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Numerical investigation of spray combustion in aero-engines: from single droplet autoignition to the prediction of blow-off and soot

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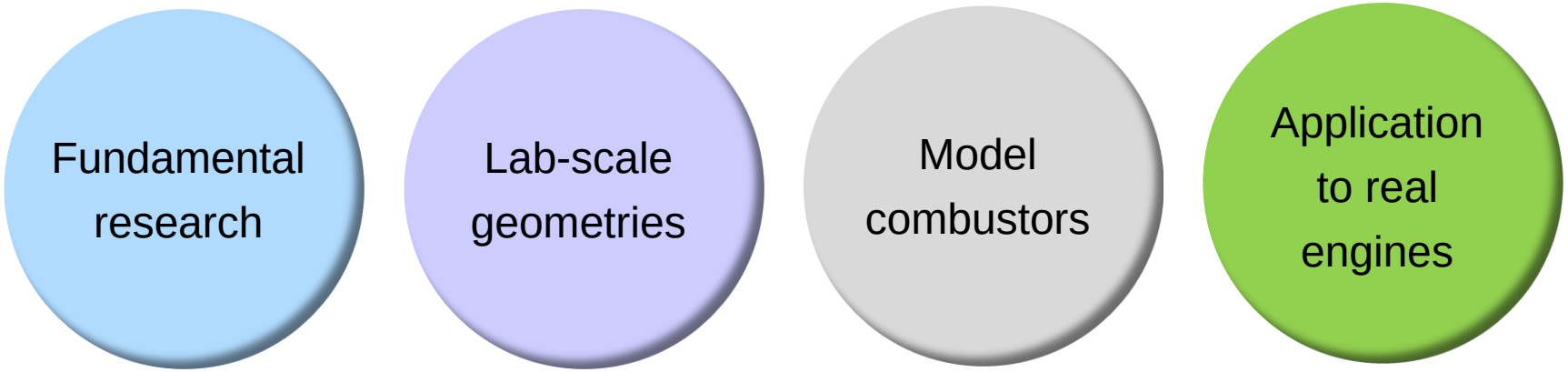
Department of Engineering

Overview



- Improve the understanding of physical phenomena
- Make CFD a reliable tool for engine predictions

- Investigate specific issues of the engine behaviour

Outline

1. Fundamental research
   - Single droplet autoignition and combustion
   - Droplet regime diagrams
2. Lab-scale spray flames
   - Local extinction in spray flames
   - Blow-off of spray flames
3. Model combustors
   - Prediction of soot

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Fundamental research

Single droplet evaporation, ignition and combustion

A. Giusti, J.A.M. Sidey,
G. Borghesi, E. Mastorakos

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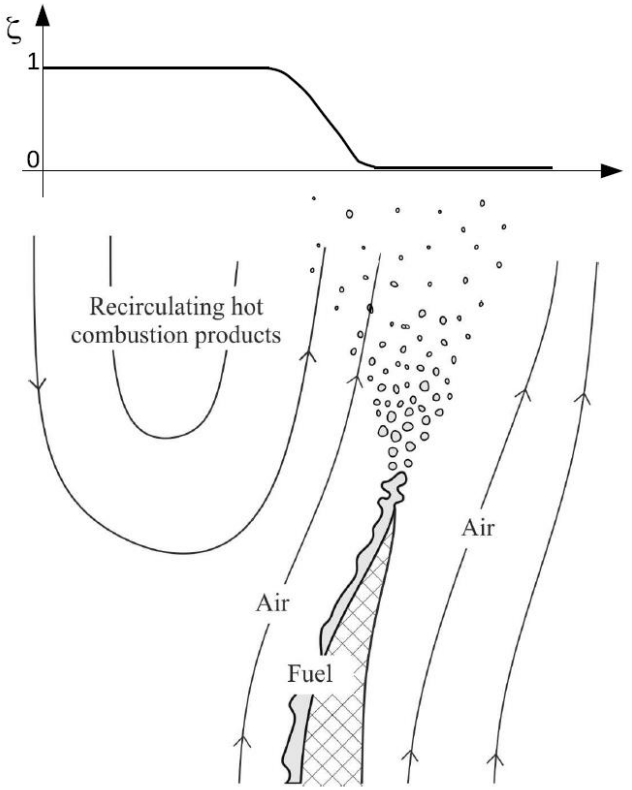
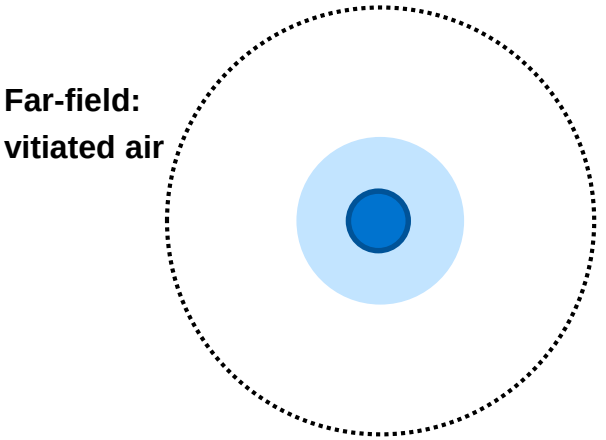
Single droplet autoignition and combustion

- Motivation
  - In real engines droplet can experience different ambience conditions, from pure air to hot combustion products
- Objective
  - What is the behaviour of the single droplet for different composition of the vitiated air?
  - Can the droplet autoignite?
  - What are the implication for the design of an combustor or an injection system?
- Method
  - Single droplet computations in a quiescent medium
  - Multi-component droplet



Numerical setup

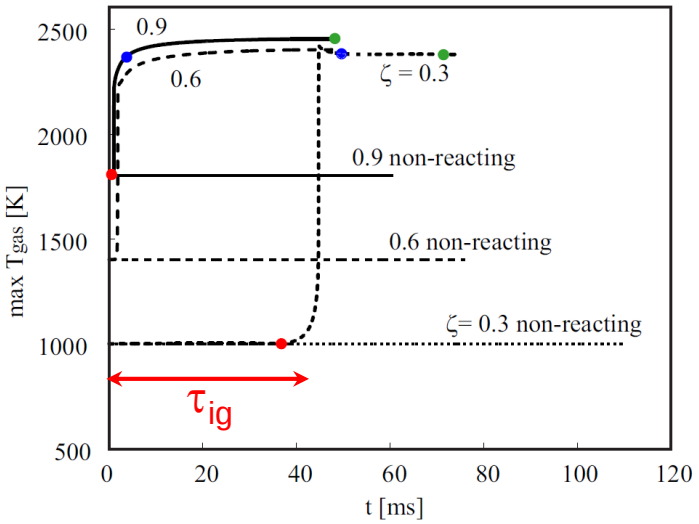
- Computations at conditions of interest for GT applications: p=11 bar
- Dagaut mechanism for kerosene: 209 species 1673 reversible reactions
  - Kerosene surrogate:
    - 74% n-decane
    - 15% n-propylbenzene
    - 11% n-propylcyclohexane
  - **Multi-component droplets**
  - Fuel initial temperature: 400 K
- Vitiated air
  - Mixture of pure air at 600 K and hot combustion products got from a premixed flame computation with reactants at 600K and ϕ=0.6.

