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STATE SPACE SENSITIVITY TO A PRESCRIBED PROBABILITY DENSITY FUNCTION SHAPE IN COAL COMBUSTION SYSTEMS: JOINT β-PDF VERSUS CLIPPED GAUSSIAN PDF

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The turbulent transport of three coal off-gas mixture fractions is coupled to a prescribed joint β-probability-density-function (β-PDF) mixing model. This physical transport and subgrid joint β-PDF mixing model is used to explore the incorporation of coal off-gas compositional disparities between the devolatilization and the char oxidation regime in detailed pulverized-coal combustion simulations. A simulation study of the University of Utah pulverized-coal research furnace is presented to evaluate the sensitivity of different mixing model assumptions. These simulation studies indicate that using a variable composition to characterize the process of coal combustion does not appreciably change the predicted gas-phase temperature field. Moreover, neglecting fluctuations in the char off-gas stream was found to change gas-phase temperature predictions by approximately 15%. State space variable sensitivity to the assumed shape of the PDF (clipped Gaussian vs. joint β) is presented. Simulation results indicate differences in temperature profiles of as much as 20% depending on the chosen shape of the PDF. Integration accuracy issues for the joint β-PDF are presented and are found to be acceptable. A robust β-PDF function evaluation procedure is presented that accommodates arbitrarily high β-PDF distribution factors. This robust algorithm simply transforms the joint β-PDF function evaluation into a logarithmic form. The assumption that a joint PDF, as rigorously required within a prescribed subgrid mixing model, can be written as the product of $N - 1$ statistically independent probability density functions is quantified and shown to be less accurate.

Introduction

The ability to accurately numerically simulate pulverized-coal furnaces relies on adequately describing the transfer of coal off-gas to the gas phase. Assuming that the reaction process is micromixing limited, the chemical state of the particular node in the reactor domain can be calculated based on equilibrium considerations alone given the degree of "mixedness" [1]. Under the assumptions of equal mass diffusivities, individual transport equations for the species present in each physical stream can be replaced by $N - 1$ scalar transport partial differential equations, where N represents the total number of distinguishable physical streams (e.g., primary air, secondary air, and coal off-gas).

Current pulverized-coal simulators frequently treat the coal off-gas originating from the devolatilization pathways and char oxidation pathways as a single stream [1–3]. Therefore, the use of a single coal off-gas turbulent mixture fraction progress variable falsely assumes that the composition of coal off-gas throughout the combustion regime is uniform.

Flores and Fletcher [4] postulated that there indeed exists a coal off-gas compositional effect by utilizing two coal off-gas mixture fractions in the coal combustion simulation code PCGC-3. In this multiple mixture fraction formulation, the coal off-gas was separated into two streams: one stream was used to describe the transfer of coal off-gas originating from the devolatilization pathway, while the second coal off-gas stream described the transfer of mass to the gas phase due to the heterogeneous char oxidation pathway. Furthermore, it was assumed that fluctuations in the char off-gas stream were negligible, and the required joint probability density function (PDF) was written as the product of individual clipped Gaussian probability density functions [1,3]. Therefore, Flores and Fletcher [4] wrote the overall joint PDF as

$$P(f, \eta_v, \eta_h) = P(f)P(\eta_v) \quad (1)$$

where f is defined as the mixture fraction of primary stream; η_v and η_h are defined as the mixture fraction of volatiles and char off-gas, respectively.

Recently, Sami et al. [5] and Dhanapalan et al. [6] constructed a multiple mixture fraction formulation in coal-blend combustion applications. In this formulation, the three independent mixture fractions for primary air, coal off-gas, and manure off-gas were

calculated, and mean state space variables (e.g., temperature, species concentration) were again computed by convolution over the product of the assumed statistically independent clipped Gaussian PDFs. No quantification of simulation sensitivity to this presumed statistical independence assumption was provided.

