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Spatial gradients of conditional averages in turbulent flames

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ABSTRACT

Data from the two different methane/air jet experimental databases is examined to understand the effects of spatial variations in the conditional averages of reactive scalars in the context of the Conditional Source-term Estimation (CSE) model, with particular emphasis on the double-conditional version, DCSE. Data from all spatial locations and from the four turbulent flames in the Sandia/TUD database are averaged together to generate a global, two-condition (mixture fraction and a species-based reaction progress variable) conditional average; it is found that the conditional fluctuations around this new, two-condition conditional average do not exhibit any significant dependence on either spatial location or even on Reynolds number. Furthermore, the normalized RMS of the conditional fluctuations are found to be dramatically lower than those seen using only one condition. These results indicate that the two-condition conditional averages in the Sandia/TUD piloted methane/air flame series do not vary in space, nor vary with Reynolds number. In the Sydney Swirl burner data, the two-condition conditional averages exhibit modest gradients in space which are attributed to heat transfer with the bluff body in the flow; when a third condition is added – based on the total enthalpy – the spatial gradients in the conditional average of temperature a dramatically reduced. In both of the cases tested, the normalized RMS of the conditional fluctuations around both the two- and three-condition conditional averages are relatively small. These results imply that, in a simulation of these flames using DCSE, one would be better off ignoring spatial variations in the conditional averages and instead collecting all of the spatial data together for the integral equation inversion using either two or three conditioning variables in a single, global ensemble species involved in relatively slow chemistry, such as NO. The results also imply that the underlying assumptions in DCSE – that the conditional variances and the spatial gradients in the conditional averages are both negligible – are valid when sufficient conditioning variables are used, at least for the flames considered.

1. Introduction

In Conditional Moment Closure (CMC) models [1], one derives and solves transport equations for the conditional averages of reactive scalars. These transport equations require closure for several terms. A common closure for several of these terms is often to simply neglect them. The solution space in which the equations are then solved includes the conditioning variable as a new independent variable. To reduce the computational cost, a common practice is to solve on a very coarse computational grid in space [2,3], taking advantage of the fact that spatial gradients in conditional averages tend to be small.

The closure for the chemical source-term is usually made using first (conditional) moment closure. The underlying assumption here is that the fluctuations around the conditional average are small and can be neglected. In flames far from ignition and extinction, this assumption has been shown to lead to an acceptably low error [4], such that predictions of experimental data using this approach have been very good – often within the error extents of the measurements.

One approach to expand CMC methods to address flames that do include local extinction, re-ignition or autoignition is to use a second (conditional) moment closure for the chemical source-terms [5–7]. Here, the idea is to use a Taylor series expansion of the reaction rate expressions with truncation at the second order terms. The result depends on the conditional variance and covariance of the reactive scalars involved in the reactions, which then necessitates deriving, closing and solving additional transport equations for these additional quantities. The method has been found to not perform well when the conditional fluctuations are large [8], but it does allow one to predict flames with local extinction well, provided the chemistry can be either simplified to a very small number of reaction steps [9] or at least a very small number

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of reaction steps within a larger mechanism can be identified for which the second moment closure is needed [10].

It has been suggested that adding a second condition to the CMC approach could further reduce the conditional fluctuations and possibly even account for the effects of ignition and extinction, provided the right conditioning variable can be found [11–14]. Unfortunately, adding a second condition leads to adding yet another independent variable to the system of equations, which makes the method much more expensive if it is to be used to model a flame in a complex geometry. Also, several new terms arise in the doubly-conditioned transport equations that need to be modeled.

It is worth mentioning also that CMC has been successful largely only in the non-premixed turbulent flame context: premixed implementations of CMC have suffered up until recently from insufficiencies in the models for the scalar dissipation, a term that is of paramount importance in the conditionally averaged transport equations. Improved models for that term have made it possible to get good predictions for premixed flames in RANS [15], although the models used may have to be well-tuned – including, as they do, several tunable parameters – and this suggests that they may not be appropriate as LES models, where there is usually a disinclination from invoking models that require tunable parameters. Partially premixed flames, however, would obviously necessitate a two-condition CMC approach with the difficulties mentioned above.

Conditional Source-term Estimation (CSE) is an off-shoot of the CMC model in which, rather than solving transport equations for the conditional averages of the reactive scalars, one obtains them by inverting integral equations [16,17]. It has been shown to predict both non-premixed [4,18–23] and premixed [24–26] flames well in both the RANS and LES contexts, however, there remains work to be done, particularly with respect to premixed flames, to demonstrate that CSE can accurately reproduce flame dynamics in turbulent flames. The two-condition version of CSE – Doubly-Conditional Source-term Estimation (DCSE) – has been shown to be able to excellent predictions of MILD combustion [27–30] and partially premixed flames in the form of a stratified V-flame [31,32] and lifted flames [33]. Recently, in a head-to-head comparison between CSE and CMC methods where both models were implemented in the code and used to predict the same flames, CSE was found to be significantly less computationally time-consuming than CMC while providing predictions that were, for the most part, considerably closer to the experimental measurements than the CMC ones [34].