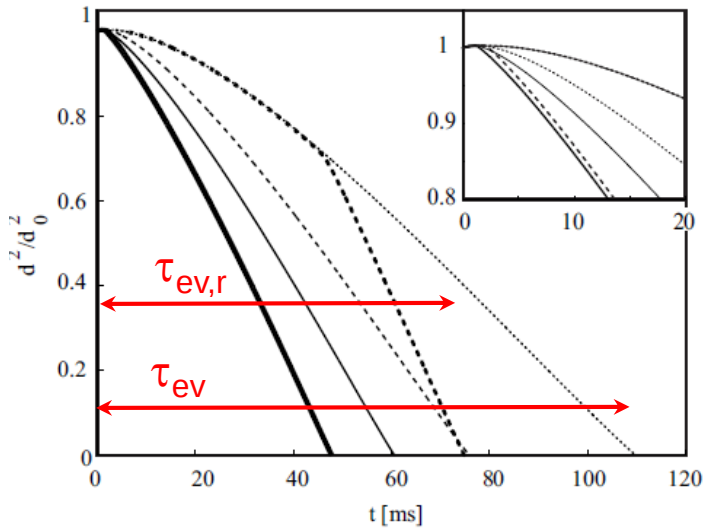


Isolated kerosene droplet in a quiescent medium

Evaporation and autoignition

d_0=200 μm

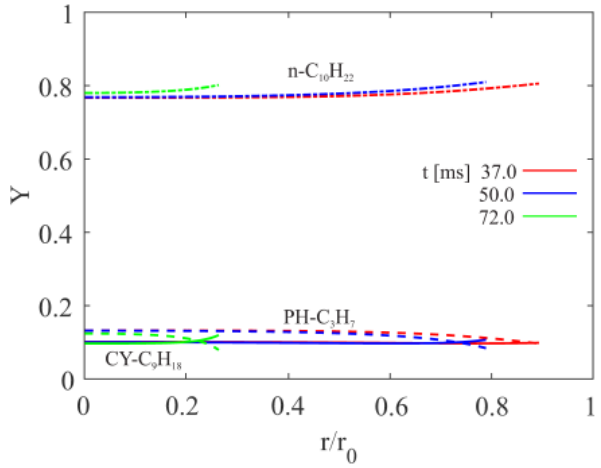


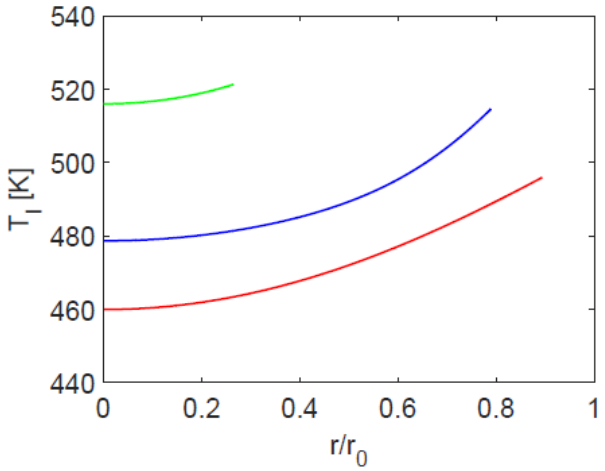


Fuel components behavior
Inside the liquid droplet

ζ=0.3

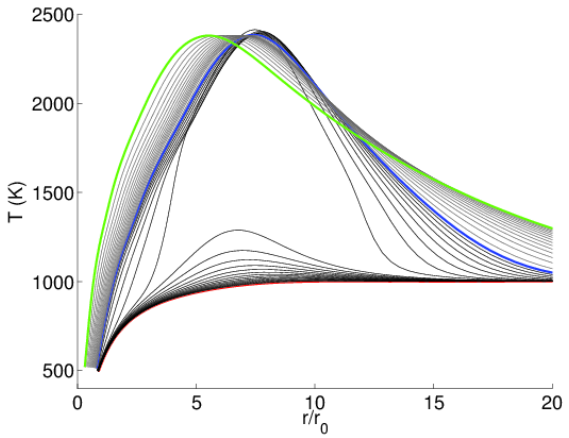
d_0=200 μm





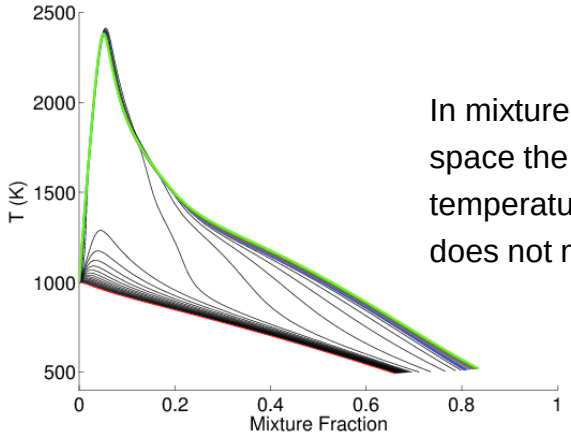
Physical *vs* mixture fraction space

Physical space

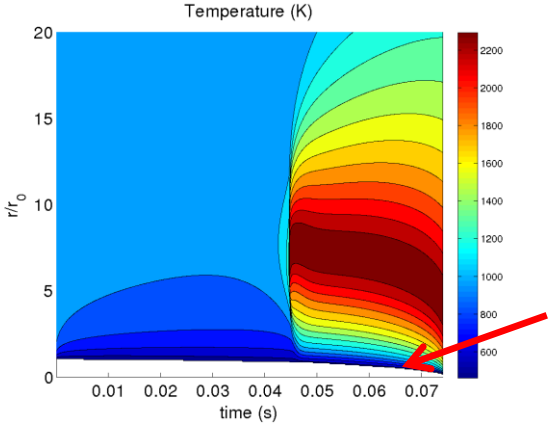


The peak of temperature moves to smaller radius as the droplet evaporates.

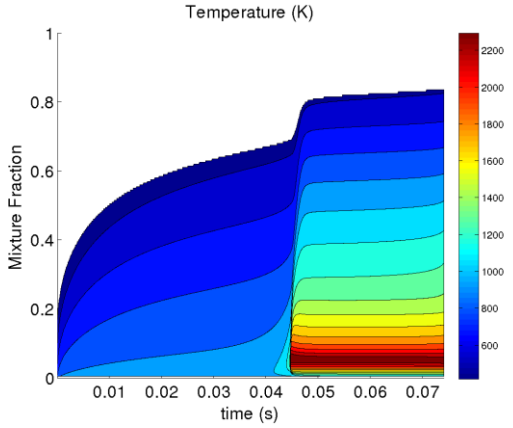
Mixture fraction space



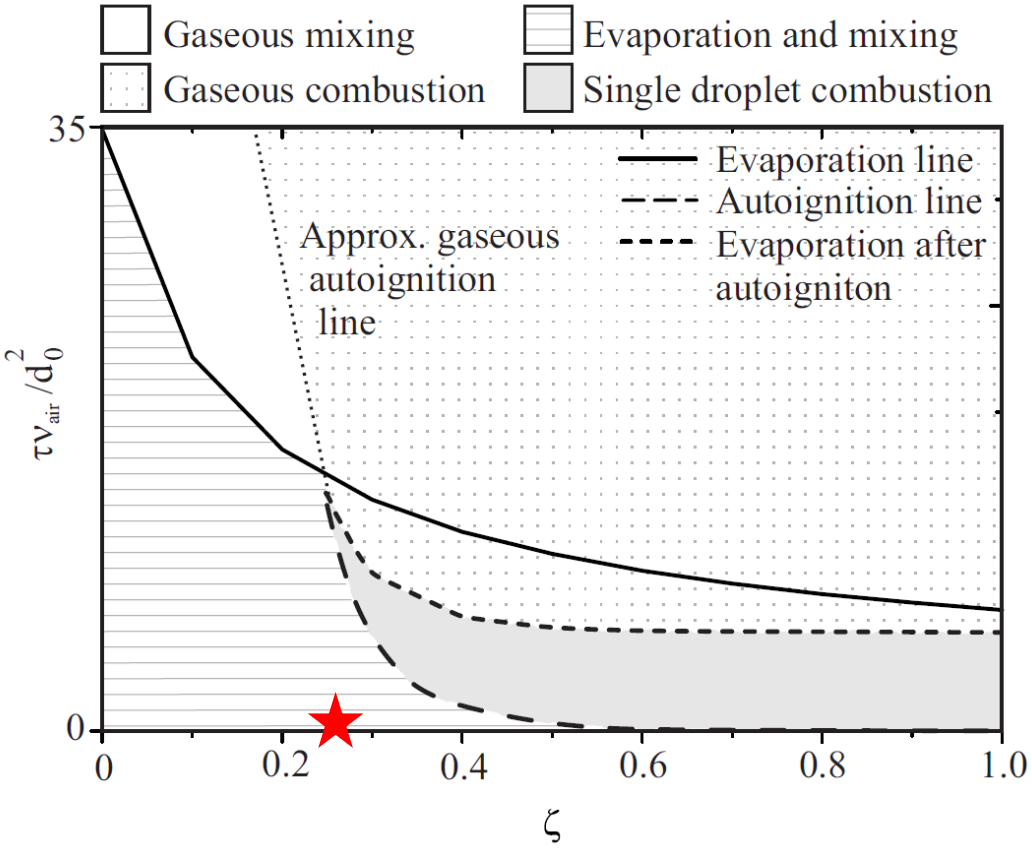
In mixture fraction space the temperature peak does not move.



Droplet surface



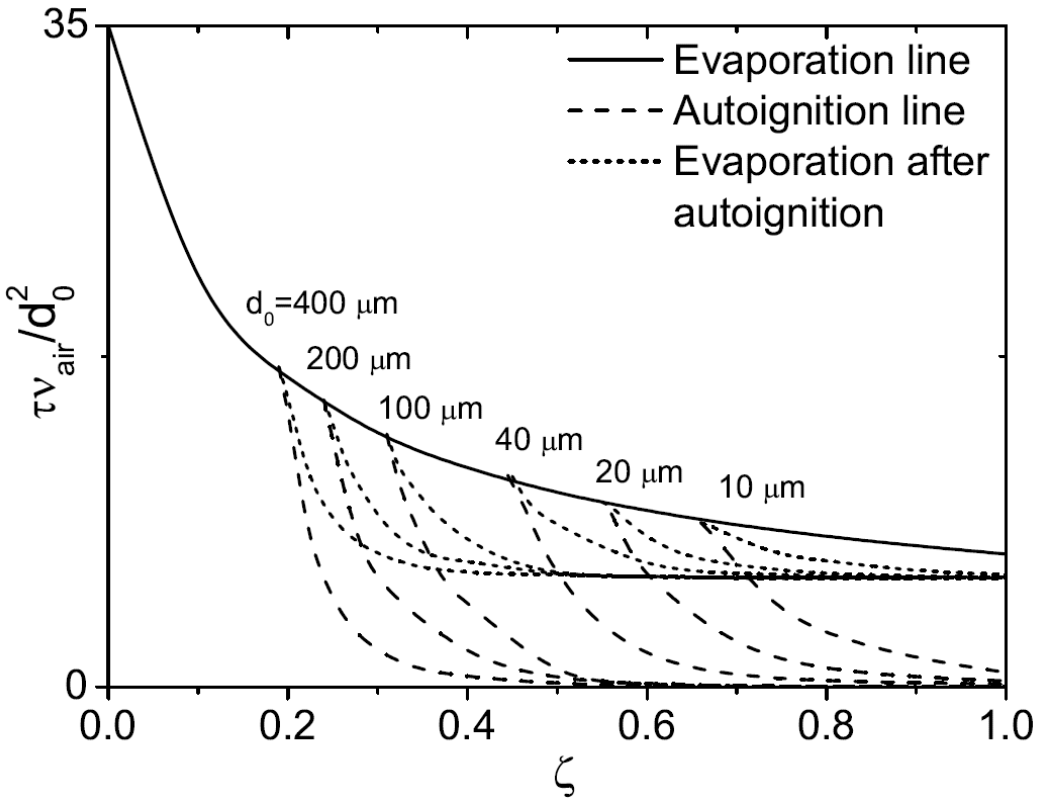
Regime diagrams



Droplet with initial diameter = 200 μm

- The behaviour of the single droplet can be summarized by plotting the time delays as a function of the dilution variable.
- It is possible to define a **critical value of dilution** below which no single droplet autoignition is possible.

