Modelling of **Spray flames** with **Double Conditional Moment Closure**

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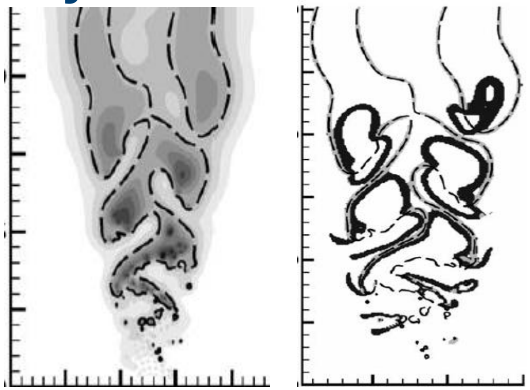
Objectives

Modelling of **Spray Flames** with **Double Conditional Moment Closure**

Spray flames



Domingo et al., CNF, 2005

- Max. mixture fraction
- Non premixed & premixed

CMC

- Statistical model
- Non-premixed — Klimenko & Bilger, PECS, 1999
- Spray — Mortensen & Bilger, CNF, 2009; Borghesi et al., CTM, 2011
- Premixed — Mantel & Bilger, CST, 1995; Amzin et al., CST, 2012
- Double-conditioning — Kronenburg, Phys. Fluids, 2004

➢ Present the **DCMC equation for spray flames**.

➢ Propose **closure**.

➢ **Preliminary test case** and **comparison with experiments**.

Governing Equations

- Governing equations of a two-phase reacting flow.

  Following Mortensen & Bilger, CNF, 2009

  Separate flow mode (Kataoka, Int. J. Multiphase Flow, 1986)

$$\frac{\partial \theta}{\partial t} + \nabla\theta = \Pi$$

here, θ = gas phase

$\bar{\theta}$ is the volume fraction of gas phase in a cell

$$\frac{\partial \theta\rho}{\partial t} + \mathrm{div}(\theta\rho\boldsymbol{u}) = \rho\Pi$$

$$\frac{\partial \theta\rho Y_\alpha}{\partial t} + \mathrm{div}(\theta\rho Y_\alpha\boldsymbol{u}) = \mathrm{div}(\theta\rho D_\alpha\nabla Y_\alpha) + \theta\rho\dot{\omega}_\alpha + \rho Y_\alpha\left(\hat{V}_\alpha + \Pi\right)$$

$$Y_\alpha\hat{V}_\alpha = \nabla\theta\cdot(-D_\alpha\nabla Y_\alpha)$$

$$Y_\alpha\hat{V}_\alpha = (\delta_\alpha - Y_\alpha)\Pi$$

DCMC equation for sprays

$\xi = 0$ in pure air

$\xi = 1$ in pure fuel vapour

$$c_\psi(\boldsymbol{x},t) \equiv \frac{\psi_0\big(\xi(\boldsymbol{x},t)\big) - \psi(\boldsymbol{x},t)}{\psi_0\big(\xi(\boldsymbol{x},t)\big) - \psi_{\mathrm{Eq}}\big(\xi(\boldsymbol{x},t)\big)}$$

Bray et al., CNF, 2005

$$\frac{\partial \theta\rho\xi}{\partial t} + \mathrm{div}(\theta\rho\xi\boldsymbol{u}) = \mathrm{div}\big(\theta\rho D_\xi \nabla\xi\big) + \rho(1-\xi)\Pi + \rho\xi\Pi$$

$$\frac{\partial \theta\rho c}{\partial t} + \mathrm{div}(\theta\rho c\boldsymbol{u}) = \mathrm{div}(\theta\rho D_c \nabla c)$$

$$+\frac{\theta\rho}{\partial\psi/\partial c}\left[\dot{\omega}_\psi + N_\xi \frac{\partial^2\psi}{\partial\xi^2} + 2\,N_{\xi c}\frac{\partial^2\psi}{\partial\xi\partial c} + N_c\frac{\partial^2\psi}{\partial c^2}\right]$$

