sum_{m=1}^M k_m(g) + \sum_{m=1}^M \sigma_{sm} \quad (63)$$

Then the heat sources are split at each g value. The heat source for a phase is the spectral heat source integrated over g and calculated numerically through a quadrature scheme, i.e.,

$$S_m = \int_0^1 S_m(g) dg = \sum_n w_n S_m(g_n) \quad (64)$$

where g_n is the quadrature abscissa and w_n the corresponding quadrature weight.

The P_1 equation is subject to Marshak boundary conditions for the incident radiation field of

$$\frac{2 - \epsilon_w}{\epsilon_w} \frac{2}{3\beta_g} \hat{n} \cdot \nabla G_g + G_g = E_{wg} \quad (65)$$

where ϵ_w is the wall emittance, β the extinction coefficient of the medium adjacent to the wall, $\hat{n}$ the wall normal direction from the medium to the wall and $E_{wg} = 4\pi a_{wg}(T_w, T^0, g) I_b(T_w)$ the wall emission. The Marshak boundary condition degenerates to a zero normal gradient boundary condition when the boundary emissivity is zero, i.e.,

$$\hat{n} \cdot \nabla G_g = 0 \quad \text{when } \epsilon_{wg} = 0 \quad (66)$$

3. Experimental and numerical configurations for a pulverized flame

3.1. Experimental configurations

The target flame for validation purposes is a pulverized coal ignition jet flame piloted by a methane flame [2–4]. The fuel injector, as shown in Fig. 2, has two co-axial jets. The central jet has an inner diameter of 6 mm and an outer diameter of 7 mm, while the annular jet has an inner diameter of 8 mm and an outer diameter of 10 mm. Coal particles are entrained by air through a central jet. Methane is injected through the annular slit between co-axial central and annular jets.

The kinematic configurations include a coal feed rate of 1.49×10^{-4} kg/s, central jet air flow rate of 1.8×10^{-4} m³/s, methane flow rate of 2.33×10^{-5} m³/s. The corresponding Reynolds number was reported as 2544. Both Shadow Doppler Particle Analyser (SDPA) and Laser Doppler Velocimetry (LDV) were used for particle velocity measurements. The two independent techniques showed strong agreement for velocity. Particle temperature was determined from a two-color radiation pyrometer operating on wavelengths of 0.9 and 1.0 μ m. The reported particle thermodynamic properties are listed in Table 2. Species concentration measurements of O₂, N₂, CO₂ and CO were performed with sample probes along the burner centerline.

3.2. Numerical configurations

The thermophysical properties of the coal employed in the simulation are based on reported values with some simplifications, and are listed in Table 2. Moisture contained in the coal is added to the carrier gas, because drying is a fast process under high heating rates and completes before coal particles are ignited. Sulfur and

Fig. 3. Comparison of the axial mean and fluctuating velocity between simulation and experiments. Axial mean velocity predictions of gas (V_g) and three solid phases (V_{s1} , V_{s2} and V_{s3}), shown by lines, are compared with the mean particle velocity from experiments (exp, shown as symbols). The predicted Favre velocity fluctuation of the gas phase (line) inferred from turbulent kinetic energy is also compared with measurements (symbols).

nitrogen components are combined with oxygen in ultimate analysis, as this study focuses on combustion and heat transfer modeling instead of pollution prediction. Because the majority of oxygen in the central stream comes from the carrier air, this substitution causes a 5% over-injection of oxygen, as if an oxygen mass fraction of 24% instead of 23% is used.

Three solid phases are considered in this study for particle size distributions in the Eulerian–Eulerian framework. The underlying particle size distribution is assumed to be a truncated Rosin–Rammler distribution, with a minimum particle diameter of 5 μ m, a maximum particle diameter of 61 μ m, a mean diameter of 25 μ m and a spreading parameter of 4.0. A mean number-based particle size of 25 μ m was reported in the original experimental paper. This distribution is binned into three phases with equal probability. The nominal particle sizes (d_{32}) of the three phases

Fig. 4. Gas phase composition compared with experiments.

are 16.6, 24.8 and 35.9 μm , respectively. Their volume fractions relative to the total solid phases are 0.063, 0.237 and 0.70, respectively. The dependency of results on the number of solid phases is examined and discussed in Section 4.4.