Regime diagrams



Regime diagrams for various initial droplet diameters

- For each ζ It is possible to define a **critical value of the initial diameter** below which no single droplet autoignition is possible.

- IMPLICATIONS
  - Injector design
  - Residence time
  - Flow path design

NOTE: a similar diagram can be produced for every condition and every fuel.

Concluding remarks

- Detailed numerical simulations of fundamental cases can give very important insight and useful indications for practical systems
  - Droplet regime diagrams
  - Implications for combustor design
- **Based on this methodology, we can define criteria for the design of injection systems to avoid locally rich combustion in a Lean-Burn strategy**
- Solutions can be exploited for the development of models to be used in LES

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Lab-scale geometries

Local extinction and blow-off of turbulent spray flames

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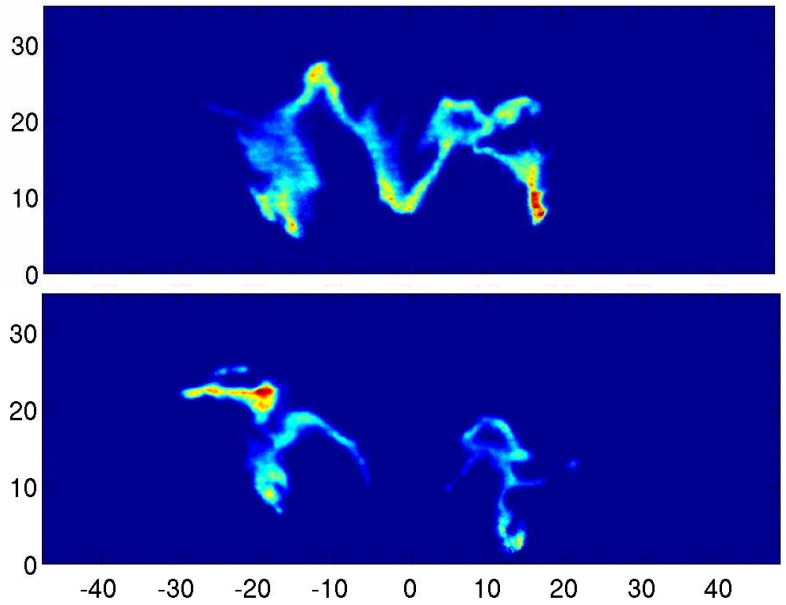
Local extinction and blow-off of an ethanol spray flame

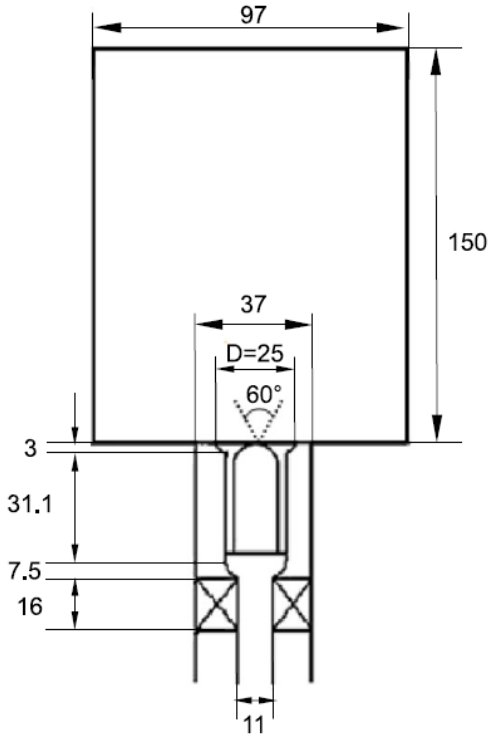
Experiment by R. Yuan [1]

OH-PLIF measurements



$U_{air}=0.79U_{BO}$

$U_{air}=U_{BO}$



Is the CFD able to predict such phenomena?

What is the mechanism of blow-off?

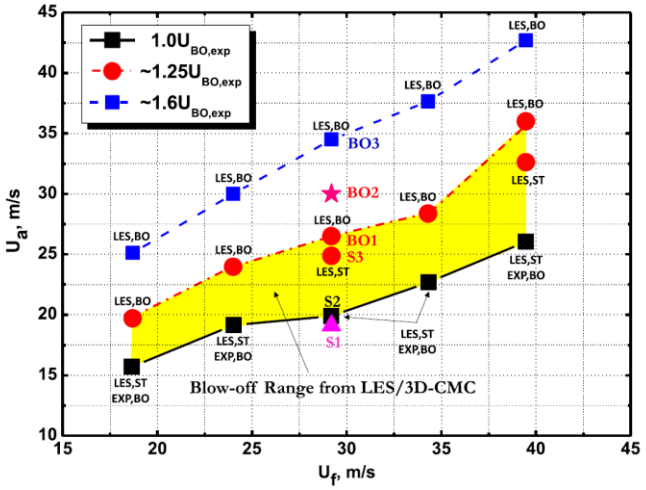
Is the evaporation important?

[1] R. Yuan, PhD thesis, University of Cambridge (2015)

Prediction of local extinctions and blow-off in turbulent flames

Turbulent gaseous non-premixed flames

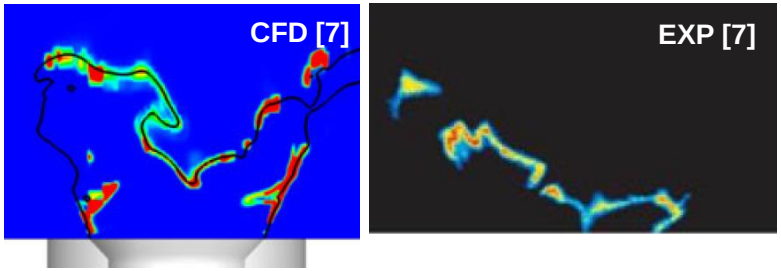
- Some success already demonstrated with Eulerian transported PDF [2], CMC [3] and flamelet [4] models
- LES/CMC, good prediction of the lift-off height PDF and blow-off curve



From Zhang and Mastorakos, FTaC (2016)

Turbulent spray flames

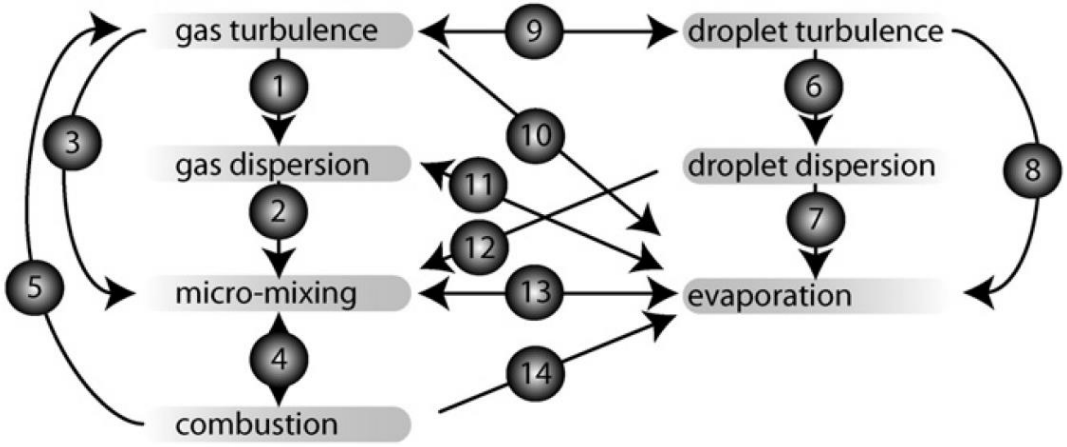
- Very few attempts: LES/CMC of a n-heptane spray flame



- Modified 1-step chemistry model
- Some success in predicting local ext.

[2] W. Jones, V. Prasad, Combust. Flame 157 (2010)
[3] A. Garmory, E. Mastorakos, Proc. Combust. Inst. 33 (2011)
[4] M. Ihme, H. Pitsch, Combust. Flame 155 (2008)
[5] H. Zhang et al., Proc. Combust. Inst. 35 (2015)
[6] H. Zhang, E. Mastorakos, Flow Turbul. Combust. 96 (2016)
[7] A. Tyliszczak et al., Flow Turbul. Combust. 92 (2014)

A simplified picture of turbulent spray combustion…



Jenny et al., Progress in Energy and Comb. Sci. 38 (2012)

Spray combustion involves many length and time scales with a strong coupling between evaporation, turbulence and chemical reactions

The ideal model should include:

- On-line solution of the chemistry
- Interaction between micro-mixing and evaporation
- Interaction between the macro- and micro-mixing and the flame structure
- Interaction between evaporation and the flame structure

Method: LES/CMC

Mixture fraction equation

$$\frac{\partial \bar{\rho}\tilde{\xi}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{\xi}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\bar{\rho} D \frac{\partial \tilde{\xi}}{\partial x_i}\right) + \frac{\partial J_{sgs}}{\partial x_i} + \bar{\rho}\widetilde{\Pi}$$

Solved by the LES solver

$$J_{sgs} = \bar{\rho} D_t \frac{\partial \tilde{\xi}}{\partial x_i}$$

Mixture fraction variance

$$\frac{\partial \bar{\rho}\widetilde{\xi''^2}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\widetilde{\xi''^2}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\bar{\rho}(D + D_t)\frac{\partial \widetilde{\xi''^2}}{\partial x_i}\right) - 2\bar{\rho}\widetilde{N}$$

$$+2\bar{\rho}(D+D_t)\frac{\partial \tilde{\xi}}{\partial x_i}\frac{\partial \tilde{\xi}}{\partial x_i} + \underbrace{2\bar{\rho}(\widetilde{\xi\Pi} - \tilde{\xi}\widetilde{\Pi})}_{\bar{\rho}W^+} - \underbrace{\bar{\rho}(\widetilde{\xi^2\Pi} - \tilde{\xi}^2\widetilde{\Pi})}_{\bar{\rho}W^-}$$