The clipped Gaussian formulation assumes that the intermittency of stream i can be represented by the portions of the integrals that are beyond the physical limits of the mixture fraction [1,3]. Therefore, the continuous PDF can be expressed as

$$P(f) = \alpha_p + \alpha_s + P(f)|_0^1 \tag{2}$$

where α_p and α_s are the intermittency of the primary and secondary stream, respectively, and are defined as

$$\alpha_p = \int_1^\infty P(f)df \tag{3}$$

and

$$\alpha_s = \int_{-\infty}^0 P(f)df \tag{4}$$

The convolution of the state space function over the required PDF, under the presumed shape of the clipped Gaussian PDF, introduces $4(2^{N-1}) - 1$ total terms to be evaluated [7]. This increase in the total number of terms is a natural consequence of the clipped Gaussian mathematical construct. Therefore, the numerical convolution can be highly computationaly intensive as the dimensionality of the PDF increases, as noted by Sami et al. [5].

Joint β-PDF Formulation

In each of the aforementioned studies, the required joint PDF has been substituted in favor of the product of the assumed, statistically independent individual mixture fraction PDF; for example, see equation 1. Methods toward the construction of the joint PDF are, therefore, warranted to evaluate the introduced error associated with this common statistically independent assumption.

The formulation described by Girimaji [8] provides a technique whereby the univariate β-PDF is extended to an arbitrary dimensional joint β-PDF. The joint PDF, which can be used to model the mixing of N scalars, is given by

$$P(f_1, f_2 \ldots f_{N-1}) = \frac{\Gamma(a_1 + a_2 \ldots + a_N)}{\Gamma(a_1)\Gamma(a_2)\ldots\Gamma(a_N)} f_1^{a_1-1} f_2^{a_2-1} \ldots f_N^{a_N-1} \tag{5}$$

where f_i is the mass fraction of species originating from stream i, a_i represents the joint β-PDF distribution parameters given by equation 6, and $\Gamma(a_i)$ represents a gamma function evaluation of argument a_i. (Note that the joint PDF is written for mixture fractions such that $\Sigma_{i=1}^N f_i = 1$.)

$$a_i = \tilde{f}_i\left(\frac{1 - S}{\tilde{q}} - 1\right) \tag{6}$$

The variable S represents the sum of squares of the mean mixture fractions,

$$S = \sum_{i=1}^N \tilde{f}_i^2 \tag{7}$$

and the fluctuating Favre-averaged turbulent scalar energy, $\tilde{q}$, is defined as the sum over all mean variances

$$\tilde{q} = \sum_{i=1}^N \tilde{g}_i \tag{8}$$

As presented, the construction of the joint β-PDF requires only the solution of $N - 1$ transport equations and the Favre-average fluctuating turbulent scalar energy, $\tilde{q}$. The variable $\tilde{q}$ can be calculated either by solving the individual N variance equations [1,9], or by the suggested transport equation given by Girimaji [8] that calculates $\tilde{q}$ directly,

$$\frac{\partial}{\partial t}\tilde{q} + \tilde{u}_j \frac{\partial}{\partial x_j}\tilde{q} = \sum_{i=1}^N \frac{\partial}{\partial x_j}(-f_i'' \tilde{f}_i'') - 2\sum_{i=1}^N u_i' f_i' \frac{\partial \tilde{f}_i}{\partial x_i} - 2\varepsilon_f \tag{9}$$

The first term on the right-hand side represents the transport of scalar energy due to velocity fluctuations and can be modeled by a gradient-diffusion model. The next term on the right-hand side is the production of turbulent scalar energy. The last term on the right-hand side is the dissipation of turbulent scalar energy and is modeled by

$$\varepsilon_f = C\frac{\varepsilon}{k}\tilde{q} \tag{10}$$

where ε is the turbulent energy dissipation, k is the turbulent energy production, and C is a numerical constant of the order unity [8].

Since the physical range of the mixture fraction is the same as the continuous portion of the β-PDF, the process of clipping the PDF, as described in the previous section, is moot. Intermittency is a natural feature of the β-PDF and occurs when any distribution parameter is less than unity [10].

Model Description

The CFD-based combustion simulation is based on the models developed by Smith and coworkers over a time spanning the last 20 years. In this combustion simulator, turbulent momentum closure is

TABLE 1
Experimental Operating Conditions

Case	Primary Flow Rate (kg/s)	Primary Temperature (K)	Coal Firing Rate (kg/s)
U1	0.011751	505	9.79×10^{-4}
U2	0.011058	505	9.63×10^{-4}

obtained using Boussinesq gradient diffusion with a nonlinear k-ε model [11,12]. As already discussed, a prescribed PDF mixing model is used to adequately model subgrid mixing effects. The gas-phase reaction model is capable of using both equilibrium, for coal combustion applications, and a reduced manifold method for non-coal combustion applications [13,14].