$$+\theta\rho\dot{\omega}_c$$

$$+\rho\hat{C}(\xi,c)\Pi \quad +\rho c\Pi$$

$$\frac{\partial \theta\rho Y_\alpha}{\partial t} + \mathrm{div}(\theta\rho Y_\alpha\boldsymbol{u}) = \mathrm{div}(\theta\rho D_\alpha \nabla Y_\alpha) + \theta\rho\dot{\omega}_\alpha + \rho Y_\alpha\big(\hat{V}_\alpha + \Pi\big)$$

DCMC equation for sprays

Klimenko & Bilger, PECS, 1999
Mantel & Bilger, CST, 1995
Kronenburg, Phys.Fl., 2004
Mantel & Bilger, 1995; Amzin & Swaminathan, CST, 2012
Mortensen & Bilger, CNF, 2009

$$\frac{\partial Q_\alpha}{\partial t} + \langle \boldsymbol{u} | \eta, \zeta \rangle \cdot \nabla Q_\alpha =$$

$$\langle \dot{\omega}_\alpha | \eta, \zeta \rangle - \langle \dot{\omega}_c | \eta, \zeta \rangle \frac{\partial Q_\alpha}{\partial \zeta}$$

$$+ \frac{Le_\xi}{Le_\alpha} \langle N_\xi | \eta, \zeta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2} + \left(\frac{Le_\xi}{Le_\alpha} + \frac{Le_c}{Le_\alpha} \right) \langle N_{\xi c} | \eta, \zeta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta \partial \zeta} + \frac{Le_c}{Le_\alpha} \langle N_c | \eta, \zeta \rangle \frac{\partial^2 Q_\alpha}{\partial \zeta^2}$$

$$- \frac{1}{\bar{\theta} \bar{\rho} \widetilde{P}} \operatorname{div}\left(\bar{\theta} \bar{\rho} \widetilde{P} \langle \boldsymbol{u}'' Y_\alpha'' | \eta, \zeta \rangle \right)$$

$$+ (\delta_\alpha - Q_\alpha) \frac{\langle \Pi | \eta, \zeta \rangle}{\bar{\theta}} - \left[(1 - \eta) \frac{\partial Q_\alpha}{\partial \eta} + \hat{C}(\eta, \zeta) \frac{\partial Q_\alpha}{\partial \zeta} \right] \frac{\langle \Pi | \eta, \zeta \rangle}{\bar{\theta}}$$

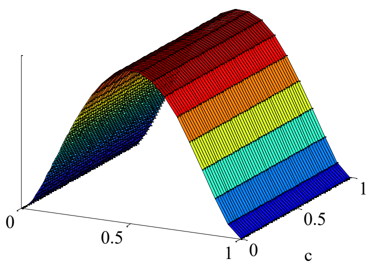
$$- \frac{1}{\bar{\theta} \bar{\rho} \widetilde{P}} \frac{\partial \bar{\rho} \widetilde{P} (1 - \eta) \langle Y_\alpha'' \Pi'' | \eta, \zeta \rangle}{\partial \eta} - \frac{1}{\bar{\theta} \bar{\rho} \widetilde{P}} \frac{\partial \bar{\rho} \widetilde{P} \hat{C}(\eta, \zeta) \langle Y_\alpha'' \Pi'' | \eta, \zeta \rangle}{\partial \zeta}$$

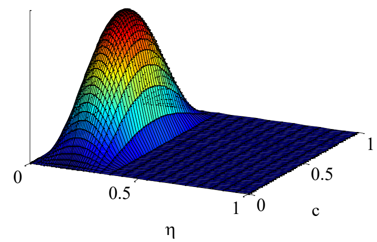
$$+ D_Q$$

Closure

- Presumed β-pdfs $\widetilde{P}\,(\eta)$ $\widetilde{P}\,(\zeta)$
- Stat. independent pdfs $\widetilde{P}\,(\eta,\zeta) = \widetilde{P}\,(\eta)\;\widetilde{P}\,(\zeta)$
- Cond. scalar dissipation rates