Scalar dissipation rate

$$\widetilde{N} = \underbrace{D\left(\frac{\partial \tilde{\xi}}{\partial x_i}\right)^2}_{\text{resolved}} + \underbrace{\frac{1}{2}C_N\frac{\nu_t}{\Delta^2}\widetilde{\xi''^2}}_{\text{subgrid}}$$

$$\widetilde{N|\eta} = N_0 G(\eta),$$

$$G(\eta) = \exp\left(-2\left[\text{erf}^{-1}(2\eta - 1)\right]^2\right)$$

$$N_0 = \frac{\widetilde{N}}{\int_0^1 G(\eta)\widetilde{\mathcal{P}}(\eta)d\eta}$$

C_N=42.0

CMC equations

Conditionally filtered mass fraction

$$\frac{\partial Q_\alpha}{\partial t} + \widetilde{u_j|\eta}\frac{\partial Q_\alpha}{\partial x_j} = e_\alpha + \widetilde{N|\eta}\frac{\partial^2 Q_\alpha}{\partial \eta^2} + \widetilde{\omega_\alpha|\eta} + \underbrace{\delta_{\alpha,f}\widetilde{\Pi|\eta} - \left(Q_\alpha + (1-\eta)\frac{\partial Q_\alpha}{\partial \eta}\right)\widetilde{\Pi|\eta}}_{\text{contribution from the liquid phase}}$$

A similar equation is solved for the conditional enthalpy

First order closure for chemical source terms.

Spray source terms in the variance equation

Mixture fraction variance equation

$$\frac{\partial \bar{\rho}\widetilde{\xi''^2}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_i\widetilde{\xi''^2}}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\bar{\rho}(D+D_t)\frac{\partial \widetilde{\xi''^2}}{\partial x_i}\right)-2\bar{\rho}\widetilde{N}+2\bar{\rho}(D+D_t)\frac{\partial \tilde{\xi}}{\partial x_i}\frac{\partial \tilde{\xi}}{\partial x_i}$$
$$+2\bar{\rho}\left(\widetilde{\xi\Pi}-\tilde{\xi}\tilde{\Pi}\right)-\bar{\rho}\left(\widetilde{\xi^2\Pi}-\tilde{\xi}^2\tilde{\Pi}\right)$$

$$\bar{\rho}W^+=2\bar{\rho}\left(\widetilde{\xi\Pi}-\tilde{\xi}\tilde{\Pi}\right)=\mathbf{2\bar{\rho}\tilde{\Pi}(\bar{\xi}_s-\tilde{\xi})}$$

$$\bar{\rho}W^-=\bar{\rho}\left(\widetilde{\xi^2\Pi}-\tilde{\xi}^2\tilde{\Pi}\right)=\mathbf{\bar{\rho}\tilde{\Pi}(\bar{\xi}_s^2-\tilde{\xi}^2)}$$

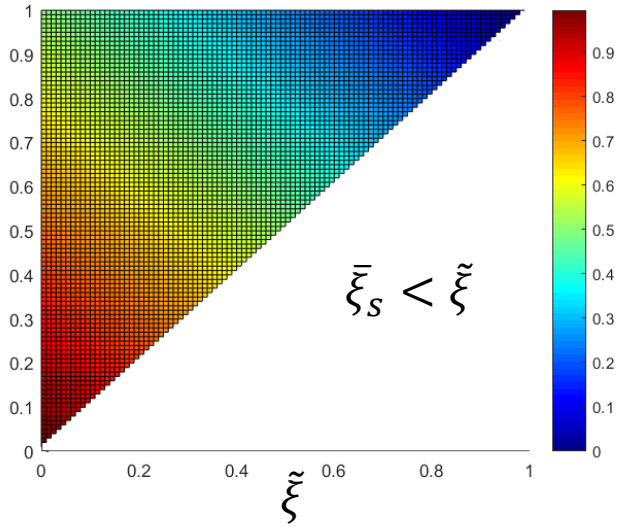
$$\widetilde{\Pi|\eta}=\frac{\tilde{\Pi}\delta(\eta-\bar{\xi}_s)}{\tilde{P}(\eta)}$$

$\bar{\rho}W^+ \gg \bar{\rho}W^-$ Pera et al. CNF (2008), very dilute spray, cold flow

?

$\bar{\rho}W^-$ in general cannot be neglected

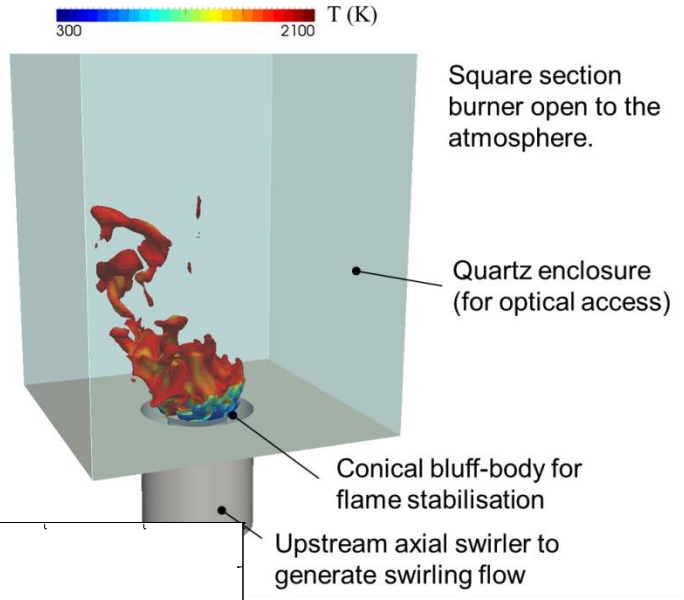
$(W^+-W^-)/W^+$

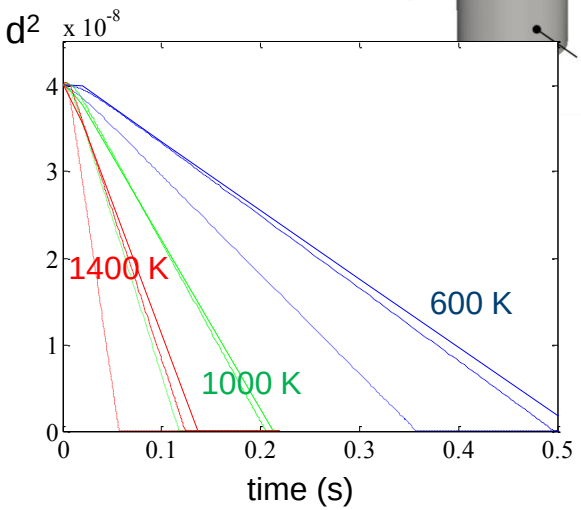


Thanks to M.P. Sitte for the useful discussions

Configuration: Cambridge spray flame

- PRECISE-UNS + unstructured CMC
- Three different conditions
  - 2 stable cases (79.2% and 92.6% U_{BO})
  - Blow-off case
- Dilute spray Lagrangian formulation for the spray. A&S evaporation model (infinite conductivity in the liquid phase)
- Numerical details
  - Vreman model for the sgs stress tensor
  - Detailed chemistry: Marinov mechanism
    - 57 species
    - 383 reactions
  - LES mesh: 5M cells
  - CMC mesh: 45k cells



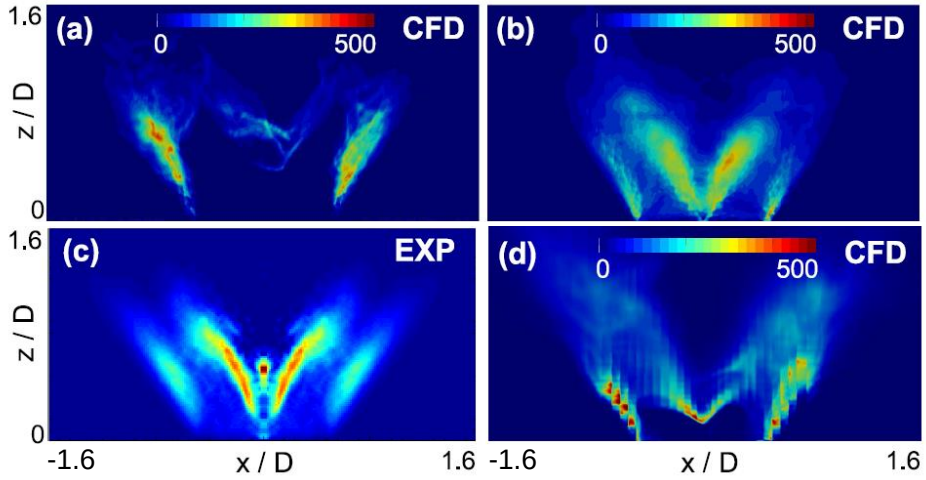


Single droplet code
A & S (1989)
Classic rapid mixing

[1] Borghesi & Mastorakos, CNF, 2015
[2] Borghesi & Mastorakos, FTC, 2016
[3] Miller et al., Int. J. Multiphaseflow, 1998

Stable condition: E1S2

- Effect of spray source terms
  - Preliminary simulations performed using 1-step chemistry model



