

Assessment of conditional source-term estimation for temporally developing flame kernels using DNS results

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1 Introduction

The successful transition from a spark to a stable flame in a turbulent flow is of importance to many combustion based energy conversion devices. Under traditional conditions this process is generally straightforward. However, the drive towards higher efficiency and lower emissions means that many devices are now employing lean and potentially stratified mixtures, where it is less certain that the flame will develop successfully. Combustion submodels typically used for turbulent combustion are challenged by the kernel growth problem; there is a need to develop more successful approaches. The primary objective for turbulent combustion models is to obtain accurate closure for the mean chemical source terms. Determined by highly non-linear reaction rate expressions, these are impossible to evaluate directly in either the RANS or LES contexts where only averaged compositions and temperatures are available. Typically, especially in the premixed regime, assumptions are made that the flame is thin and can be approximated based on a laminar flame structure. Whilst in many circumstances this is valid, the rapidly changing structure of the initial flame front evolution is clearly in conflict with these assumptions. In this paper, the conditional source-term estimation (CSE) approach — flavours of which have been used successfully in both LES[4] and unsteady RANS[1] for non-premixed situations — is reformulated for application to a premixed flame. Direct numerical simulation (DNS), where all relevant length and time scales are fully resolved, has been undertaken for the development of a nascent flame kernel. The results are spatially filtered and used to perform an *a priori* test of the CSE model's ability to predict filtered reaction rates.

2 Model Formulation

The objective is to use the first conditional moments to close the chemical source term conditionally averaged on a progress variable, i.e.:

$$\langle \dot{\omega} | c \rangle \approx f(\langle Y_\alpha | c \rangle, \langle T | c \rangle), \quad (1)$$

without resorting to solving the CMC equations to obtain the conditionally averaged species mass fractions and temperature. If the conditioning variable is well chosen, the fluctuations about the conditional average will be small, and Eq. 1 will be a much better approximation than the equivalent using unconditional averages [3]. Instead, evolution equations are solved for unconditionally averaged quantities. The

relation between the conditional and unconditional averages (using the pdf of the conditioning variable) is exploited to invert a set of integral equations for the conditional averages under the assumption of spatially homogeneous conditional averages. This is consistent with previous formulations of this method used for non-premixed combustion. The starting point is to note the identity for an arbitrary scalar Θ :

$$\overline{\Theta} = \int_{\zeta} \langle \Theta | c \rangle p(c = \zeta) d\zeta. \quad (2)$$

Eq. (2) can be discretized and written as the approximate equality where the quadrature is a form of product integration:

$$\overline{\Theta} \approx \sum_{j=1}^J \psi_j \langle \Theta | c \rangle_j; \quad \psi_j \equiv \left[\int_{\zeta_{j-1}}^{\zeta_{j+1}} p(c = \zeta) d\zeta \right], \quad (3)$$

where $\langle \Theta | c \rangle_j$ is the discrete value of the conditional average at the quadrature points. Eq. 3 can be written simultaneously for all of M averaged values of Θ in the domain where the conditional average is constant. In matrix form, the system becomes:

$$\overrightarrow{\overline{\Theta}} \approx \mathbf{M} \overrightarrow{\langle \Theta | c \rangle}, \quad \text{where} \quad \mathbf{M} \equiv \begin{pmatrix} \psi_{m=1,j=1} & \cdots & \psi_{1,J} \\ \vdots & \ddots & \vdots \\ \psi_{M,1} & \cdots & \psi_{M,J} \end{pmatrix}. \quad (4)$$

The solution for the conditional average $\overrightarrow{\langle \Theta | c \rangle} \approx \mathbf{M}^{-1} \overrightarrow{\overline{\Theta}}$ is typically ill-posed, as is often the case with integral equations. To rectify this, we follow previous work [1] and turn to Tikhonov Regularization and solve the augmented minimization problem:

$$\min \left\{ \|\mathbf{M} \overrightarrow{\langle \Theta | c \rangle} - \overrightarrow{\overline{\Theta}}\| + \lambda \|\overrightarrow{\langle \Theta | c \rangle} - \overrightarrow{\langle \Theta | c \rangle}_0\| \right\}. \quad (5)$$

The quantity $\overrightarrow{\langle \Theta | c \rangle}_0$ is an *a priori* estimate of the solution which guarantees that a unique solution exists. It is expected that the solution will evolve smoothly in time. Making use of this expectation, the solution for the conditional average at an earlier time was proposed and used successfully in [1], and used here as well to obtain $\overrightarrow{\langle \Theta | c \rangle}_0$.