The carrier gas is modeled as ideal. Seven gas species are considered, namely N_2 , O_2 , CO_2 , CO , H_2O , H_2 and CH_4 . The Eddy Dissipation Concept model employed here does not involve any chemical kinetic mechanism. Concentrations of radical species are not solved for. The devolatilization products are modeled as a gas mixture consisting of 54.9% CH_4 , 42.5% CO and 2.6% H_2 by mass. Additional devolatilization at high temperature required by the two-rate devolatilization model is achieved by subtraction of extra mass from char. The volatile products are combined with gas phase species before the EDC combustion model is applied during each time step.

The computational domain shown in Fig. 2 is two-dimensional axisymmetric that covers 3 cm in radius from the jet axis and 25 cm in height from the jet exit. Radial and axial directions are uniformly discretized into 120 and 100 cells respectively. A radially parabolic velocity profile is used for the central jet inlet velocity. A uniform axial velocity of 2 m/s is used for the methane inlet. The coflow has a velocity of 0.6 m/s. A free slip wall boundary condition is used at the far field, and a pressure outlet boundary condition is used at the downstream exit. All other pressure boundary conditions are specified as zero gradient. Inlet and radially far field temperatures are 300 K, while the outlet is set to zero gradient. Central inlet air has a composition of 75.7% N_2 , 22.9% O_2 , and 1.4% H_2O by mass, because coal moisture is added to the central air stream assuming drying is instant. The coflow has the composition of dry air. The minimal number of the total extinction coefficient is lower bounded by $1 \times 10^{-4} \text{ m}^{-1}$ to avoid zero radiative properties that destabilize the P_1 equation. All boundary conditions for the P_1 equation are the Marshak boundary condition.

The numerical models are implemented in Multiphase Flow with Interphase eXchanges (MFIx) [20], a general multiphase reacting flow solver. The programming language is Fortran. The

partial differential equations employed are discretized using the finite volume method on a structured staggered grid. The SIMPLE algorithm is used for pressure–velocity coupling. All convection terms are discretized with the upwind scheme. The simulation uses an unsteady solver, and a time marching scheme is used to reach steady state. All comparisons are at steady state.

Mesh dependency was examined by comparing predicted flow variables between the current mesh and a refined mesh. The refined mesh had mesh cells doubled uniformly along both the axial and radial directions. Major flow variables including velocities, temperatures, volume fractions and species mass fractions of both the gas and solid phases were compared. It was found that the velocity difference is within 2% throughout the computational domain for both gas and solid phases. The outer branch of the methane flame front ($r \approx 7 \text{ mm}$) shifted toward the centerline by 0.3 mm and became slightly thinner within 1 cm of the inlets. However, this region contains very low concentrations of solids, and therefore the deviation did not lead to any further deviation in temperature predictions at downstream locations, e.g., the difference in temperature was found within 2% above 3 cm from the inlets. Similarly, there were spatial shifts of gas species mass fractions near the inlets. The solid species were found to be less sensitive to mesh refinement (within 2% through the domain). The difference in predicting flow variables was smaller than the potential uncertainties of coal reactions, as well as the measurements. The null difference in temperature predictions at downstream locations suggests that the rate-controlling solid reactions and radiative heat transfer are not affected by mesh refinement. Therefore, the current mesh was considered sufficient for the current study.

4. Results and discussions

In this section, simulation results using a baseline model set are compared to experimental measurements first. The baseline model set consists of 3 solid phases, Ubhayakar's devolatilization model

Fig. 5. Temperature of each phase with radiation feedback. From left to right: gas, solid phase 1 (16.6 μm), solid phase 2 (24.8 μm) and solid phase 3 (35.9 μm). White space indicates areas with negligible particle contents.