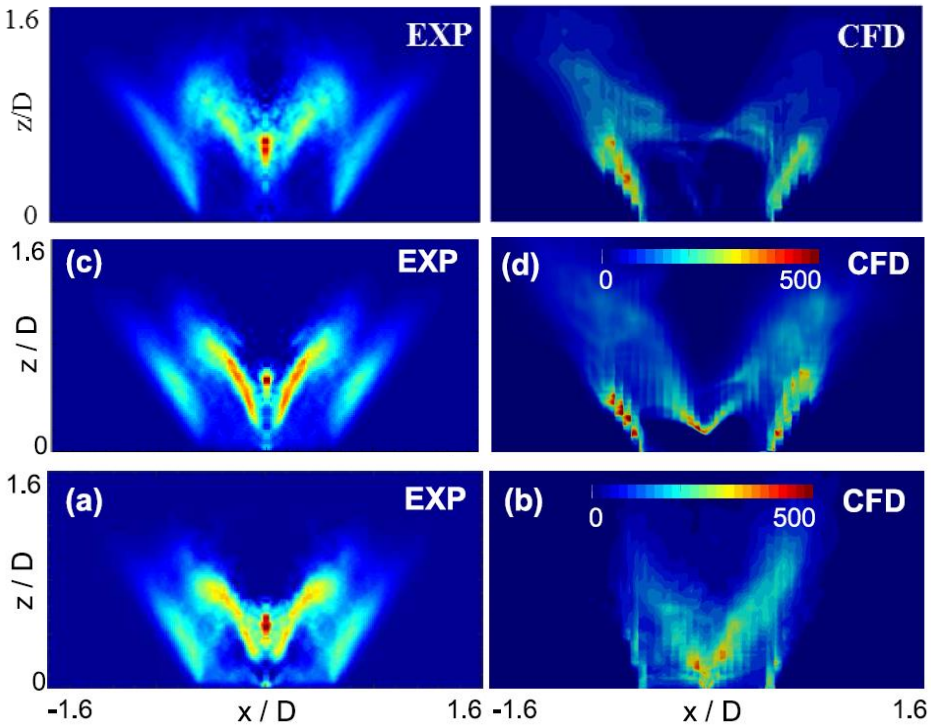
a) mean HRR predicted without spray source terms (1-step chemistry)
b) mean HRR predicted with spray source terms (1-step chemistry)
c) Inverse Able-transformed time-averaged OH*
d) mean HRR predicted with spray source terms and detailed chemistry

  - Spray source terms increase the scalar dissipation rate in the inner region of the flame generally leading to higher values of HRR

Mean flame shape

- Comparison with experiments for different values of the air flow bulk velocity.

Inverse Abel-transformed mean OH* - Mean HRR



$U_{air}=0.79U_{BO}$

$U_{air}=0.92U_{BO}$

$U_{air}=U_{BO}$

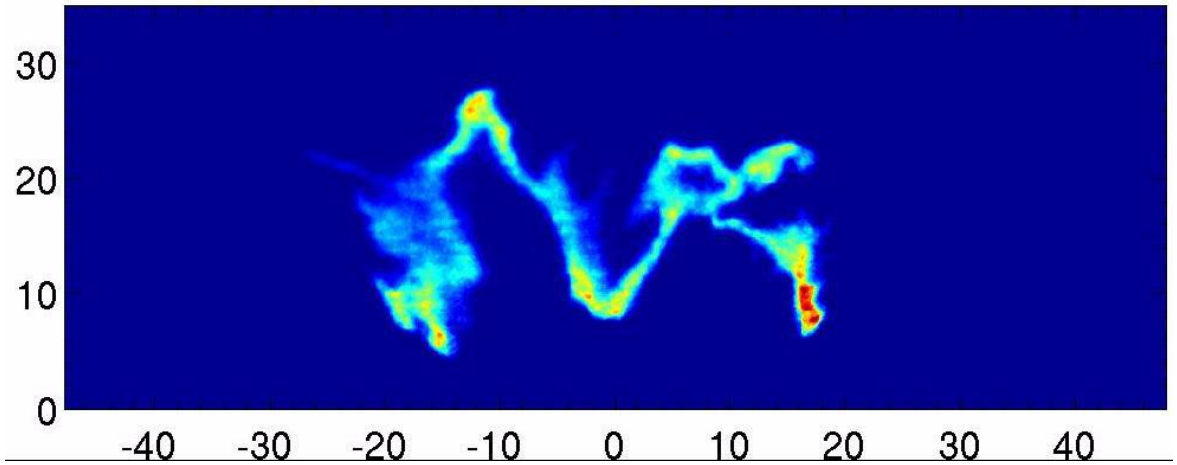
Spray source terms increase the scalar dissipation rate in the inner region of the flame generally leading to higher values of HRR

NOTE: the mean values where computed by considering the time interval before blow-off.

Giusti and Mastorakos, Proc. Combust. Inst., (2017)
Giusti and Mastorakos, ETMM-11, Palermo (2016)

Stable flame close to blow off (U_b = 79%U_{BO})

Giusti and Mastorakos, Proc. Combust. Inst., (2017)



Experiment by R. Yuan [1]

OH-PLIF measurements

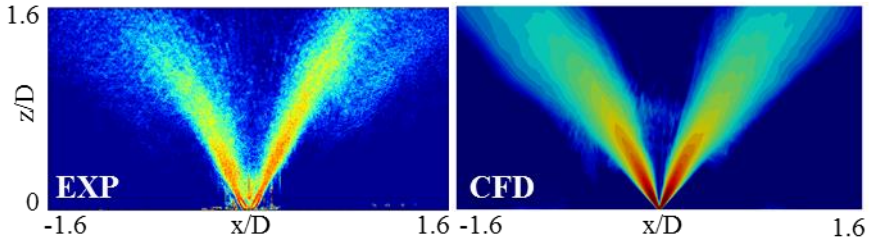
Challenges: flame lift-off, local extinction both in the inner and outer flame brush

[1] R. Yuan, PhD thesis, University of Cambridge (2015)

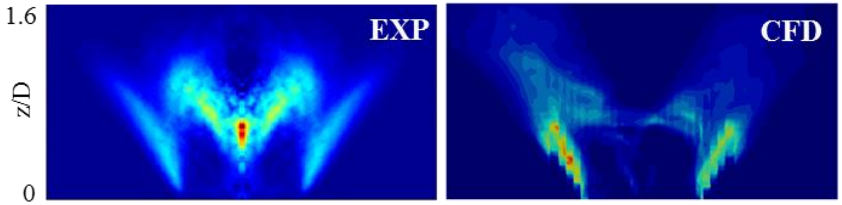
Cambridge spray flame – case E1S1

- Mean properties

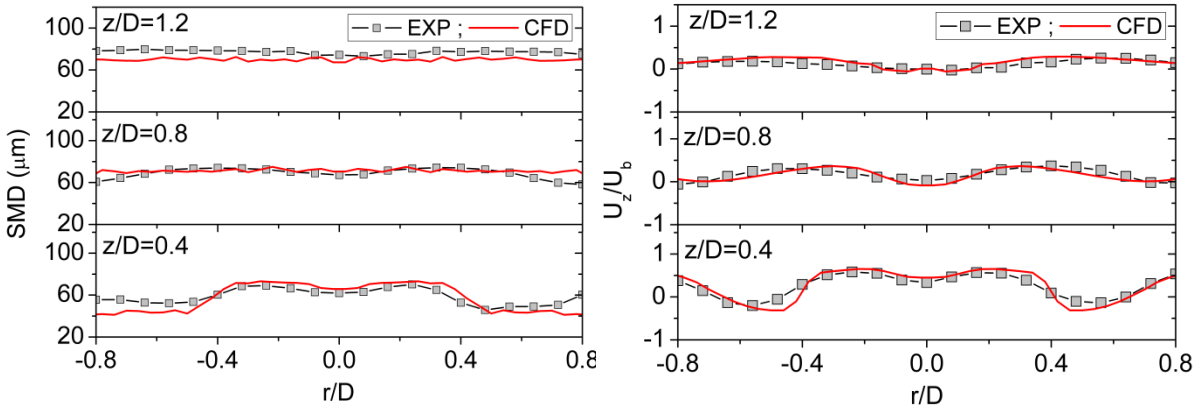
MIE scattering comparisons



Inverse Abel-transformed OH* - Mean HRR



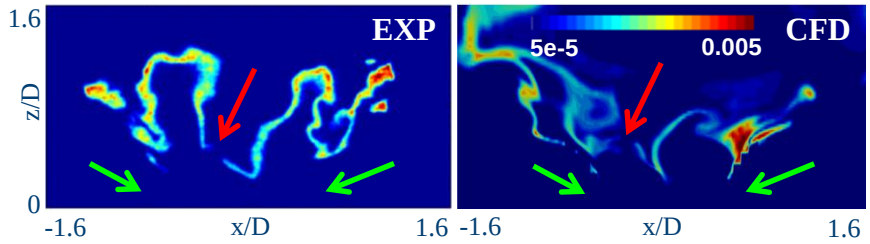
Droplet characteristics

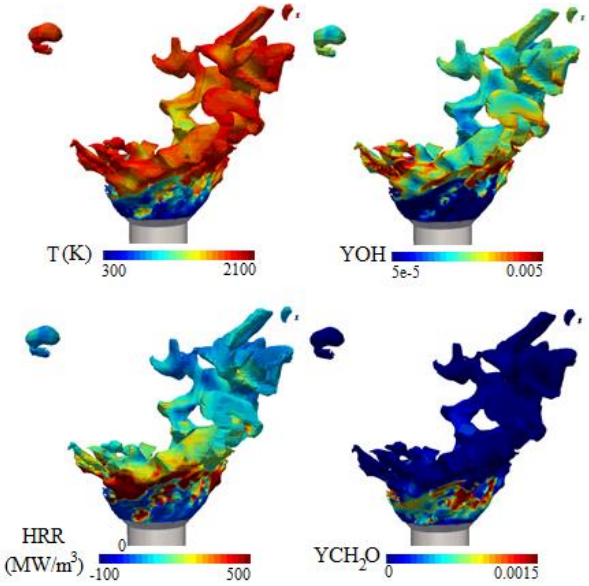


Spray characteristics and main features of the flame are well predicted.