$\langle N_\xi | \eta, \zeta \rangle$ $\langle N_c | \eta, \zeta \rangle$ $\langle N_{\xi c} | \eta, \zeta \rangle = 0$





as proposed by Nguyen et al., CNF, 2010
and discussed by Kronenburg & Mastorakos in Echekki & Mastorakos eds., Springer, 2011

- No conditional spray terms and dilute spray assumed
- No radiation or wall heat loss
- Unity Lewis number

RANS Implementation

$$\frac{\partial \bar{\rho}\tilde{\xi}}{\partial t} + \mathrm{div}\left(\bar{\rho}\tilde{\xi}\,\tilde{\boldsymbol{u}}\right) = \mathrm{div}\left(\bar{\rho}(D_T + D)\,\nabla\tilde{\xi}\,\right) + \bar{\rho}\widetilde{\Pi}$$

$$\frac{\partial \bar{\rho}\widetilde{\xi'^2}}{\partial t} + \mathrm{div}\left(\bar{\rho}\widetilde{\xi'^2}\,\tilde{\boldsymbol{u}}\right) = \mathrm{div}\left(\bar{\rho}(D_T + D)\nabla\widetilde{\xi'^2}\,\right) - 2\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\widetilde{\xi'^2} + 2\bar{\rho}D_T\nabla\tilde{\xi}\cdot\nabla\tilde{\xi}$$

$$+2\bar{\rho}\left(\widetilde{\xi\Pi} - \tilde{\xi}\,\widetilde{\Pi}\,\right) - \bar{\rho}\left(\,\widetilde{\xi^2\Pi} - \tilde{\xi}^{\,2}\,\widetilde{\Pi}\,\right)$$

$$c = c_{\mathrm{CO2}}$$

$$\frac{\partial \bar{\rho}\tilde{c}}{\partial t} + \mathrm{div}(\bar{\rho}\tilde{c}\,\tilde{\boldsymbol{u}}) = \mathrm{div}(\bar{\rho}(D_T + D)\,\nabla\tilde{c}\,) + \bar{\rho}\widetilde{\dot{\omega}_c}$$

$$\frac{\partial \bar{\rho}\widetilde{c'^2}}{\partial t} + \mathrm{div}\left(\bar{\rho}\widetilde{c'^2}\,\tilde{\boldsymbol{u}}\right) = \mathrm{div}\left(\bar{\rho}(D_T + D)\nabla\widetilde{c'^2}\,\right) - 2\bar{\rho}\tilde{\varepsilon}_c + 2\bar{\rho}D_T\nabla\tilde{c}\cdot\nabla\tilde{c} + 2\bar{\rho}\widetilde{c'\dot{\omega}'_c}$$

where $$\tilde{\varepsilon}_c = \frac{1}{\beta'}\left[(2K_c^* - \tau C_4)\frac{S_L}{\delta_L} + C_3\frac{\tilde{\varepsilon}}{\tilde{k}}\right]\widetilde{c'^2}$$

