Simulation of Autoignition of Methane Jets

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1 Introduction

Natural gas has been seen as a viable alternative fuel to replace diesel in compression ignition engines because of its relative abundance, lower emissions and lower cost. This has motivated recent studies of the autoignition of methane. In this work, numerical simulation of autoigniting jets have been done as a parallel effort to shock-tube experiments.

Conditional Source-term Estimation (CSE) [1] has been used in this study because of its computational efficiency and accuracy of closure. In CSE, conditional means are solved by inverting integral equations and chemical source terms are closed by invoking the fist moment hypothesis of Conditional Moment Closure (CMC) [3].

To include the detailed chemistry in the model, two different methods can be combined with CSE: the Trajectory Generated Low-Dimensional Manifold (TGLDM) [9] and Laminar Flamelet Decomposition (LFD) [2]. Manifold methods reduce chemical systems based on the separation of time scales between fast and slow time-scales by neglecting the effect of the fastest time-scales [6]. The TGLDM manifold is generated by tracing chemical reaction trajectories, which are the paths the reaction system takes when integrating the reaction rates in time from selected initial states in the composition space. LFD describes the conditional averages as a linear combination of basis functions generated by solving the unsteady laminar flamelet equations[8] using different time trajectories for scalar dissipation chosen to approximate scalar dissipation histories one might expect to see in the flow being simulated.

Both the TGLDM and LFD approaches have been used in the past to predict autoignition of methane jets, however the two approaches have never been compared "head-to-head", simulating the same experiments with the same underlying numerics and the same criterion used for defining ignition delay. This paper presents the results of an attempt to compare the two different approaches.

2 Background

The CSE method adopts the first moment hypothesis of CMC, which evaluates chemical source terms using quantities conditional on mixture fraction Z:

$$\overline{\dot{\omega}\left(T, Y_i, \rho\right)|\zeta} \approx \dot{\omega}(\overline{T|\zeta}, \overline{Y_i|\zeta}, \overline{\rho|\zeta}) \tag{1}$$

where ζ is in the sample space for mixture fraction, $\dot{\omega}$ is the chemical reaction rate, T is the temperature, Y_i is the mass fraction of species i and ρ is the density. Unlike CMC, where transport equations for the conditional averages are closed and solved, CSE solves for conditional averages of different quantities by inverting integral equations, taking advantage of the statistical homogeneity of conditional averages on pre-determined surfaces in the reaction field. Ensembles of points can be selected on surfaces where the conditional means at different points are equal to those of the ensemble:

$$\overline{< f|\zeta >}(\boldsymbol{x}, t) = \overline{< f|\zeta >}(t; A). \tag{2}$$

Here, A denotes the ensemble of homogeneity and $\boldsymbol{x}$ denotes a point within that ensemble.

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Mathematically, the unconditional average of a scalar is related to the conditional mean through the probability density function of the conditioning variable, presuming this is known. For a selected ensemble of statistical homogeneity, such integrals may be written for different points:

$$\overline{f}(\boldsymbol{x},t) \approx \int_0^1 \overline{< f|\xi >}(t;A)P(\boldsymbol{x},t;\xi)d\xi. \tag{3}$$

where $P(\boldsymbol{x},t;\xi)$ is the local probability density function at point $\boldsymbol{x}$. Assuming that the probability density function of mixture fraction can be well-approximated by a β-PDF with the same mean and variance (which can be obtained by solving their respective transport equations), Eq. 3 becomes a relatively simple linear system that can be inverted using linear regularization. Thus, the conditional averages of different scalars can be approximated. Chemical closure can then achieved by invoking the CMC hypothesis, Eq. 1. The chemical source term in the transport equations of the unconditional means is closed by integrating over the sample space of ζ, using Eq. 3.

In the CSE-TGLDM model, a three-dimensional manifold is generated using TGLDM; the three dimensions retained are mixture fraction and two progress variables: the mass fractions of $Y_{\mathrm{CO_2}}$ and $Y_{\mathrm{H_2O}}$. The manifold is stored in a library, where reaction scalars and source terms are tabulated and can be obtained using a simple linear interpolation based on the local mixture fraction and progress variables. In the CSE-TGLDM model, the conditional means of the progress variables are obtained by inverting integral equations as explained above; these are used to look up other reaction scalars and source terms in the TGLDM library.