We used the S6 approximation in the discrete ordinates method for solving the radiative transfer equation as demonstrated in complex combustion applications by Smith and Adams [15]. Particle history effects including heterogeneous particle phase chemistry [2] and coal devolatilization [16] are included.

A Lagrangian cloud tracking model is used to determine the mean location of a cloud of particles and its spatial variance, or dispersion [17]. Properties within the cloud are ensemble averaged over the entire domain encompassed by the cloud [18]. This coupled computational fluid dynamics code has served as a tool for the simulation of a wide range of applications including coal-fired and natural-gas-fired boilers [2,14], process heaters [15], and both metallurgical and waste incineration processes [19].

Simulation Results

In this section, simulation cases of the University of Utah pulverized-coal furnace are presented to evaluate the sensitivity of an assumed non-fluctuating char oxidation off-gas stream, state space sensitivity to the chosen PDF shape, and the assumption of writing the joint PDF as a product of $N - 1$ statistically independent PDFs.

The University of Utah multifuel combustion research furnace is down-fired with a nominal firing rate of 29 kW. The combustion chamber is 0.16 m in diameter with an overall length of 7.3 m. Ports along the length of the furnace are available for extracting samples and injecting air or fuel. Gas-phase temperature measurements were obtained using a suction pyrometer with an estimated suction velocity of 180–210 m/s, depending on sampling location. Detailed plans and sampling protocols for the University of Utah bench-scale furnace were presented by Spinti [20].

In each of the three-dimensional premixed burner simulation studies presented, a coarse mesh size of $20 \times 17 \times 17$ is used. Only the first 2.2 m of the furnace is simulated. The low-resolution simulation grid allows a multitude of simulation cases to be efficiently run, which is useful in evaluating the sensitivity to different mixing model assumptions. All cases were run on an SGI Octane work station. Each of the reported simulation cases includes a six-particle-size bin with five Lagrangian cloud starting locations for each particle size and reactivity. The char oxidation submodel was described by Domino and Smith [2]; salient features of the model include thermal annealing, ash film resistance, and a char oxidation reactivity distribution.

The finite difference equations for the three components of velocity, k, ε, the pressure correction, the pressure and all appropriate mean mixture fraction and variance progress variables were solved until the maximum of all the finite difference equation residuals was less than 3.5 [13]. Table 1 presents the operating conditions taken from the literature for the two experimental cases simulated where Pittsburgh #8 coal was fired: experimental case U1 and U2 [21].

Char Fluctuation Effects

The specification of the residual char off-gas stream to be that of the parent coal results in a multiple-η case with a uniform coal off-gas composition. This specification allows direct validation of the assumption of a non-fluctuating char off-gas stream and the validity of writing the joint PDF as a product of individual uncorrelated PDFs.

Previous pulverized-coal simulation studies postulated that fluctuations in char off-gas can be ignored [4,22]. In this formulation, the turbulent mixing of coal off-gas comprises two streams: volatile and char. A char composition is specified and an average volatile composition is calculated based on an overall conversion of raw coal to volatiles [22]. Therefore, assuming that a variable volatile:char split is available (i.e., the devolatilization model affords the prediction of a non-uniform split, as is the case when using two independent devolatilization reactions), this technique conserves overall mass balance, yet allows a breach in local mass balance. Flores [22] did not provide sensitivity studies to the stated assumptions of a non-fluctuating char oxidation stream and local mass non-conservation. Moreover, quantification of the inherent assumption mathematically shown in equation 1 was not provided.

