Sensitivity calculations in PDF particle methods

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Abstract

In combustion modeling, it is desirable to know how sensitive the predictions are to certain parameters in the model formulation. In this study, we develop a method for accurate and efficient sensitivity calculation in PDF modeling of turbulent combustion. This method enables the calculation of the sensitivities for each particle in PDF particle methods. These particle-level sensitivities are very revealing. They allow one to examine the particles with the largest sensitivities, and the corresponding compositions reveal the sensitive region of composition space. By ensemble averaging the particle sensitivities, sensitivities of mean (and conditional mean) quantities can be extracted. The method is applied to the PDF calculations of the oxidation of diluted hydrogen in a partially stirred reactor (PaSR) using three different mixing models. It is demonstrated that the method is capable of accurately calculating the sensitivities at the particle level. The study also illustrates the qualitatively different behavior of the three mixing models as revealed by both the particle composition and the particle sensitivities. The sensitivities of mean (and conditional mean) quantities reveal the controlling processes in a PaSR. They confirm that when combustion is controlled by mixing, the combustion is insensitive to chemistry; when the system is close to global extinction, the combustion is extremely sensitive both to mixing and to chemistry.
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1. Introduction

Modeling combustion phenomena requires the knowledge of chemical kinetics, transport properties, turbulence/combustion model parameters, etc. as input parameters, and produces predictions (such as species concentration profiles, flame speed, etc.) as the output, with the input and the output connected by the governing model equations. Often it is desirable to know how sensitive the predictions are to certain parameters in the model formulation. Sensitivity analysis is a formal approach to examine quantita-

tively the relationship between the parameters and the output of the model. Since it was introduced to combustion research, it has been widely used in understanding and improving chemical kinetic models, in uncertainty analysis, and in gaining insight into the model performance. Examples of the application of sensitivity analysis in chemical kinetics and laminar flames can be found in [1–9]. For example, sensitivity analyses have been performed on elementary reaction rates. Thus, without solving the problem repetitively with different values for the rate constants, sensitivity analysis allows one to understand how the model responds to changes in the rate parameters. It also provides insight about how important certain reaction pathways are to the model's predictions.

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In the fields of chemical kinetics and laminar flames, tools and softwares for sensitivity analysis are well developed. For example, a series of computer codes (e.g., SENKIN [10], CHEMKIN [11], CANTERA [12]) have been developed. These codes have been used as a routine procedure in kinetic modeling and sensitivity analysis for homogeneous gas phase reactions.

For turbulent combustion calculations, it would be equally valuable to perform sensitivity analysis, but the tools are less well developed. For example, in modeling turbulent reactive flows based on PDF methods [13], it is valuable to know the sensitivity of the predictions to the mixing model constant as well as to other parameters. In the past, somewhat crude analyses have been performed to evaluate sensitivities by repeating a calculation with a single parameter changed by a small amount. This divided difference technique has been used to show the strong sensitivity of some PDF calculations of turbulent flames to the temperature of a pilot stream [14,15], to a reaction rate [16], and to the mixing model constant C_ϕ governing the rate of turbulent mixing [14,17–19]. However, using divided differences in the Monte Carlo methods used to solve the PDF equations is costly and inefficient, as the statistical errors need to be reduced so as to be small compared to the differences in the two calculations.

In this study, we develop a method for the accurate and efficient calculation of sensitivities in PDF modeling of turbulent combustion. This method is demonstrated in the PDF calculation of a partially stirred reactor (PaSR) burning a hydrogen–air mixture with three different mixing models: interaction by exchange with the mean (IEM or LMSE) model [20,21]; the modified Curl mixing (MC) model [22]; and the Euclidean minimum spanning tree (EMST) model [23,24]. With the IEM model, accurate sensitivities can be obtained by other means and hence can be used to validate the accuracy of the method.

The remainder of the paper progresses as follows. In Section 2, the mathematical formulation of the sensitivity calculation in PDF particle methods is outlined. In Section 3, the sensitivity calculations in a PaSR are described. Results and comparisons are shown in Section 4. Conclusions are drawn in Section 5.

2. Formulation

2.1. Sensitivity equation

In a PDF calculation of a reactive flow involving n_s species, with the Monte Carlo techniques [13], the

distribution of compositions is represented by an ensemble of N particles. The composition $\boldsymbol{\phi}^{(n)}$ of the nth particle consists of the n_s species-specific moles (denoted by $\mathbf{z}$, kmol/kg, mass fractions divided by the corresponding species molecular weights) and enthalpy, i.e., $n_\phi = n_s + 1$ quantities. In the PDF calculation, the change in particle composition due to reaction is treated exactly, while molecular mixing is represented by mixing models (e.g., IEM, MC, EMST) which prescribe the evolution of the particles in composition space such that they mimic the change in the composition of a fluid particle due to molecular mixing in a turbulent reactive flow. We consider a set $\mathbf{a} = \{a_1, a_2, \ldots, a_{n_a}\}$ of n_a sensitivity parameters. These could be the temperature of an inflowing stream; a species mass fraction in an inflowing stream; a pre-exponential factor or an activation energy in a reaction rate; or the mixing model constant. In a fuller notation, $\phi_i^{(n)}(t; \mathbf{a})$ denotes the ith composition of the nth particle at time t for a PDF calculation performed with the sensitivity parameters having the values $\mathbf{a}$. The $n_\phi \times n_a$ sensitivity matrix $\mathbf{W}^{(n)}(t; \mathbf{a})$ (for the nth particle at time t) is then defined by

$$W_{ij}^{(n)}(t; \mathbf{a}) \equiv \frac{\partial \phi_i^{(n)}(t; \mathbf{a})}{\partial a_j}. \tag{1}$$

In general, in the PDF calculation of a reactive flow, the evolution equation for $\boldsymbol{\phi}^{(n)}(t; \mathbf{a})$ is given by

$$\frac{d\phi_i^{(n)}(t; \mathbf{a})}{dt} = S_i\big(\boldsymbol{\phi}^{(n)}(t; \mathbf{a}); \mathbf{a}\big) + C_\phi M^{(n)}\big(\{\phi_i(t; \mathbf{a})\}\big), \tag{2}$$

where $\mathbf{S}$ is the rate of change due to chemical reactions, C_ϕ is the mixing model constant, and $M^{(n)}$ denotes the effect of the mixing model, which depends on the ensemble $\{\boldsymbol{\phi}\}$ of particle compositions. For the IEM model we have

$$M^{(n)}\big(\{\phi_i(t; \mathbf{a})\}\big) = \frac{1}{2\tau_t}\big(\tilde{\phi}_i - \phi_i^{(n)}\big), \tag{3}$$

where $\tilde{\boldsymbol{\phi}}$ is the Favre mean composition (i.e., the ensemble average of particle compositions $\{\boldsymbol{\phi}\}$) and τ_t is the characteristic turbulence time scale. To compute the sensitivity matrix $\mathbf{W}^{(n)}(t; \mathbf{a})$ for each particle, we make the following assumptions:

- We neglect the change in density $\rho^{(n)}(t)$ due to changes in the parameters, i.e., we assume that $\partial \rho^{(n)}(t)/\partial a_j$ is negligible. Hence the velocity and turbulence fields are (by assumption) independent of infinitesimal changes in $\mathbf{a}$.
- We neglect nonlinear effects in the mixing models. The IEM (see Eq. (3)) and MC mixing models are linear in the composition, as is the under-