To approximate the unconditionally averaged reaction rates necessary to close the scalar evolution equations, Eq. 5 is first solved independently for each scalar. The resulting set of conditional means is used to evaluate the conditional reaction rates which are then integrated over the pdf of the conditioning variable.

3 Direct Numerical Simulation

The DNS code SENGAs[2] is used to conduct a fully resolved simulation of a nascent flame kernel developing in a turbulent environment. SENGAs solves the fully compressible Navier-Stokes equations in a finite-difference formulation using 10th order spatial differences and third-order Runge-Kutta time advance. It has been modified to incorporate multi-step chemistry capable of capturing the effect of variable mixture composition on reaction rates. A model chemical mechanism is adopted which can capture some of the physics of multi-step chemistry (chemical quenching, natural variation of flame speed with mixture composition) without undue computational burden. This is a two step mechanism involving model fuel, oxidizer, intermediate and product species.

The turbulent velocity field is created in Fourier space from a one-dimensional turbulent kinetic energy spectrum. The initial turbulent Reynolds number based on Taylor micro-scale is 50 and the box size is 2.5mm³; 128 points were used to discretize the solution in each direction. The boundary conditions

are periodic in two directions, and an inflow-outflow arrangement is adopted in the third direction to allow any pressure waves to escape the domain. The mean flow velocity is low, such that the calculation is effectively performed in decaying turbulence. The unburnt mixture field was initialized to be slightly lean, with an equivalence ratio of 0.8.

A spherical kernel is placed into the turbulent field by modifying the scalar field so that $a = F_1 a_0 + (1 - F_1) a_K$, where a is the mass fraction of the fuel, oxidizer and product, or the temperature, at either the unburnt mixture (a_0) or kernel value (a_K). The mass fraction of the intermediate is initialized as $Y_I = F_2(Y_I)_0 + (1 - F_2)(Y_I)_K$. The functions describing the kernel are $F_1 \equiv e^{-r^2/(2r_0^2)}$, $F_2 \equiv 4(F_1)(1 - F_1)$. The radius r_0 is set at 0.1mm so that the transition from the kernel composition to the unburnt mixture was comfortably resolved on the spatial grid. The kernel composition, chosen based on laminar flame solutions, is $(Y_F, Y_O, Y_I, Y_P, T)_K = (0, 0.06, 0.02, 0.15, 3240)$, with the balance of the mixture taken as N_2 .

Contours of the reaction rates for the first step are shown in Fig. 1 below for 4 different times during the kernel development.

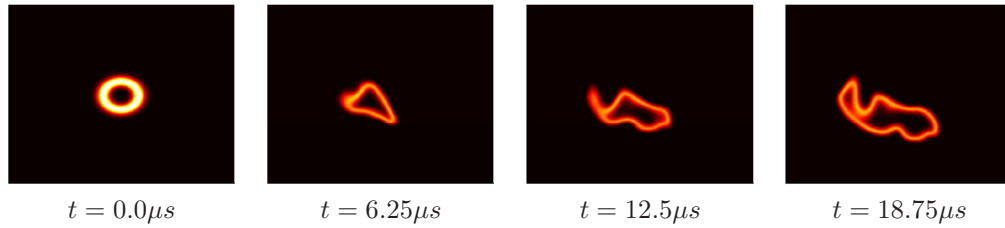


Figure 1: Reaction rates on slice through centroid of kernel. Maximum value of colourmap at $t = 0$ is twice that for later times.