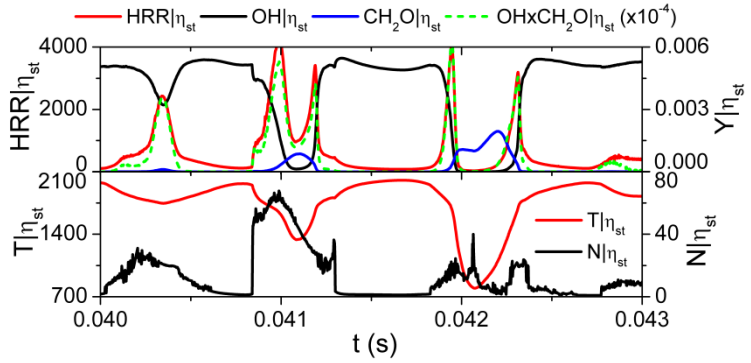
Local extinction behavior – case E1S1

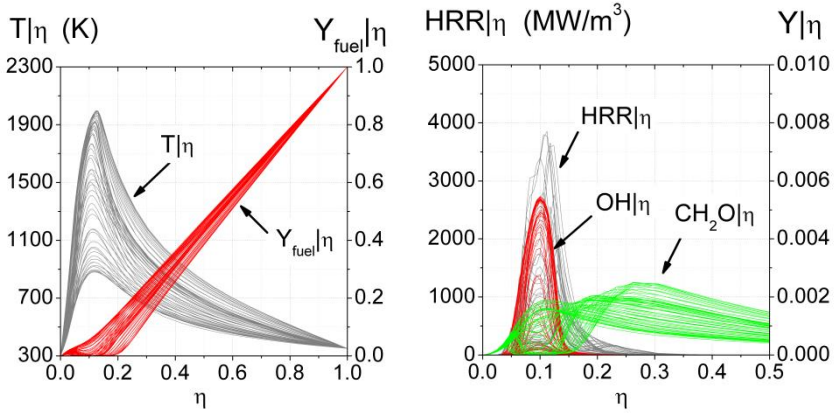
Comparison between an instantaneous OH-PLIF snapshot and OH mass fraction





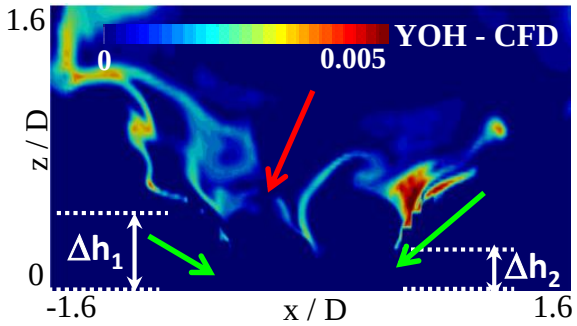
Stoichiometric mixture fraction iso-surface colored with different quantities





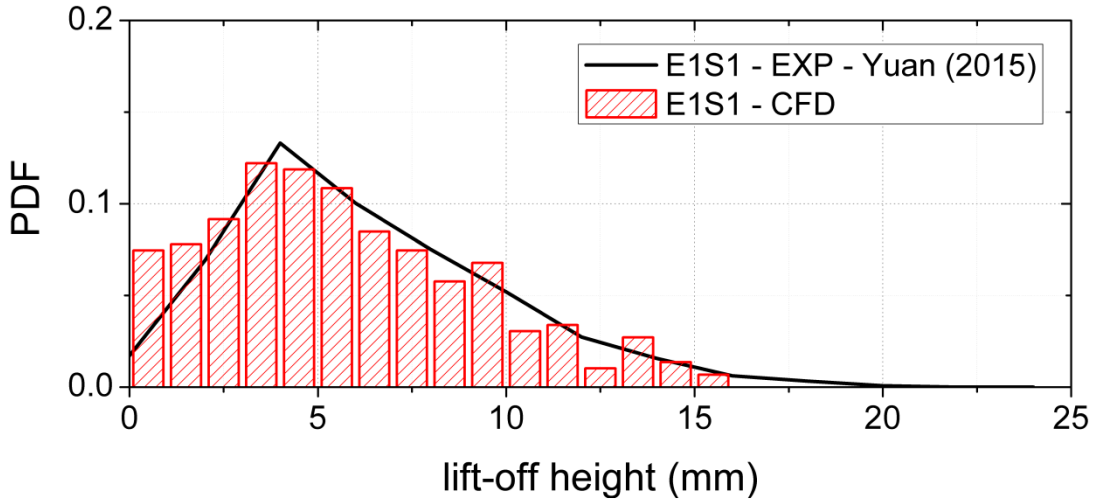
Time evolution of conditional quantities at a selected location along the outer flame brush

Lift-off height statistics – case E1S1



Definition of the lift-off height.

- Lift-off height computed from OH mass fraction snapshots
- Sampling frequency 5kHz (as in the exp)
- 2 values for each snapshot



Good agreement between numerical simulations and the experiment

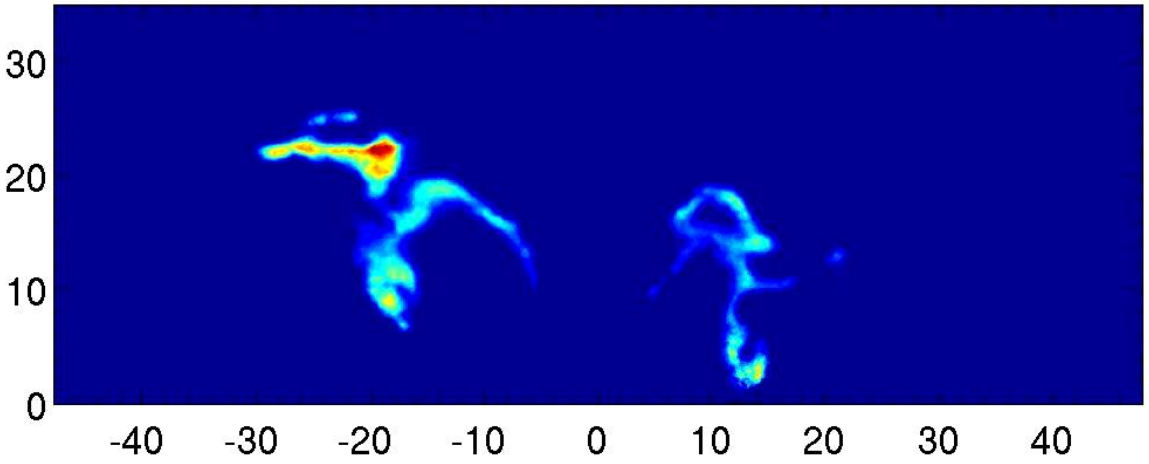
The prediction of the lift-off height statistics is a very important challenge for combustion CFD

The degree of local extinction is captured quantitatively

Giusti and Mastorakos, Proc. Combust. Inst., (2017)

blow-off case

Giusti and Mastorakos, ETMM-11 (2016)



Experiment by R. Yuan [1]

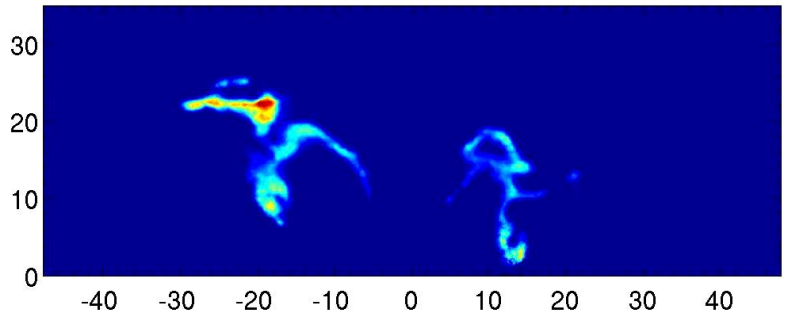
OH-PLIF measurements

Challenges: capturing the blow-off of spray flames

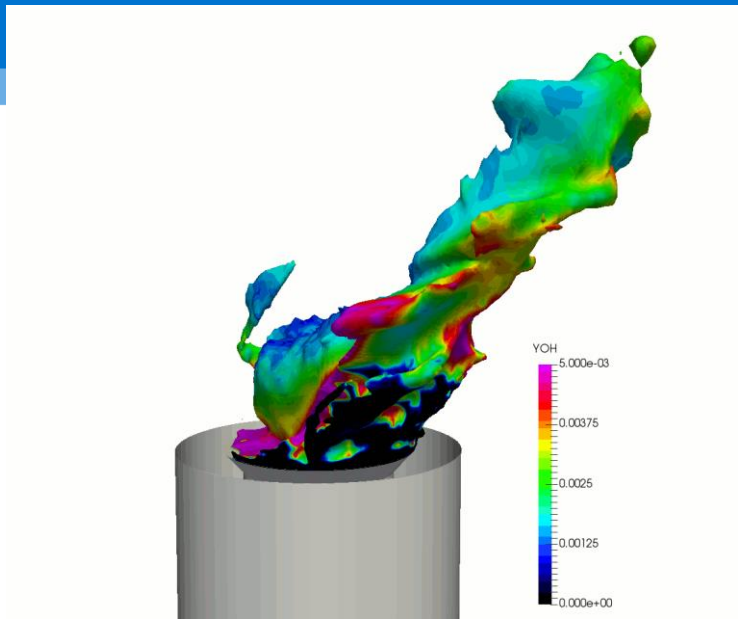
[1] R. Yuan, PhD thesis, University of Cambridge (2015)

Blow-off transient - case E1B

- Transient leading to blow-off



OH-PLIF from the experiment (R. Yuan, 2015)