In the CSE-LFD model, a flamelet library is generated by solving the unsteady laminar flamelet equation:

$$\rho\frac{\partial\psi_i}{\partial t} = \frac{\rho}{Le_i}\frac{\chi}{2}\frac{\partial^2\psi_i}{\partial Z^2} + \dot{\omega}_i \tag{4}$$

where Z is the mixture fraction and $\chi(Z,t)$ is the scalar dissipation rate. Solutions at different flamelet times are stored and used as the basis functions for decomposition.

In the decomposition algorithm, conditional means are approximated as a linear combination of basis functions:

$$\overline{< f|\xi >}(t;A) = \sum_{i=1}^{N_f} a_i\Theta_i(\xi) \tag{5}$$

where $\Theta_i(\xi)$ are the basis functions (the solutions to the flamelet equation). Now, Eq. 3 can be rewritten as:

$$\overline{f}(\boldsymbol{x},t) \approx \int_0^1 (\sum_{i=1}^{N_f} a_i\Theta_i(\xi))P(\boldsymbol{x},t;\xi)d\xi. \tag{6}$$

Now, rather than solving for the conditional average directly, one solves for the coefficient vector a_i. In the present implementation, this is done for selected scalars that are seen to be different between different solutions in the library: temperature, and the mass fractions of CO and CH_3OH [4]. Other scalars are estimated with the coefficient vector and the basis functions. The reaction rates are also obtained from Eq. 5, which makes this version of CSE more similar to flamelet methods, rather than CMC methods.

3 Simulation Results and Discussion

In the experiments, a shock-tube was used to compress air to the desired initial conditions; then, the fuel jet was injected along the centerline of the shock-tube and a high-speed camera was used to detect the onset of ignition from the luminosity of the resulting flame. Important characteristics are listed in Table 1. Details of the experimental facilities are presented by Huang et al [5] and the experiment data are provided by Wu et al [10].

Table 1: Characteristics of the Investigated Jets

d_{nozzle}(mm)	P_{inj}(bar)	m_{inj} (mg)	Fuel	T_{fuel} (K)	P_0 (bar)	T_0 (K)
0.28	120	1.941	90% CH_4 + 10% C_2H_6	300	30	1200–1400

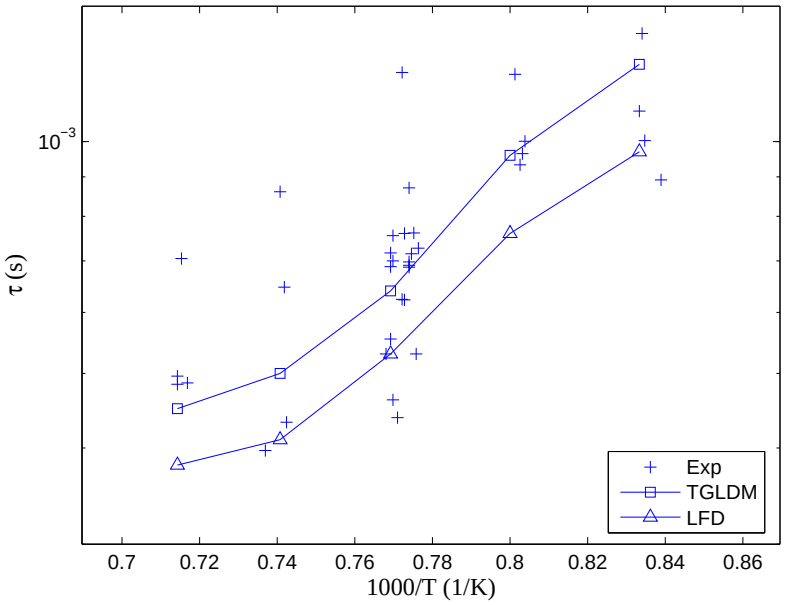

Figure 1: Comparison of CSE-TGLDM and CSE-LFD predictions to experimental results

The two different CSE approaches were implemented in OpenFOAM[7]. The detailed chemical mechanism used in generating the TGLDM and flamelet libraries includes 71 species and 379 reactions [5]. Simulations of the jets were performed in an axisymmetric computational domain using the standard $k-\epsilon$ turbulence model. In addition to the Navier-Stokes and energy equations, transport equations were solved for mixture fraction, variance of mixture fraction and selected reaction scalars.