Additional simulations were conducted where the unburnt mixture equivalence ratio was stratified with varying length scales and fluctuation levels. These ranged from the uniform case to an equivalence ratio range of 0.2 – 1.3. Differences were observed between these cases, including global characteristics such as mean product formation rates and local effects such as the shape of the kernel. Extending the CSE framework to two conditions to address these cases is ongoing work; here, our focus is on the homogeneous case.

4 *a Priori* Test of Model Performance

Evaluation of the effectiveness of the primary closure was performed in the LES context by spatially filtering the DNS data using a top-hat filter with a width of 16 grid points, supplying the filtered data to the CSE procedure, and comparing the predicted filtered reaction rates to the true filtered reaction rates. The pdf of the progress variable was taken directly from the DNS, allowing the performance of the model to be assessed independently of any errors in modelling the pdf. Approximation of the pdf of the progress variable is non-trivial and is being pursued in separate investigations.

In a predictive simulation Eq. 5 would be constructed at each time step and solved for each of the scalars describing species composition, temperature and density. These would then be used to evaluate the conditional reaction rates, which would finally be integrated over the pdf as suggested by Eq. 2 to obtain the unconditional average source terms necessary to advance the simulation. $\langle \Theta | c \rangle_0$ would be retained from the previous time step. This *a priori* test was performed at three snapshots in time (the latter three in Fig. 1) separated by $6.25 \mu s$, each time using the conditional averages from the previous snapshot to generate $\langle \Theta | c \rangle_0$. The value of λ in Eq. 5 was set to control the error in the recovery of the unconditional average value of all scalars by forward evaluation of Eq. 2.

The predicted average rates for both reactions are compared to the actual average rates in Fig. 2.

It would appear that the prediction is very good for the first step at all three times. The second step

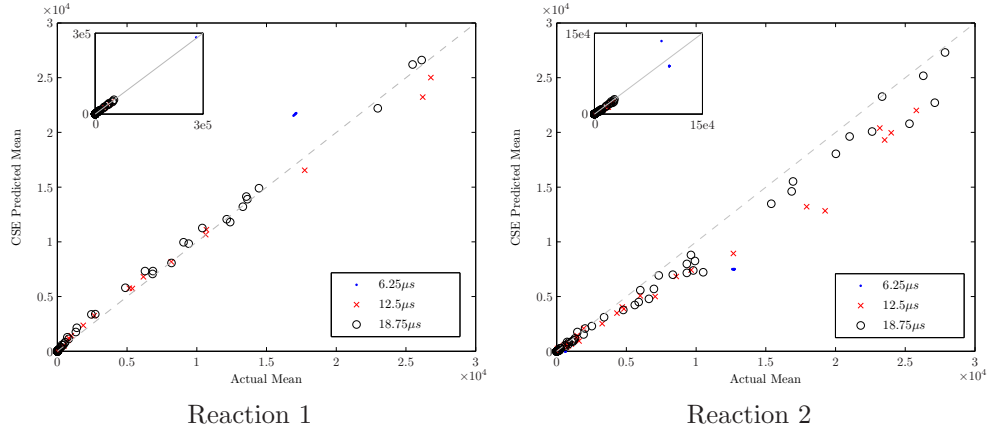


Figure 2: Comparison of estimated to actual mean reaction rates for filtered data. Inset shows extended axis to include distant points

prediction is biased slightly towards under-prediction; an under-prediction of the conditional density, especially at higher values of the progress variable, has been identified as being primarily responsible. This is due in part to rapid changes in the conditional density in the initial phases of kernel growth, and is seen to become less significant at later times.

5 Conclusion

The CSE method has been shown to be promising for the difficult problem of a developing flame kernel in a homogeneously mixed turbulent flow. Although the time step in a predictive simulation must still be small enough that the conditional averages do not change too much, the spatially unresolved features of the flame can be captured. This makes the model a good candidate for modelling subgrid combustion effects in LES simulations where the time step must be relatively small compared to uRANS. Modelling the pdf of the progress variable is still an open question, although the potential to accurately close the chemical source terms improves the feasibility of solving transport equations for higher moments of the progress variable.

References

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