Fig. 6. Predicted emission temperature (Temiss) readout of two color pyrometer compared with experiments. Also shown are the centerline temperature and maximum temperature along the line of sight of gas (Tgc) and three solid phases (Ts1c, Ts2c and Ts3c). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 7. Predicted radial temperature profiles of the smallest (16.6 μm shown as thin lines) and largest (35.9 μm shown as thick lines) particles at three downstream locations, namely 1.1 cm (solid line), 1.6 cm (dashed) and 5 cm (dash-dotted).

and radiation feedback. Then the effects of the devolatilization model on solid particle composition and temperature are investigated. The effects of radiation are demonstrated by comparing simulation results with and without radiation. Finally, the dependency on the number of solid phases is also examined.

4.1. Comparisons with experiments using baseline configurations

The calculated axial velocity along the centerline of gas and solid phases is compared with experimental measurements of particle velocity in Fig. 3. The velocity differences between phases are found to be small. The solid phase axial velocity has good agreement with measurements up to 13 cm above the nozzle. The velocities of all phases drop quickly beyond 15 cm. Compared to other

studies [7,11], our simulation shows much lower temperature at downstream locations because of the radiative heat loss. The reduced temperature might be the cause of velocity decline due to increased densities. The Favre velocity fluctuation v'' of the gas phase was estimated from turbulent kinetic energy as $\sqrt{2k/3}$ assuming locally isotropic turbulence. The velocity fluctuation showed good agreement with experiments considering the simple $k-\epsilon$ model employed here.

The mole fractions of major species (N_2 , O_2 and CO_2) along the centerline are compared with experiments in Fig. 4. The mole fractions are dry-based, i.e., mole fractions without water vapor. Predicted and measured CO_2 concentrations show good agreement, while some discrepancies were found for N_2 and O_2 . Similar trends were also found in other recent simulations of the same target flame [7,11]. However, comparing with previous studies [7,11], results from the current study demonstrate slower axial evolution of the gas compositions. Especially, the O_2 is not depleted in the central stream. It should be noted that the minimal remaining O_2 along the centerline is still more than three times the extra oxygen introduced by replacing nitrogen and sulfur with oxygen in the coal. Although the central jet is fuel-rich, particles collected downstream revealed large amounts of incomplete combustion [3]. The incomplete combustion was also observed in previous simulations because of insufficient oxygen. Our simulation suggests similar incomplete combustion, but due to reduced reaction rates at lower temperatures due to radiative heat loss.

The temperatures of gas and solid phases with radiation feedback are shown in Fig. 5. The peak gas temperature reaches in excess of 2200 K, close to the adiabatic flame temperature of CH_4 in air. Two flame fronts are formed. One is between the methane pilot and the central air-coal jet, the other one is between the methane pilot and ambient air.

The solid phase temperature profiles (Fig. 5) are left blank in regions with low volume fractions, because Eulerian phase properties are not properly defined. The solid phases have lower temperature than the gas during the ignition ($y < 10$ cm) because of particle thermal response delay. Smaller particles with shorter response time follow gas phase temperatures more closely. After being ignited solid phases experience high temperatures through char oxidation. The solid temperatures approach thermal equilibrium with the gas phase gradually in the downstream (i.e., $y > 15$ cm). Upstream solid phases follow gas temperature in the outer front ($r > 5$ mm) of the CH_4 flame closer than the inner flame front, because smaller solid phase velocity in the outer front leads to longer residence time.

In the original flame measurements [2–4], the particle temperature was inferred from a two-color pyrometer operating at 0.9 and 1.0 μm . Such a pyrometer measures flame radiation at two wavelengths along line-of-sight. The ratio of radiation intensity at two wavelengths is compared to that from blackbody emission. This method is mostly used for surface temperature measurement, as surface emissivity is close at two close wavelengths. However, its use in flame measurements requires additional caution since the pyrometer readout does not reflect the particle temperature at any location, nor the average temperature along the line-of-sight because of nonlinear dependence of radiation emission on temperature. In order to make a direct comparison, the flame emission is calculated using predicted flow field variables and particle properties at the two wavelengths before an integral along a line-of-sight. The ratio of integrated intensities is compared against a blackbody intensity ratio. This synthesizes the pyrometer readout from the simulated flow fields.

