18th Australasian Fluid Mechanics Conference
Launceston, Australia
3-7 December 2012

LES Calculations of Auto-Ignition in a Turbulent Dilute Methanol Spray Flame

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Abstract

An auto-igniting methanol spray flame is simulated using a fully coupled approach, where the reactive gas-phase is calculated from Large Eddy Simulation (LES) and the dispersed phase is represented by a Lagrangian particle method. The turbulence-chemistry interactions of the gas phase are modelled using the Eulerian stochastic field method and a detailed chemical reaction mechanism involving 18 reactive species is employed. Flame lifting was predicted with lift-off heights similar to the experiment and characteristic features such as initial kernel formations upstream of the flame base were qualitatively captured. Statistics of the droplet velocity were in very good agreement but the predictions of the mean droplet diameter with increasing downstream location indicated that the evaporation rate was deficient. Mean profiles of the temperatures were satisfactory upstream of the flame base, but were over predicted in the main flame region. Overall, the results are very encouraging given the complexities introduced by the interactions of the dispersed and gas phases along with the presence of finite-chemistry.

Introduction

Spray combustion plays a vital role in many power and heat generating devices such as gas turbines in aero-engines, industrial furnaces as well as diesel engines. Typically, liquid fuel is injected into a turbulent air stream where it produces fuel vapour which then mixes and burns. Since the droplet sizes often correspond to the width of reaction zones, changes in their properties and dynamics prove to impact the local flame structure and change its characteristics. Describing the entire process requires the knowledge of the gas phase turbulence-chemistry interactions, the dispersion and evaporation of the spray as well as the coupling between the phases. This is a challenging task to both experiments as well as numerics.

Numerically, Large Eddy Simulation (LES) has gained success in the recent past in describing turbulent reactive flows, using a wide range of *sub-grid* models for the unresolved turbulence-chemistry interactions (see e.g. [17] for a topical review). Particularly in conjunction with the Eulerian stochastic field method, a wide range of flame regimes has been captured by this approach including auto-ignition in lifted flames[10], partially premixed combustion with extinction[11], spark ignition and subsequent flame propagation in a jet flame [12] and a premixed swirl flame [9]. This methodology has been extended to spray combustion in recent years [8] by coupling a Lagrangian particle method [2, 3] to describe the dispersed phase.

The aim of this study is to extend previous work using the LES/stochastic field and Lagrangian particle approach [8] to compute a spray flame configuration with strong finite-rate effects. Recently, O'Loughlin and Masri [14, 15] investigated a series of dilute methanol spray flames auto-igniting in a wide stream of hot, co-flowing combustion products. A range of flow conditions (Mt2A, Mt2B and Mt2C) were investigated experimentally and detailed measurements of droplet statistics such as the velocity and the mean diameter, as well as low-speed and high-speed imaging of hydroxyl (OH) and formaldehyde (CH_2O) were made to visualise the flame characteristics. Being strongly controlled by finite-rate chemistry effects, one of the flames (Mt2B) has been chosen as a test case for this paper.

Mathematical modelling

Filtered gas phase equations

The density-weighted filtered equations of motions are:

Continuity:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i}{\partial x_i} = \bar{\dot{S}}_{mass}, \tag{1}$$

Momentum:

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\bar{\tau}_{ij} - \frac{\partial}{\partial x_j}\tau_{ij}^{sgs} + \bar{\dot{S}}_m^i \tag{2}$$

Species mass fraction + enthalpy:

$$\frac{\partial \bar{\rho}\tilde{\phi}_{\alpha,h}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j\tilde{\phi}_{\alpha,h}}{\partial x_j} = \frac{\partial}{\partial x_k}\left(\frac{\mu}{\sigma}\frac{\partial \tilde{\phi}_{\alpha,h}}{\partial x_k}\right) - \frac{\partial \tilde{J}_k^{\alpha,h}}{\partial x_k} + \overline{\rho\dot{\omega}_{\alpha,h}(\phi,T)} + \bar{\dot{S}}_v^{\alpha,h} \tag{3}$$