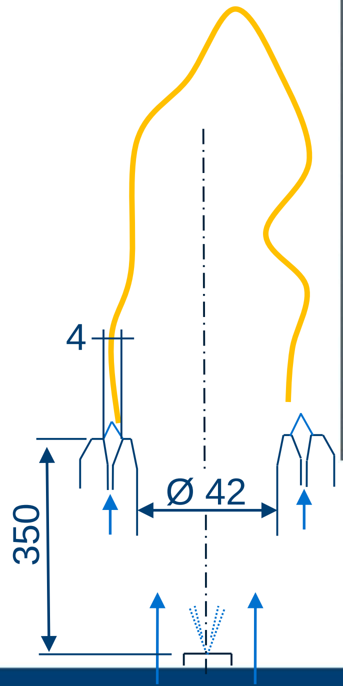
Kolla et al. CST, 2009

Test case

Piloted ethanol spray flame

Kariuki & Mastorakos, submitted to CNF, 2016

- Liquid fuel
- Pre-vaporisation
- Premixing

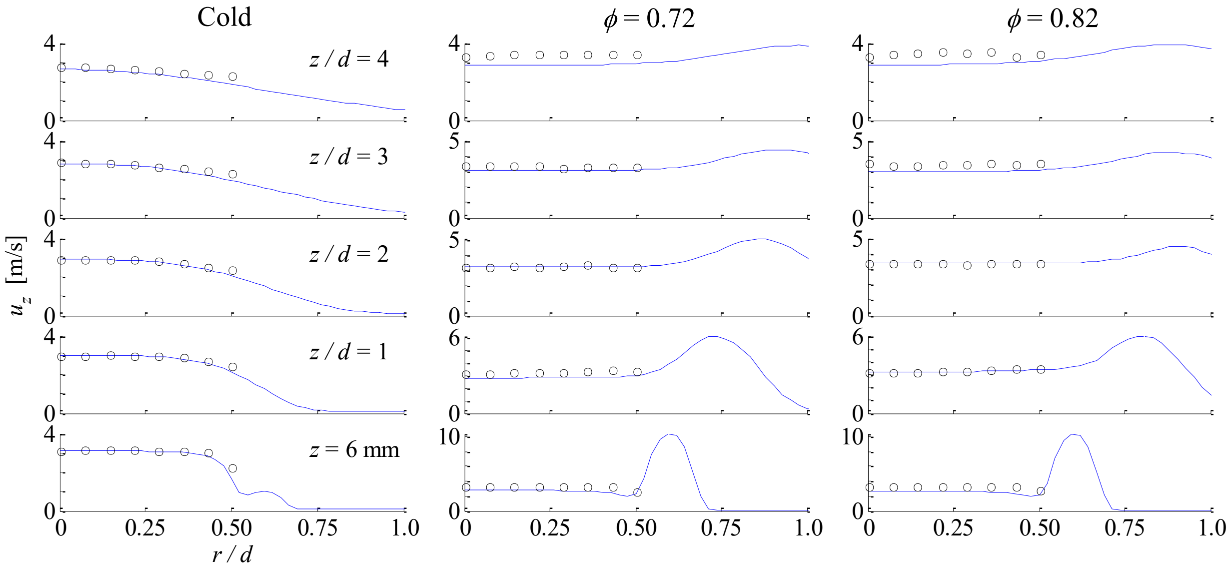


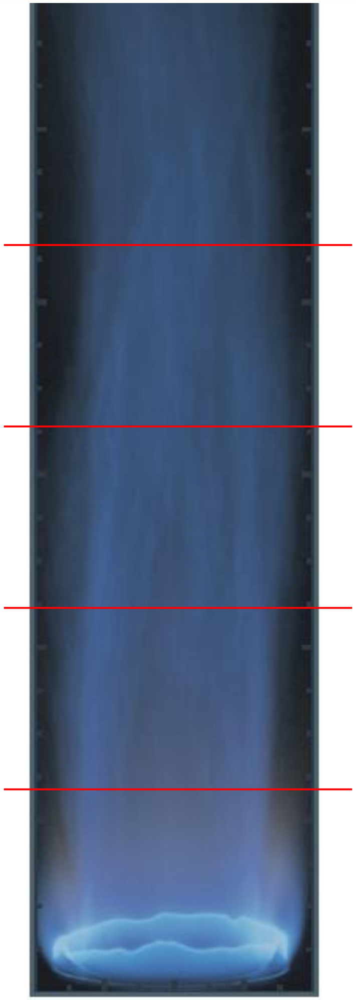
Kariuki and Mastorakos, submitted to CNF, 2016