To define ignition delay, the maximum increase in the conditional means of temperature in the reaction field is plotted against time for different pre-combustion temperatures. It is observed that this maximum value is almost zero at the beginning and later increases dramatically. Ignition is defined to have occurred when the dramatic change begins.

Predictions of ignition delay are compared with experiments, as shown in Figure 1. Both predictions appear to agree with the experimental results despite (if not because of) the scatter in the experimental data. The scatter observed in measurements can be attributed to fluctuations in turbulent mixing as well as to different realizations of chemical reaction paths. Although the present model captures the trend of ignition delay, further work is needed to account for these fluctuations.

The ignition delay predicted with CSE-TGLDM is, largely, somewhat better than that predicted with with CSE-LFD – the predictions of CSE-LFD being universally shorter than those with CSE-TGLDM. For the unsteady flamelet library, the scalar dissipation rate is modelled according to the approximate behavior of the mean scalar dissipation along the stoichiometric interface in the jets. That the modelled scalar dissipation rate cannot exactly reproduce all possible realizations of the scalar dissipation rate in

the real flame could be a source of the discrepancy.

Another issue is that the solutions in the library are exclusively igniting flamelets: the flamelet method is not able to account for the transition from igniting to burning. The TGLDM library covers a much wider range of conditions and is able to transition form igniting to burning conditions seamlessly. This, combined with the (arguably) better predictions of ignition delay, lead us to suggest that the CSE-TGLDM method appears to be the better of the two approaches available.

4 Conclusion

Numerical models have been developed to study the autoignition of methane jets. The predicted ignition delays are consistent with the experimental results, however, the scatter observed in the experiments are not accounted for in the present models. The predictions of the two different models implemented are different due differences in the methods for generating the libraries. Ultimately, it was found that the CSE-TGLDM approach appears to be superior to the CSE-LFD approach. In future work, the focus will be modelling the fluctuations in the physical and chemical processes.

References

[1] W. K. Bushe and H. Steiner (1999) "Conditional Moment Closure for Large Eddy Simulation of non-premixed turbulent reacting flows", Phys. Fluids. **11**(7), 1896-1906.

[2] W. K. Bushe and H. Steiner (2003) "Laminar Flamelet Decomposition for Conditional Source-term Estimation", Phys. Fluids. **15**(6), 1564-1575.

[3] A. Yu. Klimenko and R. W. Bilger (1999) "Conditional Moment Closure for turbulent combustion", Prog. Energy Combust. Sci. 25, 595-687.

[4] R. Grout (2004) MASc. thesis, University of British Columbia, Canada.

[5] J. Huang (2006) Ph. D. thesis, University of British Columbia, Canada.

[6] U. Maas and S. B. Pope (1992) "Implementation of simplified chemical kinetics based on intrinsic low dimensional manifold", Proc. Combust. Inst. 24, 103-112.

[7] See: http://www.opencfd.co.uk/openfoam/

[8] N. Peters (1984) "Laminar diffusion flamelet models in non-premixed turbulent combustion", Prog. Ener. Combust. Sci. 10, 319-339.

[9] S. B. Pope and U. Maas (1993) "Simplifying chemical kinetics: Trajectory-Generated Low-Dimensional Manifolds", Cornell University, report FDA 93-11.

[10] N. Wu, M. H. Davy, W. K. Bushe (2006) "Ignition and emission characteristics of methane direct injection compression ignition combustion", *CICS Spring Technical Meeting*, H3-1.