where $\tau_{ij}, \rho, u_i, \mu, p, \phi_{\alpha,h}$ represent the viscous stress tensor, density, velocity component in i-th direction, viscosity, pressure and scalar (species α or enthalpy h) respectively. The over bar and tilde denote conventional and density-weighted filtering respectively. A dynamic *Smagorinsky* approach by Piomelli and Liu [16] is employed for the unclosed *sub-grid* stresses τ_{ij}^{sgs} and equal diffusivities are assumed for the scalar and enthalpy equations. Equations 3 contain the unclosed *sub-grid* scalar fluxes $\tilde{J}_k^{\alpha,h}$ and filtered source terms $\overline{\rho\dot{\omega}_{\alpha,h}(\phi,T)}$, which in the case of the enthalpy represent heat sources and sinks such as radiation (neglected here) or spark energy and in the case of the reactive species represent the net formation rate due to chemical reactions - the main closure problem in turbulent combustion modelling.

The mass, momentum and scalar source terms $\bar{\dot{S}}_{mass}, \bar{\dot{S}}_m^i$ and $\bar{\dot{S}}_v^{\alpha,h}$ in Eqs. 1 to 3 arise from the dispersed phase and are obtained from the volume-averaged contribution of the liquid phase (see e.g. [3] for more details).

Spray formulation

The droplet dispersion is treated in a Lagrangian manner following Bini and Jones [1, 2]. The change of the droplet position of the p-th particle $\mathbf{x}_p$ is determined by:

$$d\mathbf{x_p} = \mathbf{v}_p dt \tag{4}$$

where the stochastic velocity $\mathbf{v}_p$ is obtained from:

$$d\mathbf{v}_p = \frac{(\widetilde{u} - \mathbf{v}_p)}{\tau_p} + \sqrt{C_0 \frac{k_{sgs}}{\tau_t}} d\mathbf{W} \tag{5}$$

where $\tau_p^{-1} = \frac{3}{8}\frac{\rho_g C_D}{\rho_p r_p}|\mathbf{u}-\mathbf{v}|$ denotes the particle relaxation time, ρ_p is the droplet density and ρ_g the gas phase density interpolated at the particle position. The drag coefficient C_D is determined by the drag law formulated by Yuen and Chen [24]. The stochastic contribution including the model constant C_0 assumed unity, the *sub-grid* kinetic energy k_{sgs} and containing the *Wiener* process $d\mathbf{W}$ accounts for the effects of the *sub-grid* fluctuations on the droplet dispersion and the associated time scale $\tau_t = \tau_p\left(\frac{\tau_p k_{sgs}^{1/2}}{\Delta}\right)^{0.6}$ represents the interactions between the gas-phase turbulence and the particles. The kinetic *sub-grid* energy $k_{sgs} = 2\Delta C_s^{2/3}\widetilde{S}_{ij}\widetilde{S}_{ij}$ is evaluated using an equilibrium assumption, where $\widetilde{S}_{ij}$ is the resolved strain rate tensor.

The temperature change of the particle dT_p and the change in mass dm_p is assumed as:

$$dT_p = \frac{T_g - T_p}{\tau_p}dt + \frac{h_{fg}}{C_{P_p}}\frac{dm_p}{m_p} \tag{6}$$

$$dm_p = -\frac{Sh}{3Sc_g}\frac{m_p}{\tau_p}\cdot\ln(1+B_M)dt \tag{7}$$

where the sub-script g denotes the gas phase value interpolated onto the particle position, C_p,C_g are the heat capacities, h_{fg} is the latent heat of vaporisation, Sc_g the Schmidt number and B_M the *Spalding* number [22]. The Sherwood number Sh is obtained from the *Ranz-Marshall* correlations [19, 20].