Simulation

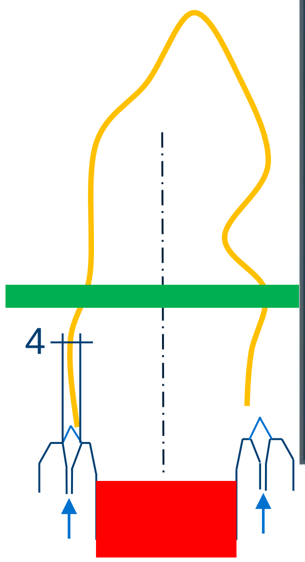
- Flow field solver **OpenFOAM**
- BCs from experiment
- Lagrangian doplets
- Abramzon & Sirignano evaporation model
- 1D CMC grid
- Detailed chem. (57 species) Marinov mechanism

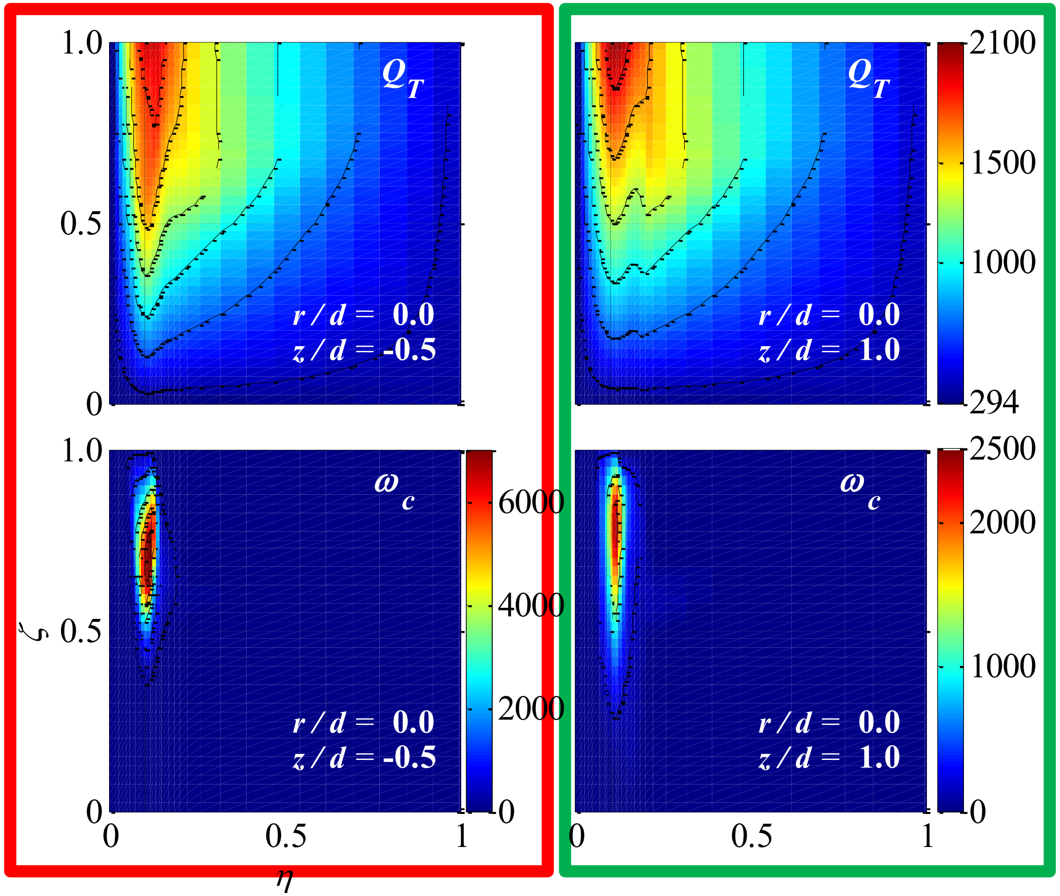
Axial velocity





Conditional moments

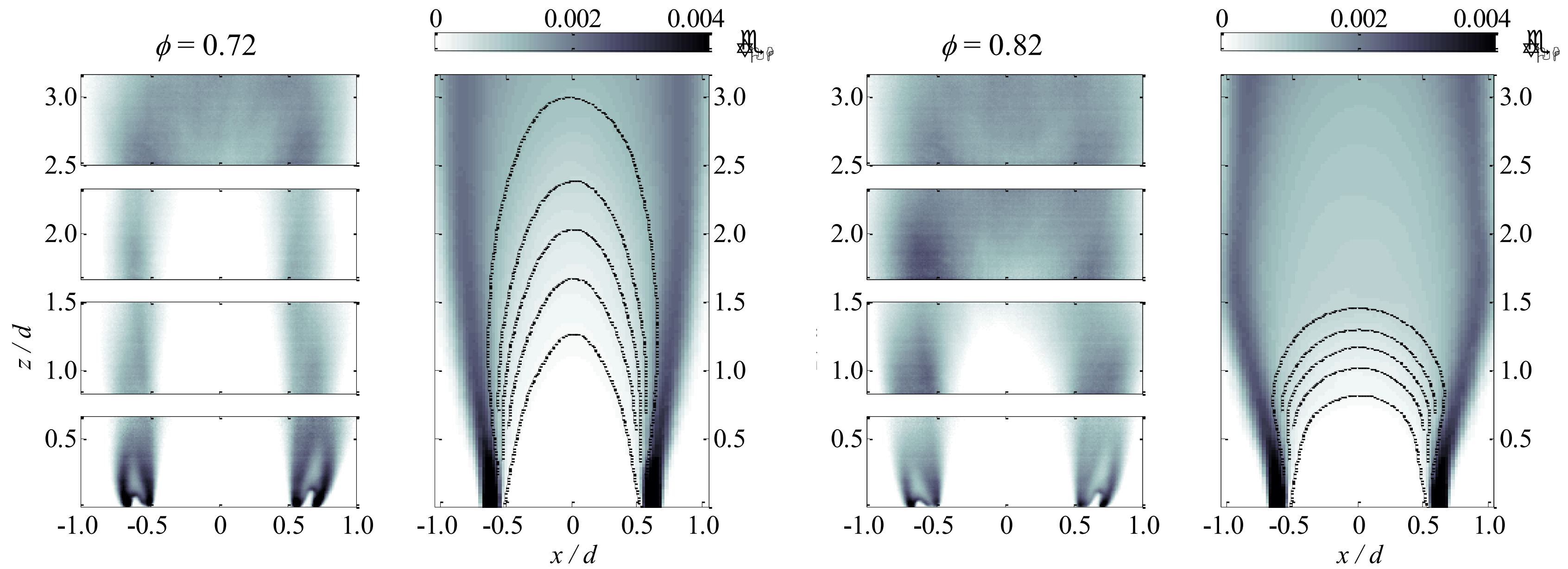