To test the assumption of a non-fluctuating char oxidation off-gas stream, a simulation case that included two coal off-gas mixture fractions was developed. This simulation case, Eta2, is based on the coal off-gas mixture fraction formulation as described by Flores [22] and Flores and Fletcher [4]. The residual

char composition was set to that of the parent coal, and two simulation cases were run: one with char off-gas fluctuations and one without. A prescribed clipped Gaussian PDF shape was used, and the joint coal off-gas compositional PDF was assumed to be separable,

$$\tilde{P}(\eta_v, \eta_h) = \tilde{P}(\eta_v)\tilde{P}(\eta_h) = \tilde{P}(\eta) \qquad (11)$$

Figure 1 is a plot that compares the effect of a non-fluctuating char oxidation stream and the PDF independence assumption. Table 1 describes the appropriate operating firing conditions for the University of Utah premixed experimental case U1. Fig. 1 clearly indicates the significance of the fluctuating char off-gas stream and indicates that ignoring fluctuation effects of the char off-gas stream can lead to differences in predicted temperature of up to 15%. Comparing case Eta2 with char fluctuations to case Eta (the uniform single coal off-gas mixture fraction PDF) indicates that the assumption of statistical PDF independence is not appropriate.

Joint β-PDF Study

As described in equation 5, the β-PDF requires a gamma function evaluation for individual distribution parameters, $\Gamma(a_i)$ and sums of distribution parameters, $\Gamma(a_1 + a_2 + \ldots + a_N)$. Unfortunately, mean values with low variances yield calculated distribution parameters that give rise to numerical overflow when the gamma function evaluation is attempted. Machine overflow occurs at approximately $\Gamma(170)$. Typical distribution parameters can range from slightly less than unity to greater than 1000.

Various techniques can be used in an attempt to extend the point at which machine overflow occurs. One such method is to replace the entire gamma function evaluation by an integration [9]. Therefore, the following integration is substituted into equation 5:

$$\int_0^1 \int_0^{1-f_1} \int_0^{1-f_1-f_2} \cdots \int_0^{1-f_1-f_2-\ldots-f_{N-1}} \tilde{P}(f_1, f_2, \ldots, f_{N-1}) df_1 df_2 \ldots df_{N-1} = \frac{\Gamma(a_1)\Gamma(a_2)\ldots\Gamma(a_N)}{\Gamma(a_1 + a_2 \ldots + a_N)} \qquad (12)$$

thereby eliminating the need for gamma function evaluations.

Although the use of equation 12 extends the robustness of the gamma function evaluation, distribution parameter values greater than approximately 800 fail due to machine underflow problems. Another technique, which has been proposed by Chen et al. [9], is renormalization of the distribution parameters. In this technique, the underflow problem is circumvented by normalizing the maximum β-PDF distribution parameter to a value that does not result in machine underflow, for example, 600 [9]. All other distribution parameters are appropriately scaled such that the ratio of any two distribution parameters is exactly equal to the prenormalized ratio. This process ensures that the maximum value of the PDF remains somewhat constant, yet it artificially augments the physical mixing effect by increasing the modeled variance of the system. Nevertheless, the technique of renormalization has been reported in the literature to perform well when the integration of equation 12 fails due to a high distribution factor and low mixture fraction [9].

The most robust β-PDF evaluation involves recasting the joint PDF to natural logarithm form, thus eliminating the overflow (equation 5) and underflow (equation 12) problem associated with large distribution factors. Function evaluations of the joint β-PDF, as required for any chosen integration algorithm, are obtained by first taking the natural logarithm of the joint β-PDF:

$$\ln(P(f_1, f_2 \ldots, f_{N-1})) = \ln\left(\frac{\Gamma(a_1 + a_2 \ldots + a_N)}{\Gamma(a_1)\Gamma(a_2)\ldots\Gamma(a_N)} f_1^{a_1-1} f_2^{a_2-1} \ldots f_N^{a_N-1}\right) \qquad (13)$$

Simplification of equation 13 yields

$$\ln(P(\eta_1, \eta_2 \ldots, a_{N-1})) = \ln(\Gamma(a_1 + a_2 \ldots + a_N)) - \sum_{i=1}^{N} \Gamma(f_i) + \sum_{i=1}^{N-1} (a_i - 1)\ln(f_i) + (a_N - 1)\ln(f_N) \qquad (14)$$

The precise function evaluation of the β-PDF is simply obtained by taking the exponential of equation 14. This novel formulation perfectly extends the use of the β-PDF to an arbitrarily high distribution factor [21], since most gamma function numerical algorithms are cast within a natural logarithm formulation. Integration of the state space function, here taken to be a Gibbs free energy minimization mapping, is done using 10-point Gaussian quadrature [23].