The calculated temperature along centerline and a predicted pyrometer temperature readout are compared with experiments in Fig. 6. The solid line shows numerical prediction of the pyrom-

Fig. 8. Solid compositions of each phase with radiation feedback using Ubhayakar devolatilization model. From left to right: mass fractions of volatile matter in solid phase 1, 2 and 3; and mass fractions of fixed carbon in solid phase 1, 2 and 3, respectively.

Fig. 9. Solid compositions of each phase with radiation feedback using Kobayashi devolatilization model. From left to right: mass fractions of volatile matter in solid phase 1, 2 and 3; and mass fractions of fixed carbon in solid phase 1, 2 and 3, respectively.

eter readout from current simulation. Different solid phases have distinct temperatures due to their size variations and size-sensitive heat transfer and reaction rates, so that pyrometer readout differs from centerline temperature profiles of all phases. The predicted readout has good agreement with experiments.

To investigate the discrepancies between predicted emission temperature and experimental measurements, including the maximum predicted temperature near $y = 1.5$ cm, we show the radial profiles of solid temperatures of the smallest and largest particles from this simulation in Fig. 7. The predicted emission temperature depends on solid volume fractions and temperatures of all solid phases. The volume fractions decrease with radius, but the temperatures increase with radius. The result of these competing effects is that the predicted temperature corresponds mostly to the temperature of particles located radially between 0.6 and 0.8 cm. Within this region solid temperature changes little between 1.1 and 1.6 cm above the nozzle, which produces the plateau. In this region the peak particle temperature is close to the gas peak temperature,

and to a large extent the solid phases are heated up by gas. The predicted emission temperature of solid phases based on both volume fractions and temperatures of all solid phases is therefore lower than experimental measurements.

4.2. Comparisons between devolatilization models

Kobayashi's devolatilization model [26] was also employed to investigate the sensitivity to devolatilization models. Reaction rates of Kobayashi's model are slower than Ubhayakar's model by several orders of magnitudes at the same temperature. Therefore, comparison between the two models may also reveal dependency on the choice of devolatilization models. The comparisons are based on predictions with radiation feedback.

The mass fractions of predicted volatile matter and fixed carbon using different devolatilization models in all three solid phases with different particle sizes are compared in Fig. 8 for Ubhayakar's model and in Fig. 9 for Kobayashi's model. In both predictions, all

Fig. 10. Predicted emission temperature between two devolatilization models. Also shown is the axial temperature profile at radius 4 mm.

particles devolatilize completely within 10 to 16 cm above the nozzle, respectively, but devolatilization by Kobayashi's model takes roughly 60% longer due to the fact that its reaction rate is several orders of magnitudes slower. Both models predict a sharp decline of volatile matter mass fraction within the flame front. Indeed, in both models the devolatilization time scale is less than 1 ms when the solid temperature exceeds 1700 K.

The particle burn-out, defined as mass loss fraction of combustible contents (volatile matter and fixed carbon) in this study, depends strongly on particle sizes. However, the predictions on burn-out are close between the two devolatilization models. The

original experiments reported a low combustion efficiency of 38.3%, a volatile release of 44.6% and remaining fixed carbon of 65% [3]. In comparison, the simulations suggest complete devolatilization using either Kobayashi's or Ubhayakar's models. The conversion of char varies with particle sizes at the exit of the simulation domain. The largest particles (35.9 μm) represented in this simulation showed a radial variation of char conversion percentage from 90% to 60% at the exit.

The same emission temperature calculation was also applied to the two temperature predictions with different devolatilization models, as shown in Fig. 10, and was found to be very close for both models. Also shown in the figure are the axial temperature profiles at radius $r = 4$ mm, approximately where the largest temperature deviation between the two devolatilization models is observed. Although temperature predictions of gas and particles may be different by up to 200 K, the prediction of the pyrometer readout is only weakly affected by the choice of devolatilization model.

4.3. Comparisons between with and without radiation

Temperature predictions without radiation feedback are shown in Fig. 11. Temperature differences between the with and without radiation cases are further illustrated in Fig. 12 to emphasize the effects of radiation. Temperature differences are calculated between with and without radiation at each grid point.