Eulerian stochastic field method

To account for the unresolved filtered rate terms $\overline{\rho\dot{\omega}_{\alpha,h}(\phi,T)}$ in Eq. 3, a joint *sub-grid* probability density function (*pdf*) $\widetilde{P}_{sgs}$ is introduced for all involved scalars (reactive species and enthalpy). All statistical moments such as the filtered mean or the *sub-grid* variance can be obtained from this quantity. The resulting modelled transport equation of the *sub-grid pdf* (see e.g [6]) is highly dimensional and cannot be feasibly solved with conventional finite-different schemes when a large number of scalars are involved. Instead, equivalent stochastic differential equations are usually solved. This is commonly achieved via the introduction of notional Lagrangian particles (see e.g. [18]). Alternatively, fully Eulerian formulations have become available using stochastic fields [23],[21]. The ensemble of N stochastic fields ξ_α^n for each scalar α represents the joint *sub-grid pdf*:

$$\widetilde{P}_{sgs} = \frac{1}{N}\prod_{\alpha=1}^{N_s}\sum_{n=1}^{N}\delta(\psi_\alpha - \xi_\alpha^n) \tag{8}$$

Following the approach by Valiño [23], based on an *Ito* interpretation of the stochastic integral, the N stochastic fields for each reactive scalar α and the enthalpy h then evolve according to:

$$\begin{aligned}\overline{\rho}\mathrm{d}\zeta_\alpha^m = &-\overline{\rho}\widetilde{u}_i\frac{\partial\zeta_\alpha^m}{\partial x_i}\mathrm{d}t + \frac{\partial}{\partial x_i}\left[\Gamma'\frac{\partial\zeta_\alpha^m}{\partial x_i}\right]\mathrm{d}t + \overline{\rho}\sqrt{\frac{2\Gamma'}{\overline{\rho}}}\frac{\partial\zeta_\alpha^m}{\partial x_i}\mathrm{d}W_i^m \\ &- \frac{\overline{\rho}}{2\tau_{sgs}}\left(\zeta_\alpha^m - \widetilde{\phi}_\alpha\right)\mathrm{d}t + \overline{\rho}\dot{\omega}_\alpha^m(\zeta^m)\mathrm{d}t + \dot{S}_\alpha\end{aligned} \tag{9}$$

where Γ' represents the total diffusion coefficient and where dW_i^n represent increments of a vector *Wiener* process, different for each field but independent of the spatial location $\mathbf{x}$. This stochastic term has no influence on the first moments (or mean values) of $\xi_{\alpha,h}^n$ but is responsible for the generation of the scalar variance. The micro-mixing term on the other hand, which is closed with the *Linear Mean Square Estimation* (LMSE) model (e.g. [5]) acts as a scalar variance dissipation term. The additional source term $\dot{S}_\alpha$ accounts for the change in mass fraction due to evaporation of the droplets. In this study, this source term is assumed independent of the *sub-grid* fluctuations, i.e. $\dot{S}_\alpha$ is evaluated using the filtered properties. The stochastic fields given by (9) are fully Eulerian and not to be mistaken with any particular realisation of the real field, but rather form an equivalent stochastic system (both sets have the same one-point *pdf*) smooth on the scale of the filter width. Statistical moments such as the filtered mean can be computed by simple unweighted ensemble averages of the stochastic fields, i.e.:

$$\widetilde{\phi}_\alpha = \frac{1}{N}\sum_{n=1}^{N}\xi_\alpha^n \tag{10}$$

Test case configuration

Experiment

The investigated burner comprises of a central fuel tube with an inner diameter of 4.6 mm, embedded in a vitiated co-flow of an equilibrium composition of hydrogen-air at 1430 K at 3.5 m/s. The spray is formed upstream of the pipe exit by an ultrasonic generator (Sonotek) producing droplets with a *Sauter mean diameter* of approximately 40 μm and carried with a co-flowing air-stream of air. More details of the burner configuration can be obtained from[14, 15].

A series of methanol flames with this geometry, labelled as Mt2A,Mt2B and Mt2C were investigated by O'Loughlin and Masri [14], differing only in the liquid fuel loading while the carrier air velocity and the co-flow temperatures are identical. In this study, the flame Mt2B is investigated. For this case, the bulk jet carrier velocity was set to 75 m/s and the mass flow rate of the liquid fuel was adjusted to 23.8 g/min. Experimental data of the droplet statistics are available from Particle Doppler Anemometry (PDA), the gas phase temperature was measured using thermocouples and low and high-speed imaging of hydroxyl (OH) and formaldehyde (CH_2O) was performed to characterise the flame (see [14, 15] for more details).