Figure 2 is a comprehensive plot of all uniform composition simulation cases run for experimental case U2. The operating conditions for this experimental case are given in Table 1. The simulation cases presented are as follows: no mixing model, single clipped Gaussian PDF, joint β-PDF with renormalization, joint β-PDF without renormalization, joint β-PDF with three assumed independent clipped Gaussian at distribution parameter overflow, robust joint β-PDF method, and three independent clipped Gaussian PDFs that neglect intermittency effects. A total of three coal off-gas mixture fractions are computed within the context of a two-step devolatilization mechanism [24]. They are the mixture

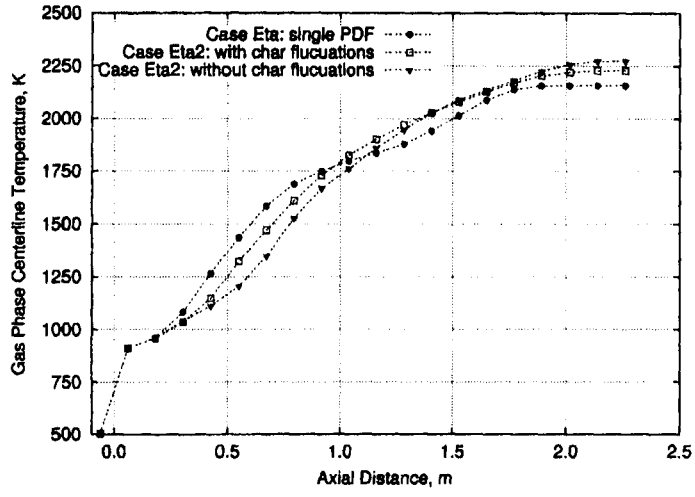

FIG. 1. Simulation comparison of case Eta2, with and without char off-gas fluctuations, to case Eta.

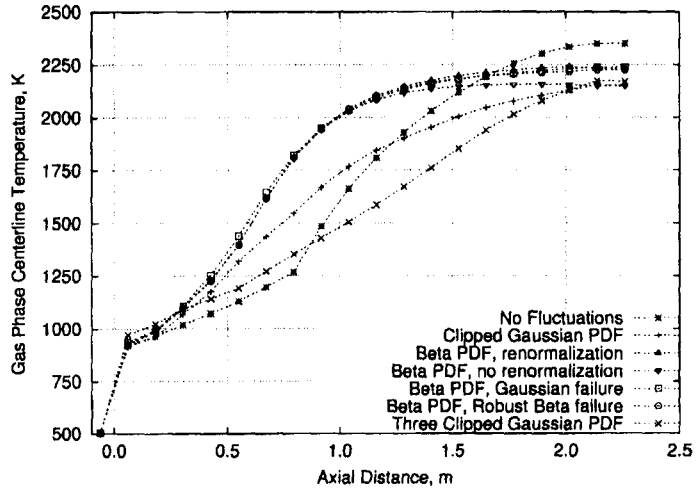

FIG. 2. Summary of the University of Utah bench-scale furnace U2 simulation.

fraction of coal off-gas originating from devolatilization reaction pathway 1, pathway 2, and the coal off-gas originating from the heterogeneous char oxidation pathway. Therefore, the total number of physical streams is four. Four physical streams requires a three-dimensional PDF integration,

$$\tilde{\phi} = \int_0^1 \int_0^{1-\eta_1} \int_0^{1-\eta_1-\eta_2} \phi(\eta_1, \eta_2, \eta_3) \cdot \tilde{P}(\eta_1, \eta_2, \eta_3) d\eta_1 d\eta_2 d\eta_3 \quad (15)$$

Note that the above equation arbitrarily includes the three coal off-gas mixture fraction progress variables.

The plot indicates that the use of three independent clipped Gaussian PDFs at machine overflow is nearly identical to using the robust joint β-PDF. This is expected because the β-PDF is known to coalesce to a Gaussian form at fully mixed conditions. Moreover, the results indicate that the use of renormalization does not augment the physical variance in any appreciable manner. This indicates that machine underflow occurs at nearly negligible mixing effects.

Of clear concern is the disparity of predictions between the joint β-PDF and the single clipped Gaussian shape. In this simulation case, the two differed as much as 20%. The experimental data only serve to indicate that both are in the correct range, not in the applicability of each prescribed PDF shape. The use of three independent clipped Gaussian PDFs also displays a great disparity in predictions both when compared to the single clipped Gaussian PDF case and for all joint β-PDF cases. This substantial difference may be caused by the independence assumption and neglecting the clipped Gaussian intermittent terms.