The temperatures of gas and solid phases have similar trends to those with radiation since they are controlled by chemical reactions (Fig. 5). However, the gas phase temperature drops by about 280 K at the centerline 20 cm above the nozzle due to radiation. Although the CH_4 combustion has finished within 10 cm above the nozzle, where the gas phase temperature peaks, gas phase temperature without radiation (Fig. 11) does not drop with gas phase diffusion. This is due to the heat transfer from burning particles to gas.

Fig. 11. Temperatures of separate phases without radiation. From left to right: gas, solid phase 1 (16.6 μm), solid phase 2 (24.8 μm) and solid phase 3 (35.9 μm). White space indicates areas with negligible particle contents.

Fig. 12. Temperature differences of each phase between with and without radiation. From left to right: gas, solid phase 1 (16.6 μm), solid phase 2 (24.8 μm) and solid phase 3 (35.9 μm). White space indicates areas with negligible particle contents.

Fig. 13. Radiative heat sources of each phase. From left to right: gas, solid phase 1 (16.6 μm), solid phase 2 (24.8 μm) and solid phase 3 (35.9 μm). Unit is $\text{cal}/(\text{cm}^3 \text{ s})$.

Solid phase temperatures demonstrate stronger cooling effects due to radiation (Fig. 12). The temperature differences demonstrate consistent variations with respect to the flame temperatures. This suggests that within this flame the primary cooling effects overrule other potential secondary effects, such as dilation, velocity, a shift of flame position, etc. The smallest particles (solid phase 1 in this study) may have a temperature difference over 400 K. Larger particles are more sensitive to radiation because of relatively weaker convective heat transfer. Diffused combustion products (gases and particles) away from the flame ($r > 1.5 \text{ cm}$ and

$y > 15 \text{ cm}$) at lower temperature absorb radiation from the flame and acquire slightly higher temperature. Cooler particles near the inlet also absorb radiation emitted from the flame.

Radiative heat sources are shown in Fig. 13 and appear to be mostly negative (emission is stronger than absorption) in flame regions. The magnitudes of the radiative heat source align with the temperature of that phase. Both observations confirm that emission dominates radiation in this flame. The cooling effects from these radiative heat sources are not instantaneous and depend on residence time. This is also observed in Fig. 12, e.g.,

Fig. 14. Comparison of gas species mass fraction between with and without radiation feedbacks. From left to right: CO₂ without radiation, CO₂ with radiation, H₂O without radiation and H₂O with radiation.

Fig. 15. Predicted emission temperature based on 3 and 6 solid phases.

the highest temperature drop is downstream from the peak flame temperature location.

Although radiation feedback is limited to the radiative heat sources in the energy conservation equations only, it also produces indirect effects on other flow variables, such as species concentrations through the temperature-dependent reaction rates. In Fig. 14 the CO₂ and H₂O mass fractions are compared for the cases with and without radiation. With radiation the CO₂ mass fraction is reduced downstream (i.e., $y > 10$ cm). In this region radiative heat loss causes gas and particle temperatures in the flame to drop by over 200 K and 400 K, respectively. This temperature drop significantly reduces char reaction rates and leads to a lower prediction of CO₂ levels. However, as shown in Fig. 4, the CO₂ prediction with radiation has satisfactory agreement with experiments. This indicates the success of the radiation model. The mass fraction of

H₂O is also affected, but to a lesser extent. This is because in the current model H₂O is formed from hydrogen elements in coal particles through devolatilization and volatile combustion. Both processes complete in the upstream (i.e., $y < 15$ cm) where coal particles are heated and yield the same H₂O generation.

This laboratory coal flame was found to be optically thin. The amounts of self absorption for both gas and solid phases were found to be less than 1%. Therefore, the nongray radiation model employed here might be an overkill since an optically thin approximation is sufficient. However, the k -distribution model that we employed here is based on the latest spectroscopic databases that ensure correct calculation of emission. Additionally, the new radiation model introduced here is applicable for arbitrary optical thickness. Its high accuracy assures that the bottleneck for accuracy will never be the radiation among this set of multiphysical models. A demonstration of an optically thicker flame is underway.