Numerics

The in-house code BOFFIN [7] developed at Imperial College London was used for the LES simulation. The code is based on a semi-implicit low-Mach number formulation, with all spatial gradients being discretised with an energy conserving second order schemes except for the scalar convection, for which a TVD scheme is applied. Eight stochastic fields along with a micro-mixing constant of C_D=2.0 are employed to characterise the turbulence-chemistry interactions at *sub-grid* level. The chemistry is represented by a reduced mechanism by Lindstedt and Meyer [13] which contains 18 chemical species and 14 reaction steps.

The computational domain corresponds to an inverted pyramid with a 10Dx10D inlet plane and 20Dx20D outlet plane, extending 50D in axial direction. The axial location of the inlet plane corresponds to the location of the exit plane of the pipe. Measured velocity profiles at exit plane of the pipe were imposed as boundary conditions for the velocity field. The particles were injected using the measured *pdf* of the droplet diameters. A pre-vaporised fuel mass fraction of about 4.7% was detected in [14] at the pipe exit and was considered in the boundary condi-

tions.

Results

Global features

An overall impression of the predicted flame structure can be obtained from Figure 1. Here, a temperature plot is shown along with iso-contours of the vaporised fuel mass fraction. Close to the nozzle, the presence of methanol is visible due to pre-vaporised fuel measured in the experiment and imposed as boundary condition for the simulation. The flame is clearly lifted and the base of the fully established flame is located at around x/D=25. Most of the fuel is vaporised in the jet, and the overall flame structure shows strong similarities to a purely gaseous lifted flame (e.g. the "Cabra" flame [4] which has a similar geometry).

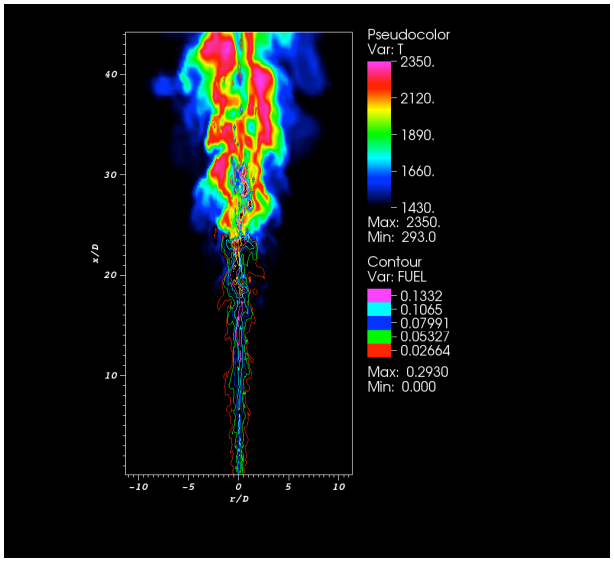

Figure 1: Snapshot of the temperature and contour levels of the vaporised fuel

A closer comparison of the experimental and predicted flame structure is shown in Figure 2 where contours of OH from the LES simulation and an experimental low-speed OH-LIF image are displayed. Note that only one side of the jet is shown and the experimental images are shown in sections, as measured. A characteristic feature of the flame is the downstream region below the fully ignited flame base where initial OH kernels preceding the established flame are formed. This has been discussed in [14] and has been qualitatively captured by the LES simulation. Upon ignition, the simulation predicts a continuos edge flame, whereas the experiments indicate disruptions in the reaction zone until about x/D=40.

