UNIVERSITY OF CAMBRIDGE

Modelling spray autoignition with CMC

Giulio Borghesi

Hopkinson Lab, Department of Engineering, University of Cambridge

Motivations and outline

Motivations:

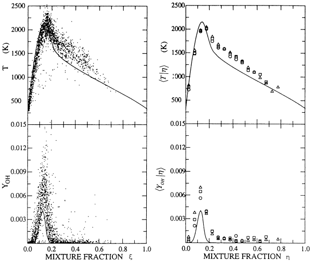
- spray combustion employed in wide range of industrial devices (gas turbines, diesel engines, furnaces);
- CFD powerful and reliable tool to assist the design process of state-of-the-art combustion chambers;
- spray effects often neglected (partially/totally) in most combustion models $\Rightarrow$ assessment of their importance needed!

Conditional Moment Closure (CMC)

Idea: key quantity exists that controls combustion process:

- non premixed flows: mixture fraction, ξ;
- premixed flows: progress variable, c.

True or not? Experiments suggest it is true.



- CMC solves for the conditional moments;
- scatter around conditional moments small;
- $\langle \dot{\omega} | \eta \rangle$ can be closed at first order;
- $\widetilde{Y}_\alpha = \int_0^1 \langle Y_\alpha | \eta \rangle P(\eta) d\eta$

The CMC equation for two-phase flows

Species transport equation [1]:

$$\frac{\partial Q_\alpha}{\partial t} + \langle u_j | \eta \rangle \frac{\partial Q_\alpha}{\partial x_j} = \langle N | \eta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2} + \langle \dot{\omega} | \eta \rangle + e_f + \dot{S} \qquad (1)$$

where:

- $\langle u_j | \eta \rangle$: conditional mean velocity;
- $\langle N | \eta \rangle = D \overline{\left\langle \frac{\partial \xi}{\partial x_j} \frac{\partial \xi}{\partial x_j} \middle| \eta \right\rangle}$: conditional scalar dissipation rate;
- $\langle \dot{\omega} | \eta \rangle$: chemical source term;
- $e_f = -\frac{1}{\overline{\rho}\widetilde{P}(\eta)} \frac{\partial}{\partial x_j} \left(\overline{\rho}\widetilde{P}(\eta) \left\langle u_j'' Y_\alpha'' \middle| \eta \right\rangle \right)$: conditional turbulent flux;
- $\dot{S}$: droplets source term.

[1] M. Mortensen, R.W. Bilger, Combustion and Flame, 156:62-72, 2009

Source terms due to droplets evaporation

$\dot{S}$ describes droplets influence on the gas phase and is given by:

$$\dot{S} = -\frac{1}{\rho_\eta \langle\theta\rangle \widetilde{P}(\eta)} \frac{\partial \left[(1-\eta)\rho_\eta \widetilde{P}(\eta) \left\langle Y''_\alpha \Pi'' \right| \eta \rangle \right]}{\partial \eta} + \left[Q_{l,\alpha} - Q_\alpha - (1-\eta)\frac{\partial Q_\alpha}{\partial \eta} \right] \frac{\langle \Pi | \eta \rangle}{\langle\theta\rangle} \qquad (2)$$

In the above equation:

- $Q_{l,\alpha}$: mass fraction of species α in liquid phase;
- $\langle \Pi | \eta \rangle$: conditional evaporation rate.

Modelling of droplets source terms

Modelling principles:

- Evaporation occurs at saturation mixture fraction ξ_s only;
- Consistency condition $\int_0^1 \langle \Pi | \eta \rangle \widetilde{P}(\eta) d\eta = \widetilde{\Pi}$ has to be satisfied.

Proposed model:

$$\langle \Pi | \eta \rangle = \frac{1}{\overline{\rho} \widetilde{P}(\eta) V} \sum_{i=1}^{N_d} \dot{m}_i \delta \left(\eta - \xi_{s,i} \right) \tag{3}$$

$\langle \Pi'' Y_\alpha'' | \eta \rangle$ difficult to model, and neglected for the moment being.

Mixture fraction PDF and conditional scalar dissipation rate

PDF shape presumed $\longrightarrow$ β-function employed.
Solution of two auxiliary equations required, modelled as in [2] :

$$\frac{\partial \overline{\rho}\widetilde{\xi}}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u}_j\widetilde{\xi}\right) = \frac{\partial}{\partial x_j}\left(\overline{\rho} D_T \frac{\partial \widetilde{\xi}}{\partial x_j}\right) + \overline{\rho}\widetilde{\Pi} \tag{4}$$

$$\frac{\partial \overline{\rho}\widetilde{\xi'^2}}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u}_j\widetilde{\xi'^2}\right) = \frac{\partial}{\partial x_j}\left(\overline{\rho} D_t \frac{\partial \widetilde{\xi'^2}}{\partial x_j}\right) - 2\overline{\rho}\widetilde{u'_j\xi'}\frac{\partial \widetilde{\xi}}{\partial x_j} - 2\overline{\rho} D\widetilde{N}$$
$$+2\overline{\rho}\left(\widetilde{\xi\Pi} - \widetilde{\xi}\,\widetilde{\Pi}\right) + \overline{\rho}\left(\widetilde{\xi}^2\widetilde{\Pi} - \widetilde{\xi^2\Pi}\right) \tag{5}$$

AMC model [3] used for conditional scalar dissipation rate

[2] F.X. Demoulin, R. Borghi, Combustion and Flame, 129:281-293, 2002
[3] E. E. OBrien, T. Jiang, Physics of Fluid A, 3:3121-3123, 1991

Chemistry, turbulent transport and conditional velocities

First-order closure of $\langle \dot{\omega} | \, \eta \rangle$ employed:

$$\langle \dot{\omega} | \, \eta \rangle = \dot{\omega}(Q_\alpha, \ldots, Q_T) \tag{6}$$