The number of Gaussian quadrature points required to accurately perform the integration represented in equation 15 depends on the PDF dimension. Fig. 3 represents a typical error plot for a

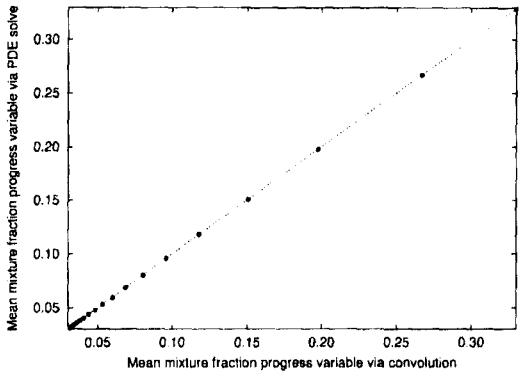

FIG. 3. Typical η_1 convolution error plot for a three-dimensional PDF.

TABLE 2
Individual Coal Off-Gas Stream Compositions

Component %	η	η_1	η_2	η_3
C	81.93	62.23	78.64	95.06
H	5.35	11.70	6.41	1.12
O	10.00	22.57	12.09	1.62
N	1.74	2.01	1.79	1.56
S	0.98	1.49	1.07	0.64

three-dimensional 10-point Gaussian quadrature integration algorithm [23]. Shown in this figure is the mean value of the volatile mixture fraction 1, η_1, calculated by two different methods. Method 1 calculates $\tilde{\eta}_1$ from a partial differential equation transport equation, while method 2 uses the definition of a mean variable within the context of a PDF integration.

$$\tilde{\eta}_1 = \int_0^1 \int_0^{1-\eta_1} \int_0^{1-\eta_1-\eta_2} \eta_1 \tilde{P}(\eta_1, \eta_2, \eta_3) d\eta_1 d\eta_2 d\eta_3 \tag{16}$$

Unfortunately, when the dimensionality of the integration is increased, the accuracy dramatically decreases at fixed Gaussian quadrature points [22]. Increases in the numerical accuracy for a higher-dimensional PDF integration can be obtained by using more fixed points or by the use of the computationally expensive adaptive Gaussian quadrature method [25]. Monte Carlo and quasi–Monte Carlo schemes also represent possible techniques, however, each needs to be further developed in the context of this multidimensional PDF integration [26].

Compositional Disparity Effects

The calculation of multiple coal off-gas mixture fraction progress variables via a partial differential equation solution affords the specification of a residual char composition. The ability to distinguish individual coal off-gas mixture fractions allows capturing the known compositional disparity throughout the devolatilization and char oxidation combustion regime [27]. The specification of the char composition for Pittsburgh #8 coal was given by Spinti [20], and the values used in this simulation study are given in Table 2. Figs. 4 and 5 are axial plots of centerline temperature comparing the effect of a varying coal off-gas composition for experimental case U2. The simulation cases presented are for the cases with and without the use of renormalization. Each plot also contains the experimental data provided within the dissertation by Spinti [20]. As seen, gas-phase temperature is rather insensitive to both the choice of mixing model used at distribution overflow and the use of a multiple coal off-gas composition.

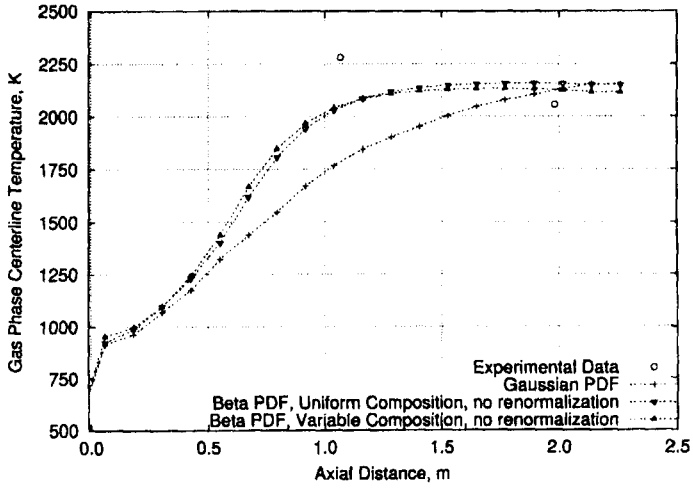

FIG. 4. Axial simulated temperature profiles comparing clipped Gaussian and β-PDF without renormalization.