Gas phase statistics

Radial profiles of the mean gas phase temperature are shown in Figure 3where comparisons are made with thermocouple measurements by O'Loughlin and Masri [14]. At x/D=10 the trend is captured. The jet core is somewhat over predicted whereas the jet/co-flow shear layer region is under predicted. This may stem from the under-predicting the occurrence of ignition kernels which were shown in Figure 2. At x/D=20 the agreement is satisfactory, particularly in the jet/co-flow region but at x/D=30, the profiles show fundamental differences. While the simulations show a peaking at around 2200 K indicating a stable fully

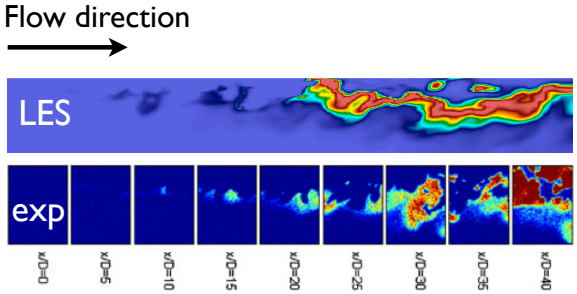

Figure 2: Snapshots of OH from the experimental OH-LIF images [14] and the LES simulation

burning flame, the mean measured temperatures are depressed to around 1500 K. This is consistent with the findings of the OH snapshot comparisons, where the LES simulations show a continuous OH contour, whereas the experiments show breakages in the reaction zones. These are indicative of extinction processes which are obviously not well captured by the simulation. Reasons for this deficiency include potential shortcomings of the droplet/gas-phase coupling as well as inadequacies in the description of the turbulence-chemistry interactions. These issues are the subject of future work.

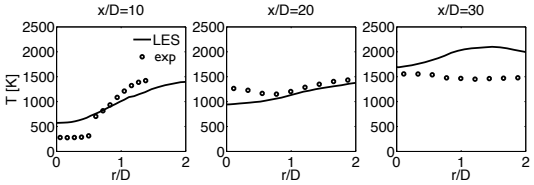

Figure 3: Mean radial profiles of the gas phase temperature at four axial locations.

Droplet statistics

Radial profiles of mean radial velocities for all droplet sizes are displayed in Figure 4. The dispersion is captured well, both in terms of reproducing the jet spreading as well as the magniude of the mean velocities.

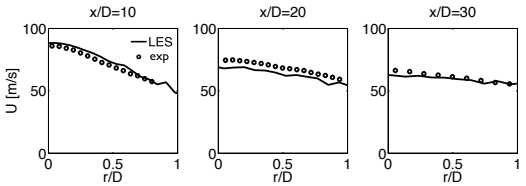

Figure 4: Mean radial profiles axial droplet velocity for all droplet sizes at three axial locations.

Radial profiles of mean droplet diameter (denoted as D_{10}) for all droplet sizes are shown in figure 5 at three axial downstream locations. While the agreement is good at x/D=10, the level of under-prediction increases further downstream at x/D=20 and x/D=30. The overall increase of the mean diameter D_{10} is related to smaller droplets evaporating quicker than larger ones. Although the simulations replicate the trend of increasing magnitude of the mean diameter with increasing distance from the nozzle exit, they under-predict the level of evaporation.

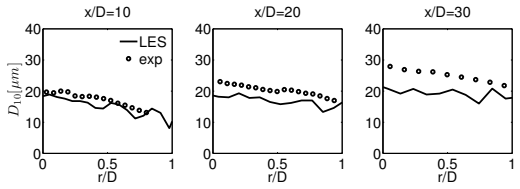

Figure 5: Mean radial droplet diameter profiles for all droplet sizes at three axial locations.

Conclusions

This study investigated an auto-igniting methanol spray flame in a vitiated co-flow. A fully coupled approach involving Large Eddy Simulation along with the Eulerian stochastic field method for the gas-phase turbulence-chemistry interactions and a Lagrangian particle methodology with a stochastic dispersion model to characterise the dispersed phase was applied. The simulation showed promising results. The droplet dispersion was captured to a large extend. The overall lift-off characteristics were reproduced by the simulations except for predicting the breakages in the established flame as seen in the experiments. To resolve these deficiencies, future work must focus on enhancing the modelling of fuel vaporisation as well as correctly accounting for the complex physics present in this spray flame such as role of the initial kernel formation upstream of the flame base.

Acknowledgements

This work is supported by the Australian Research Council. The authors gratefully acknowledge the support of Prof. W.P. Jones (Imperial College London) for providing the original subroutines of the LES code and Drs. Salvador Navarro-Martinez (Imperial College London) and Mathew Cleary (University of Sydney) for their valuable input.

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