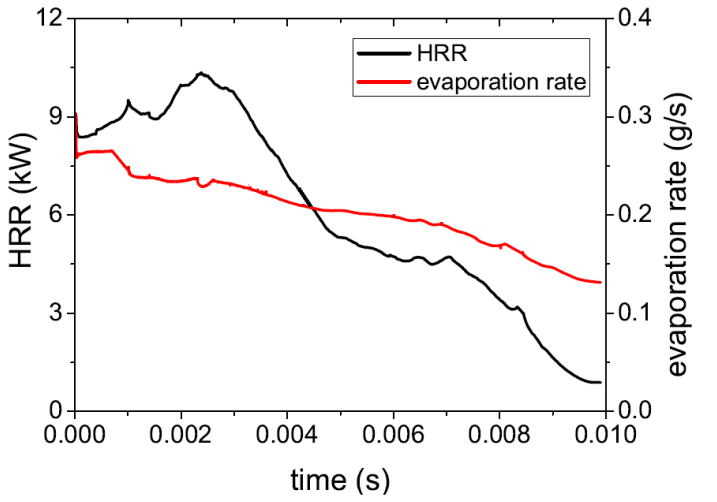


a) **The flame sheet becomes more and more fragmented**

b) **The initial V-shape is completely destroyed**

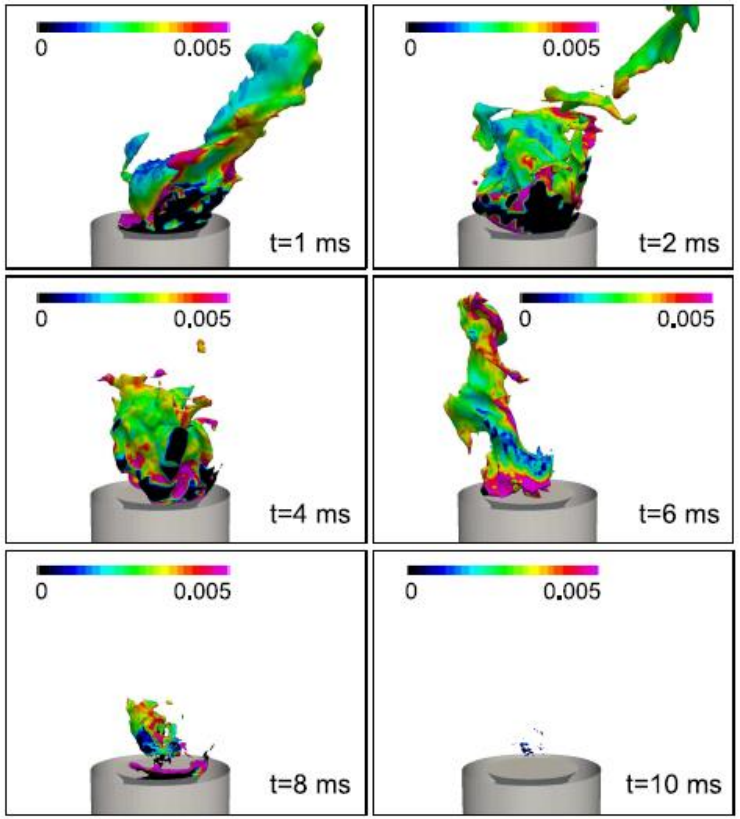
c) **The last surviving flame appears close to the injection location**

Blow-off was achieved by imposing an air mass-flow rate 20% higher than the experimental blow-off velocity



Blow-off transient - case E1B

Stoichiometric mixture fraction iso-surface colored with OH mass fraction



A combination of the following phenomena:

1. Increase of the amount of local extinction in the outer flame region;
2. Lower temperatures in the spray region and the evaporation rate decreases;
3. The stoichiometric iso-surface moves closer and closer to the injection location;
4. Strong fluctuations of the swirling air flow and further fragmentation of the flame;
5. the amount of local extinctions in the inner flame region and further decrease of the evaporation rate;
6. the flame disappear.

Concluding remarks

- The LES/CMC is able to give a quantitative prediction of the degree of local extinction in turbulent spray flames.

- The LES/CMC showed a promising degree of maturity for the prediction of blow-off in turbulent spray flames
  - Strong coupling between finite-rate turbulence chemistry interaction and evaporation

a) The flame sheet becomes more and more fragmented
- The higher air flow rate increases the amount of local extinctions

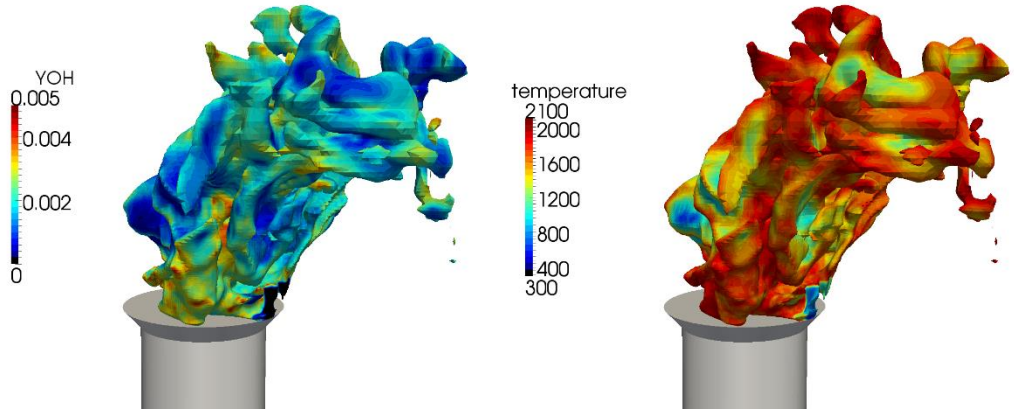
b) The initial V-shape is completely destroyed
- The lower temperature induces a decrease of the total amount of evaporated fuel
- The degree of local extinction in the inner flame brush increases
- High density fluctuations cause high fluctuations in the recirculation zone

c) The last surviving flame appears close to the injection location
- Because of the lower amount of fuel released, the flame get closer and closer to the injection location
- The amount of local extinction in this region increases

Spray flame: Jet-A1 (ongoing)

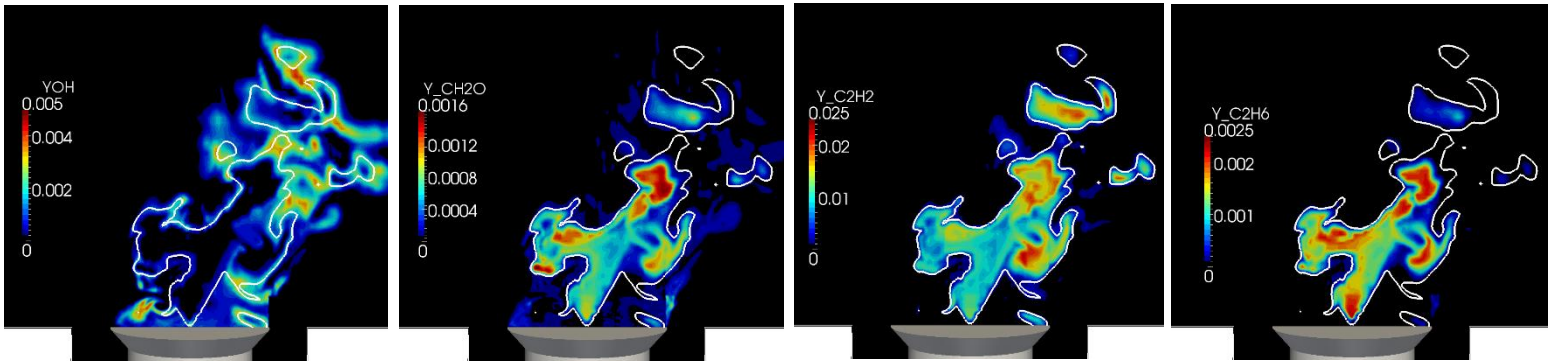
Numerical setup

- U_b = 15.6 m/s, m_{fuel}=0.27 g/s
- SGS stress model: Vreman
- Chemical mechanism: Dagaut & Cathonnet
  - 3-component surrogate fuel
  - 209 species, 1673 reactions
- LES mesh: 5M cells
- CMC mesh: 2.2k cells
- Nodes in mix. frac. Space: 51



Isosurface of the stoichiometric mixture fraction coloured with temperature and OH mass fraction

Instantaneous mass fraction of selected species in the burner cross-section



White line= stoichiometric mixture fraction

OH mass fraction | *CH_2O mass fraction* | *C_2H_2 mass fraction* | *C_2H_6 mass fraction*

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Model combustors

Soot prediction in aero-engine combustors

Department of Engineering

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Method: LES/CMC

Mixture fraction equation

$$\frac{\partial \bar{\rho}\tilde{\xi}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{\xi}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\bar{\rho} D \frac{\partial \tilde{\xi}}{\partial x_i}\right) + \frac{\partial J_{sgs}}{\partial x_i} + \bar{\rho}\widetilde{\Pi}$$

Solved by the LES solver

$$J_{sgs} = \bar{\rho} D_t \frac{\partial \tilde{\xi}}{\partial x_i}$$

Mixture fraction variance

$$\frac{\partial \bar{\rho}\widetilde{\xi''^2}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\widetilde{\xi''^2}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\bar{\rho}(D + D_t)\frac{\partial \widetilde{\xi''^2}}{\partial x_i}\right) - 2\bar{\rho}\widetilde{N}$$

$$+2\bar{\rho}(D+D_t)\frac{\partial \tilde{\xi}}{\partial x_i}\frac{\partial \tilde{\xi}}{\partial x_i} + \underbrace{2\bar{\rho}(\widetilde{\xi\Pi} - \tilde{\xi}\widetilde{\Pi})}_{\bar{\rho}W^+} - \underbrace{\bar{\rho}(\widetilde{\xi^2\Pi} - \tilde{\xi}^2\widetilde{\Pi})}_{\bar{\rho}W^-}$$

Scalar dissipation rate

$$\widetilde{N} = \underbrace{D\left(\frac{\partial \tilde{\xi}}{\partial x_i}\right)^2}_{\text{resolved}} + \underbrace{\frac{1}{2}C_N\frac{\nu_t}{\Delta^2}\widetilde{\xi''^2}}_{\text{subgrid}}$$

$$\widetilde{N|\eta} = N_0 G(\eta),$$

$$G(\eta) = \exp\left(-2\left[\text{erf}^{-1}(2\eta - 1)\right]^2\right)$$

$$N_0 = \frac{\widetilde{N}}{\int_0^1 G(\eta)\widetilde{\mathcal{P}}(\eta)d\eta}$$

C_N=42.0

CMC equations

Conditionally filtered mass fraction

$$\frac{\partial Q_\alpha}{\partial t} + \widetilde{u_j|\eta}\frac{\partial Q_\alpha}{\partial x_j} = e_\alpha + \widetilde{N|\eta}\frac{\partial^2 Q_\alpha}{\partial \eta^2} + \widetilde{\omega_\alpha|\eta} + \underbrace{\delta_{\alpha,f}\widetilde{\Pi|\eta} - \left(Q_\alpha + (1-\eta)\frac{\partial Q_\alpha}{\partial \eta}\right)\widetilde{\Pi|\eta}}_{\text{contribution from the liquid phase}}$$

A similar equation is solved for the conditional enthalpy

First order closure for chemical source terms.