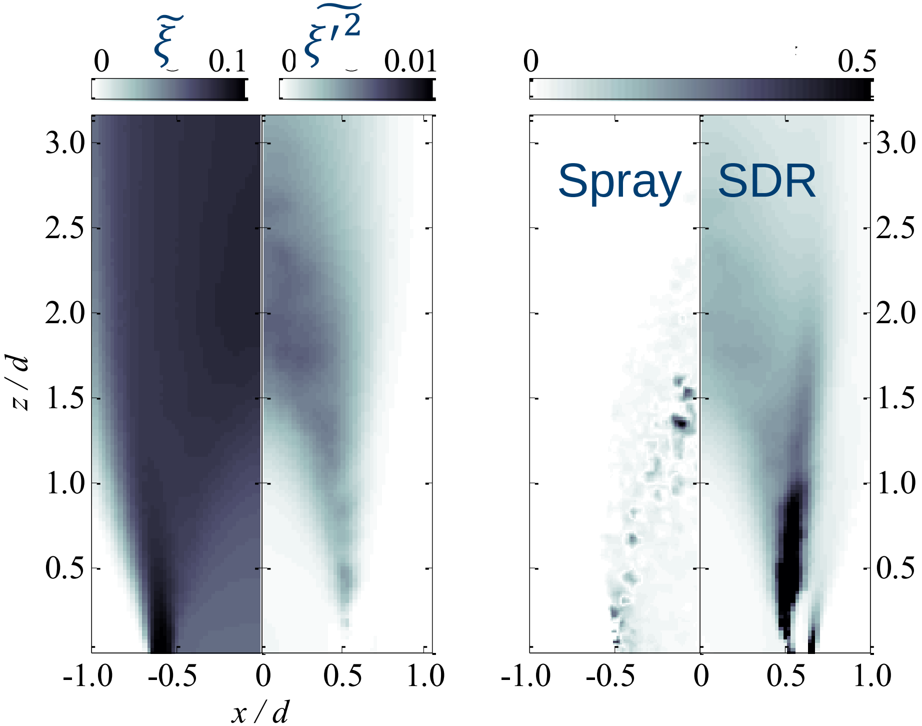
Flame shape

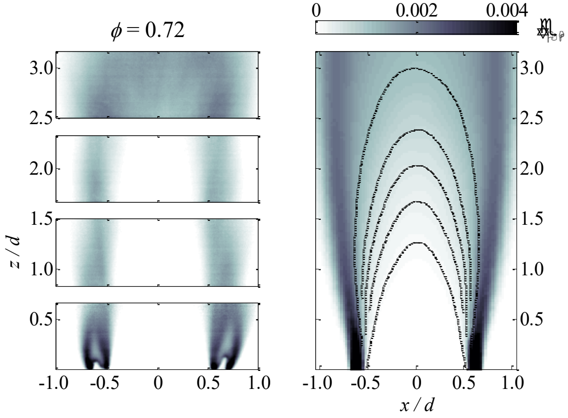
Experiment | **Simulation**

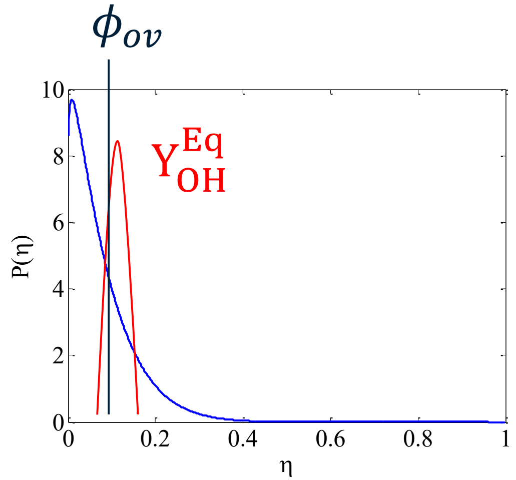
OH PLIF | $\widetilde{Y}_{OH}$



Mixture fraction variance







SDR: $2\frac{\tilde{\varepsilon}}{\tilde{k}}\widetilde{\xi'^2}$

Spray: $2(\widetilde{\xi\Pi} - \tilde{\xi}\,\widetilde{\Pi}) - (\widetilde{\xi^2\Pi} - \tilde{\xi}^2\,\widetilde{\Pi})$

Summary and conclusions

- DCMC equation for spray flames $\frac{\partial Q_\alpha}{\partial t} + \cdots$
- Preliminary application
- Experiment vs. Simulation
- Performance of the mixture fraction SDR model unsatisfactory

Future work:

Modelling of the spray terms