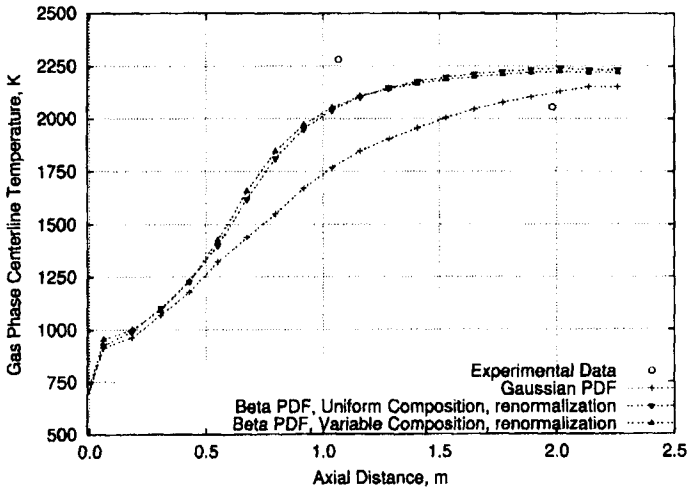

FIG. 5. Axial simulated temperature profiles comparing clipped Gaussian and β-PDF with renormalization.

Conclusions

It has been demonstrated that the procedure of neglecting char oxidation stream fluctuation effects in detailed coal combustion simulations can introduce minor differences in predicted gas-phase centerline temperature. Moreover, in this pulverized-coal combustion application, the assumption that a joint PDF can be written as the product of $N - 1$ statistically independent PDFs has been shown to be highly questionable.

The construction and use of a joint β-PDF within the mixing model has been shown to be feasible in detailed coal combustion simulations and is consistent with the stated assumptions of the prescribed PDF method. The outlined technique of constructing the joint β-PDF allows proper mixing effects when the total number of coal off-gas mixture fractions in detailed coal combustion simulations is augmented.

A robust β-PDF function evaluation technique has been presented. This technique extends the robustness of the β-PDF to arbitrarily high distribution parameters [22]. Although the technique of renormalization [9] was shown to yield similar simulation results, the use of a robust function evaluation is preferred.

The detailed pulverized-coal combustion simulations presented indicate that there exists a substantial state space variable sensitivity to the chosen shape of the PDF. This disparity of the prescribed shape is most likely caused by the highly nonlinear heterogeneous particle-phase chemistry model. Small changes in gas-phase temperature can dramatically change the placement of mass source terms on the Eulerian mesh and can dramatically change the gas-phase fluid dynamics and subsequent dispersion of the calculated Lagrangian clouds. Moreover, a sensitivity to the bulk-phase oxidizer concentration can also change the predicted char oxidation rate [22].

In this numerical simulation study, compositional disparities between the char oxidation and devolatilization regime were not found to be significant in the prediction of gas-phase temperatures. Although state space variables did not show compositional disparity sensitivity, nitric oxide centerline predictions have been shown to be extremely sensitive to coal off-gas compositional disparities [22]. Therefore, the added complexity of the joint PDF mixing model may not be warranted for simulation cases not including detailed nitric oxide calculations.

Nomenclature

a beta function distribution parameter
C model constant for dissipation term in turbulent scalar energy equation
f primary mixture fraction, general mixture fraction
g variance of mixture fraction
k turbulent kinetic energy, m^2/s^2
N number of independent streams
q fluctuating turbulent scalar energy, m^2/s^2
S sum of the squared mean mixture fractions
u gas-phase velocity, m/s

Greek

α intermittency
ε dissipation rate of kinetic energy, m^2/s^2
ϕ dummy space variable, units vary
η coal off-gas mixture fraction

Subscripts

h char
i ith velocity component/mixture fraction; $i = 1, 3$
p primary

s secondary
v volatiles
1 volatile stream 1 coal off-gas mixture fraction
2 volatile stream 2 coal off-gas mixture fraction
3 char off-gas mixture fraction

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