Conditional turbulent fluxes closed according to gradient model:

$$e_f = -D_T \frac{\partial Q_\alpha}{\partial t} \tag{7}$$

Linear model used for conditional velocities:

$$\langle u_j | \, \eta \rangle = \widetilde{u}_j - \frac{D_T}{\widetilde{\xi'^2}} \frac{\partial \widetilde{\xi}}{\partial x_j} \left(\eta - \widetilde{\xi} \right) \tag{8}$$

The Sandia bomb setup

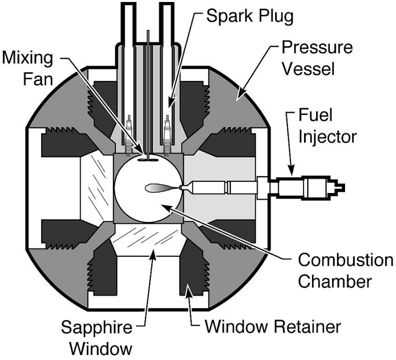


Figure 1: Experimental setup

- Operating pressure: $42.5\,\mathrm{bar}$
- Air temperature: $1000\,\mathrm{K}$
- Fuel temperature: $374\,\mathrm{K}$
- Fuel type: n-heptane
- Injector diameter: $100\,\mu\mathrm{m}$
- Injection pressure: $150\,\mathrm{MPa}$
- O_2 content: 10 to 21 %

Flame lift-off height and ignition delay time

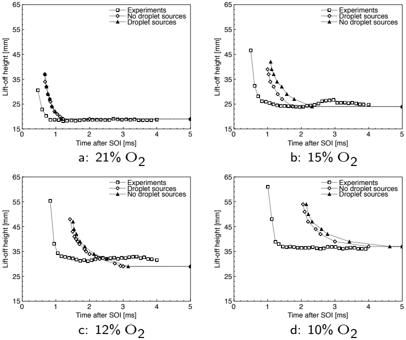


Figure 2: Lift-off height versus time

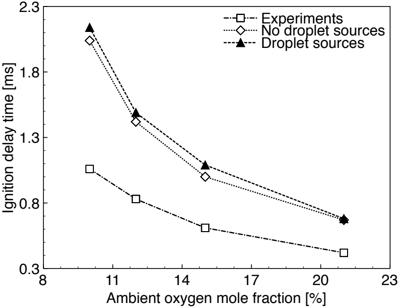


Figure 3: τ_{id} versus O_2 %

Unconditional averages - $15\,\%\,O_2$ case

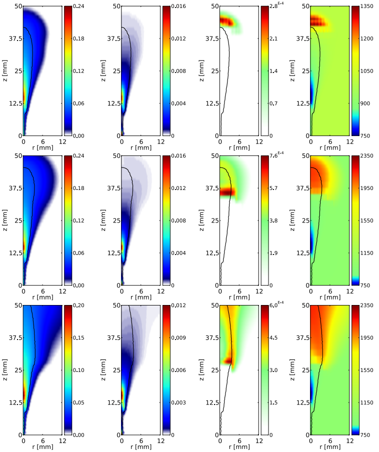
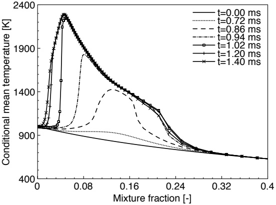


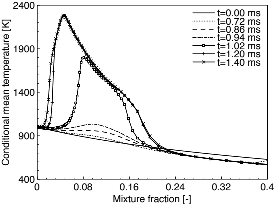
Figure 4: $\widetilde{\xi}$, $\widetilde{\xi'^2}$, $\widetilde{T}$, $\widetilde{Y}_{OH}$ vs. time

- $\widetilde{\xi'^2}$ peaks where evaporation is the strongest;
- Autoignition occurs along axis;
- flame propagates along ξ_{st};
- propagation towards axis delayed;
- anchoring occurs off-axis.

Conditional temperature evolution - $15\,\%\,O_2$ case



$\dot{S} = 0$ case, ignition spot

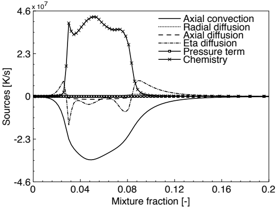


$\dot{S} \neq 0$ case, ignition spot

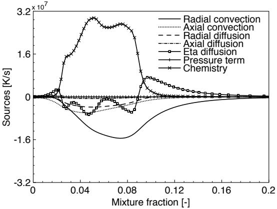
- Evaporative cooling most effective at high η values - drop in T up to $60\,\mathrm{K}$;
- ignition delay time increases when $\dot{S} \neq 0$;
- ξ_{MR} decreases when including droplets source terms in CMC equations;
- $\langle \mathrm{T} | \xi_{st} \rangle$ decreases by $\simeq 10\,\mathrm{K}$.

Anchoring mechanism

- Chemistry balanced by convection and diffusion in η space;
- radial component of convection larger than axial one;
- spatial diffusion terms less important than in lifted jet flames;
- droplet terms do not affect anchoring mechanism.



CMC source terms along axis



CMC source terms off axis

Conclusions and future work

Conclusions:

- influence of droplets terms on numerical predictions weak;
- τ_{id} overpredicted for all conditions investigated;
- lift-off height reproduced with good accuracy.

Future work:

- more accurate modeling of $\widetilde{P}(\eta)$ and $\langle N | \eta \rangle$ needed!
- modeling of $\langle Y_\alpha'' \Pi'' | \eta \rangle$ to be investigated;
- assessment of droplet effects against wider range of conditions.