4.4. Effects of number of phases

To investigate the effects of the choice of the number of solid phases, a simulation was performed using 6 solid phases, while fixing all other models in the baseline model set. The nominal particle sizes are 11.6, 17.8, 22.5, 26.4, 30.9 and 39.2 μm , respectively. It was found that the general dependency of all flow variables on particle sizes is unchanged. The comparison of the emission temperature between 3 and 6 solid phases is shown in Fig. 15. The predicted emission temperature improves slightly with the number of phases in the downstream region.

It is clear that only small particles can achieve a high temperature within a short distance (e.g., 5 cm) from the nozzle, because of their faster thermal response. It appears that the detector rejects weak radiation from large particles and returns a number biased toward maximum temperature of smallest particles along the line of sight. More information about the detectors is needed to determine the exact cause of underprediction. One cause is random ignition of the smallest particles that lead to temperature fluctuations not predicted. A second possible cause is that the detector reaches its detection limit, which is suggested by the sudden change of

over 1000 K in the experimental measurements near 2 cm. The third possible reason is that soot temperature may dominate pyrometer readout before coal particles ignite.

5. Conclusions

In this work, we report a new Favre averaging method based on gas phase density applied to the Eulerian–Eulerian approach of turbulent multiphase reacting flows. The advantages of Favre averaging in gaseous combustion are retained. Besides, the new Favre averaging method can reproduce turbulent dispersions of mass, momentum, heat and species in the solid phases from their averaged transport equations. It preserves commutation between Favre average and other linear operators, because the same gas density is employed as the Favre weight. This is found crucial in deriving interphase coupling terms. A new radiation model that can account for nongray gas–solid mixtures is developed for pulverized coal flames. The new models are validated against a pulverized coal ignition flame. Predictions of velocity, temperature and gas major species are found satisfactory.

Temperatures of solid phases demonstrate stronger dependency on sizes than velocity. Smaller particles that have shorter thermal response time follow gas phase temperature more closely. Smaller particles are crucial to the prediction of early ignition, while large particles sustain a longer flame. Pyrometer temperature measurements do not reflect either individual particle temperatures as they are size-dependent, or temperature along the centerline. A radiation transport integration along radial direction determines the radiation intensity at two wavelengths arriving at the pyrometer, and predicts pyrometer readout successfully.

Special attention is paid to demonstrate the importance of radiation in this flame. It is found that radiation cooling effects can lead to a 500 K temperature decline in solid phases. Radiation also has indirect influence on CO₂ predictions through the slow yet strongly temperature-dependent char reaction rates. The consideration of radiation improves predictions of both temperature and CO₂.

Simulation results demonstrate weak dependency on devolatilization model compared to the reaction rate differences between devolatilization models. Increasing the number of solid phases does not change general dependency of all flow variables on particle sizes.