The integral equations in the CSE and DCSE models are formed by collecting unconditional averages within control volumes into ensembles and assuming that the conditional averages within those ensembles are constant, hence (for CSE):

$$\widetilde{f}(x_k,t) = \int_0^1 \int_0^1 \langle f|\zeta\rangle(t;\mathbf{E})\,\widetilde{P}(\zeta;x_k,t)\,d\zeta, \tag{1}$$

or, for DCSE,

$$\widetilde{f}(x_k,t) = \int_0^1 \int_0^1 \langle f|\zeta,\gamma\rangle(t;\mathbf{E})\,\widetilde{P}(\zeta,\gamma;x_k,t)\,d\zeta\,d\gamma, \tag{2}$$

where f is a reactive scalar (temperature or a species mass fraction), $\widetilde{f}(x_k,t)$ is the Favre averaged value of that reactive scalar in the control volume at x_k at time t, $\langle f|\zeta,\gamma\rangle(t;\mathbf{E})$ is the conditional average of that reactive scalar for the ensemble $\mathbf{E}$ of control volumes in which that conditional average is presumed constant, ζ and γ are the conditioning variables (corresponding, for example to the random variables mixture fraction Z and progress variable c) and $\widetilde{P}(\zeta,\gamma;x_k,t)$ is the Favre joint probability density function (PDF) of those two conditioning variables.

In practice, the inversion of Eq. (1) is highly over-constrained, in that there are many more instances of the integral than discrete intervals in the conditioning space. The inversion is done in a least-squares sense, however, because the problem is ill-posed, it is necessary to add some kind of regularization, with Tikhonov regularization [35] often being the method of choice [16]. There, one solves the linear system with an additional linear constraint on the solution. In discrete form, the above integral can be written

$$\vec{b} = \mathbf{A}\vec{\alpha}, \quad \text{where} \quad A_{kj} = \widetilde{P}(\zeta;x_k,t)\Delta\zeta_j, \quad \alpha_j = \langle f|\zeta\rangle_j, \quad b_k = \widetilde{f}(\vec{x_k}) \tag{3}$$

Tikhonov proposed solving the following least-squares problem for the solution of the above equation:

$$min\left\{||\mathbf{A}\vec{\alpha}-\vec{b}||_2 + \lambda||\mathbf{L}(\vec{\alpha}-\vec{\alpha}^0)||_2\right\} \tag{4}$$

where $||\cdot||_2$ denotes the L2-norm of a vector. In this equation, $\vec{\alpha}^0$ is *a priori* knowledge of the solution and λ is the regularization parameter; $\mathbf{L}$ is either the unity matrix or a discrete approximation to a derivative operator. Bushe and Steiner [16] used a second-order derivative operator for $\mathbf{L}$ and did not assume any value for $\vec{\alpha}^0$ in a CSE simulation of a non-premixed flame. The relative weight given to the *a priori* knowledge of the solution, λ, introduces a "tunable" parameter to CSE; Bushe and Steiner used $\lambda = Tr(\mathbf{A}^T\mathbf{A})/Tr(\mathbf{I})$ where Tr is the trace of the matrix, which effectively means the tunable parameter is set by the problem itself. Grout et al. [36] performed their CSE simulation of a non-premixed flame using Tikhonov regularization with the solution at the previous time-step for $\vec{\alpha}^0$ and a unity matrix for $\mathbf{L}$. Jin et al. [37] proposed using an unstrained one-dimensional laminar premixed flame for $\vec{\alpha}^0$ in a premixed version of CSE; Salehi et al. [24] used this in combination with an L-curve method to provide a more robust means of selecting the parameter λ. Whichever approach is taken for $\vec{\alpha}^0$, it is important to note that this is effectively a paramater in the model and the model's accuracy is likely dependant on making a good choice for this function. Using a laminar flame solution seems to be a good choice because, if the flame were to actually be in the flamelet regime, that would likely be the right solution to get and CSE ends up calculating just how different the flame is from the laminar one. Having said that, there remains considerable work to be done on this point, including potentially exploring different integral inversion algorithms, perhaps within a Bayesian framework, as was done recently by Labahn et al. [38], or using a truncated singular value decomposition.

CSE usually assumes that the PDF can be well approximated by a presumed functional form, typically a function of the mean and variance of the conditioning variables – although, in principle, one could calculate the PDF in some other way. For mixture fraction, the β-PDF has proven to work well [4,39]. For progress variable, the β-PDF has proven to not work well at all; instead, recent work has suggested that using the laminar flame to construct the PDF [40] or to tabulate results of a calculation using the Linear Eddy Model [41] provides a very good approximation to the PDF of reaction progress variable in turbulent premixed flames. Chemical closure is then achieved with first (conditional) moment closure, assuming that the conditional fluctuations are small, such that, within each ensemble,

$$\langle\dot{\omega}_I|\zeta,\gamma\rangle \approx \dot{\omega}_I(\langle T|\zeta,\gamma\rangle, \langle Y_k|\zeta,\gamma\rangle, \langle\rho|\zeta,\gamma\rangle), \tag{5}$$

where $\dot{\omega}$ is the non-linear rate expression for the chemical reaction rate of reaction I. From the collection of all rates in which a given species participates, one can them make a linear combination to give the rate of formation or destruction of each chemical species $\langle\dot{\omega}_K|\zeta,\gamma\rangle$ and then the chemical rates of formation or destruction of the different species mass fractions within each control volume