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References

- [1] L.D. Smoot (Ed.), *Fundamentals of Coal Combustion*, Elsevier, 1993.
- [2] S.M. Hwang, R. Kurose, F. Akamatsu, H. Tsuji, H. Makino, M. Katsuki, *Energy Fuels* 19 (2) (2005) 382–392.
- [3] S.M. Hwang, R. Kurose, F. Akamatsu, H. Tsuji, H. Makino, M. Katsuki, *JSME Int. J.* 49 (4) (2006) 1316–1327.
- [4] S.M. Hwang, R. Kurose, F. Akamatsu, H. Tsuji, H. Makino, M. Katsuki, *JSME Int. J.* 49 (4) (2006) 1328–1335.
- [5] C.T. Crowe, J.D. Schwarzkopf, M. Sommerfeld, Y. Tsuji, *Multiphase Flows with Droplets and Particles*, second ed., CRC Press, 2011.
- [6] A. Bermudez, J.L. Ferrin, A. Linan, L. Saavedra, *Combust. Flame* 158 (9) (2011) 1852–1865.
- [7] B.M. Franchetti, F.C. Marincola, S. Navarro-Martinez, A.M. Kempf, *Proc. Combust. Inst.* 34 (2) (2013) 2419–2426.
- [8] N. Hashimoto, R. Kurose, H. Shirai, *Fuel* 97 (2012) 277–287.
- [9] K. Luo, H. Wang, J. Fan, F. Yi, *Energy Fuels* 26 (10) (2012) 6128–6136.
- [10] O.T. Stein, G. Olenik, A. Kronenburg, F. Cavallo Marincola, B.M. Franchetti, A.M. Kempf, M. Ghiani, M. Vascellari, C. Hasse, *Flow Turbul. Combust.* 90 (2013) 859–884.
- [11] X. Zhao, D.C. Haworth, *Combust. Flame* 161 (7) (2014) 1866–1882.
- [12] L. Zhou, *Numer. Heat Transfer B* 47 (2) (2005) 179–197.
- [13] R. Jackson, *Chem. Eng. Sci.* 52 (15) (1997) 2457–2469.
- [14] T. Poinsot, D. Veynante, *Theoretical and Numerical Combustion*, second ed., R.T. Edwards, Inc., 2005.
- [15] F. Mashayek, R.V.R. Pandya, *Progr. Energy Combust. Sci.* 29 (4) (2003) 329–378.
- [16] M.F. Modest, *Radiative Heat Transfer*, third ed., Academic Press, New York, 2013.
- [17] R. Viskanta, M.P. Mengüç, *Progr. Energy Combust. Sci.* 13 (1987) 97–160.
- [18] J. Cai, R. Marquez, M.F. Modest, Comparisons of radiative heat transfer calculations in a jet diffusion flame using spherical harmonics and k-distributions, *J. Heat Transfer* 136 (11) (2014) 112702, <http://dx.doi.org/10.1115/1.4026169>.
- [19] J. Cai, M.F. Modest, Absorption coefficient regression scheme for splitting radiative heat sources across phases in gas particulate mixtures, *Powder Technol.* 265 (2014) 76–82, <http://dx.doi.org/10.1016/j.powtec.2014.01.026>.
- [20] M. Syamlal, W. Rodgers, T.J. O'Brien, *MFI Documentation: Theory Guide*, Technical Note, DOE/METC-94/1004, 1993.
- [21] D. Merrick, *Fuel* 62 (1983) 540–546.
- [22] S.B. Pope, *Turbulent Flows*, Cambridge University Press, Cambridge, 2000.
- [23] B.F. Magnussen, The Eddy dissipation concept: a bridge between science and technology, in: *ECCOMAS Thematic Conference on Computational Combustion*, Lisbon, Portugal, 2005.
- [24] S.B. Pope, *Comb. Flame* 139 (2005) 222–226.
- [25] Shivadev K. Ubhayakar, David B. Stickler, Charles W. Von Rosenberg Jr., Richard E. Gannon, *Symp. (Int.) Combust.* 16 (1) (1977) 427–436.
- [26] H. Kobayashi, J.B. Howard, A.F. Sarofim, *Symp. (Int.) Combust.* 16 (1) (1977) 411–425.
- [27] R.J. Hamor, I.W. Smith, R.J. Tyler, Kinetics of combustion of a pulverized brown coal char between 630 and 2200K, *Comb. Flame* 21 (2) (1973) 153–162.
- [28] R. Viskanta, A. Ugnan, M.P. Mengüç, Predictions of Radiative Properties of Pulverized Coal and Fly-Ash Polydispersions, ASME paper no. 81-HT-24, 1981.
- [29] R.O. Buckius, D.C. Hwang, *J. Heat Transfer* 102 (1980) 99–103.
- [30] M.F. Modest, *J. Quant. Spectrosc. Radiat. Transfer* 76 (1) (2003) 69–83.
- [31] A. Wang, M.F. Modest, *J. Quant. Spectrosc. Radiat. Transfer* 93 (2005) 245–261.
- [32] J. Cai, M.F. Modest, *J. Quant. Spectrosc. Radiat. Transfer* 141 (2014) 65–72.