Method: soot model

2-Eq. soot model

Solution in the CMC framework of:

- Soot mass fraction: $Q_\alpha = \widetilde{Y_S|\eta}$
- Soot number density: $Q_\alpha = \widetilde{N_S|\eta}$

Chemical source terms

$$\widetilde{\omega_{Y_S}|\eta} = \underbrace{w_{Y_S,inc}}_{\text{nucleation}} + \underbrace{w_{Y_S,gro}}_{\text{surf. growth}} + \underbrace{w_{Y_S,ox}}_{\text{oxidation}}$$

$$\widetilde{\omega_{N_S}|\eta} = \underbrace{w_{N_S,inc}}_{\text{nucleation}} + \underbrace{w_{N_S,coa}}_{\text{coagulation}}$$

Soot chemistry (Lindstedt and co-workers)

(I) $C_2H_2 \xrightarrow{R_{inc}} 2C_{(S)} + H_2$ $\quad R_{inc} = k_{inc}[C_2H_2]$

(II) $C_2H_2 + nC_{(S)} \xrightarrow{R_{gro}} (n+2)C_{(S)} + H_2$ $\quad R_{gro} = k_{gro}[C_2H_2]$

Acetylene as soot precursor

(III) $C_{(S)} + 0.5O_2 \xrightarrow{R_{ox,O_2}} CO$ $\quad R_{ox,O_2} = k_{ox,O_2}[O_2]$

(IV) $C_{(S)} + OH \xrightarrow{R_{ox,OH}} CO + H$ $\quad R_{ox,OH} = k_{ox,OH}[OH]$

Oxidation by both O2 and OH

(V) Soot coagulation from Ma et al., CST, (2005)

Soot chemistry coupled with gas-phase chemistry

$$k_j = AT^b \exp(-T_a/T)\, S_S^c$$

Surface growth and oxidation dependent on the soot surface area

Overview

Configuration:

- BOSS rig, pilot only configuration
- Fuel: kerosene, airblast atomizer
- Experimental investigation: DLR
- Combustion model: 3D-CMC
- Detailed chemistry: 38 species
- Soot model: 2Eqs-model (Leung et al., 1991)

Operating condition

- Mid-power condition
- FS: 100% pilot
- Global AFR = 120

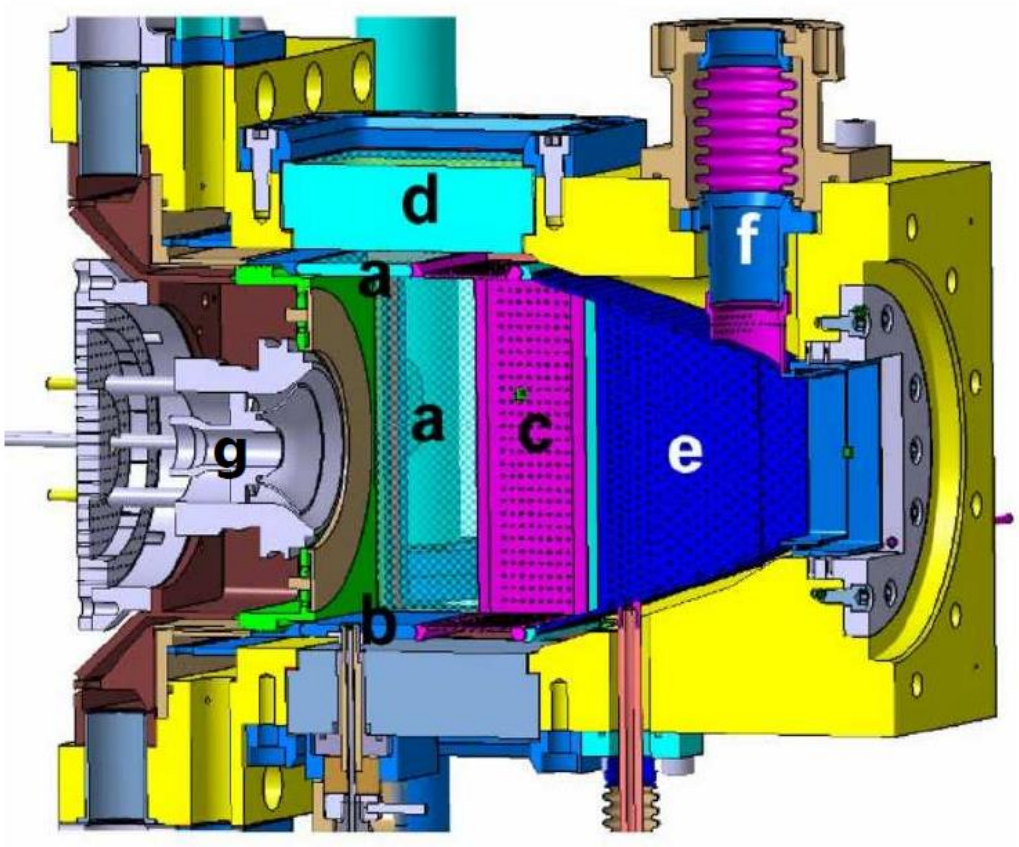
Objective:

- Analyse the combustor behavior at the pilot only condition.
- Analysing the soot formation in an aero-engine combustor using the 3DCMC model

Investigated configuration

BOSS rig (DLR Cologne):

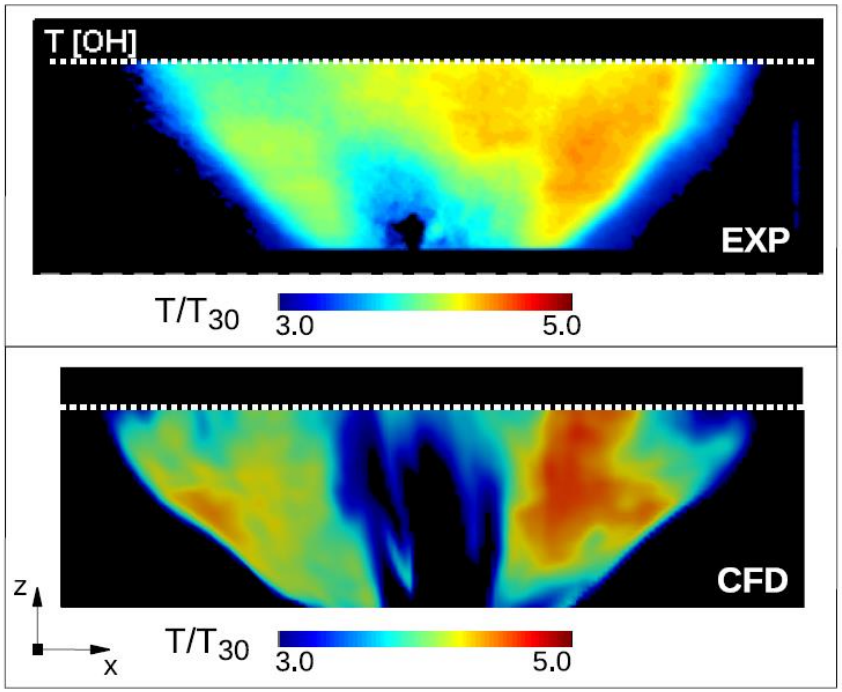
- High pressure
- High temperature
- Real scale airblast atomizers
- Wide range of measurements available: OH-PLIF, PDA, MIE scattering…

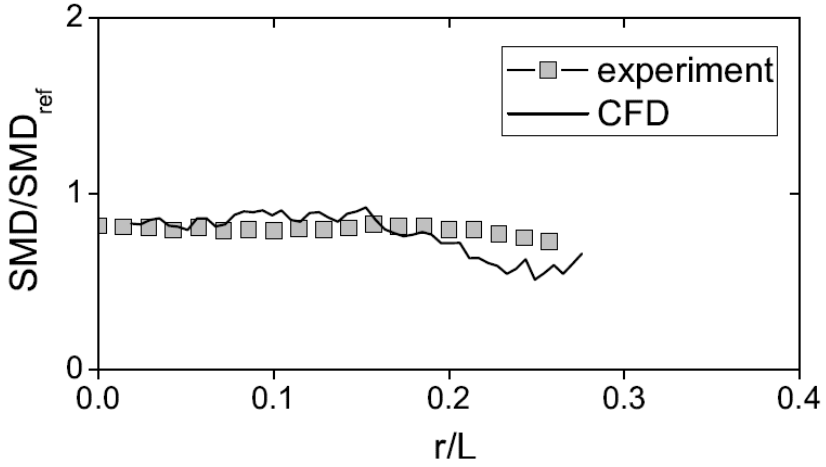


BOSS = Big Optical Single Sector

Comparison with experiments

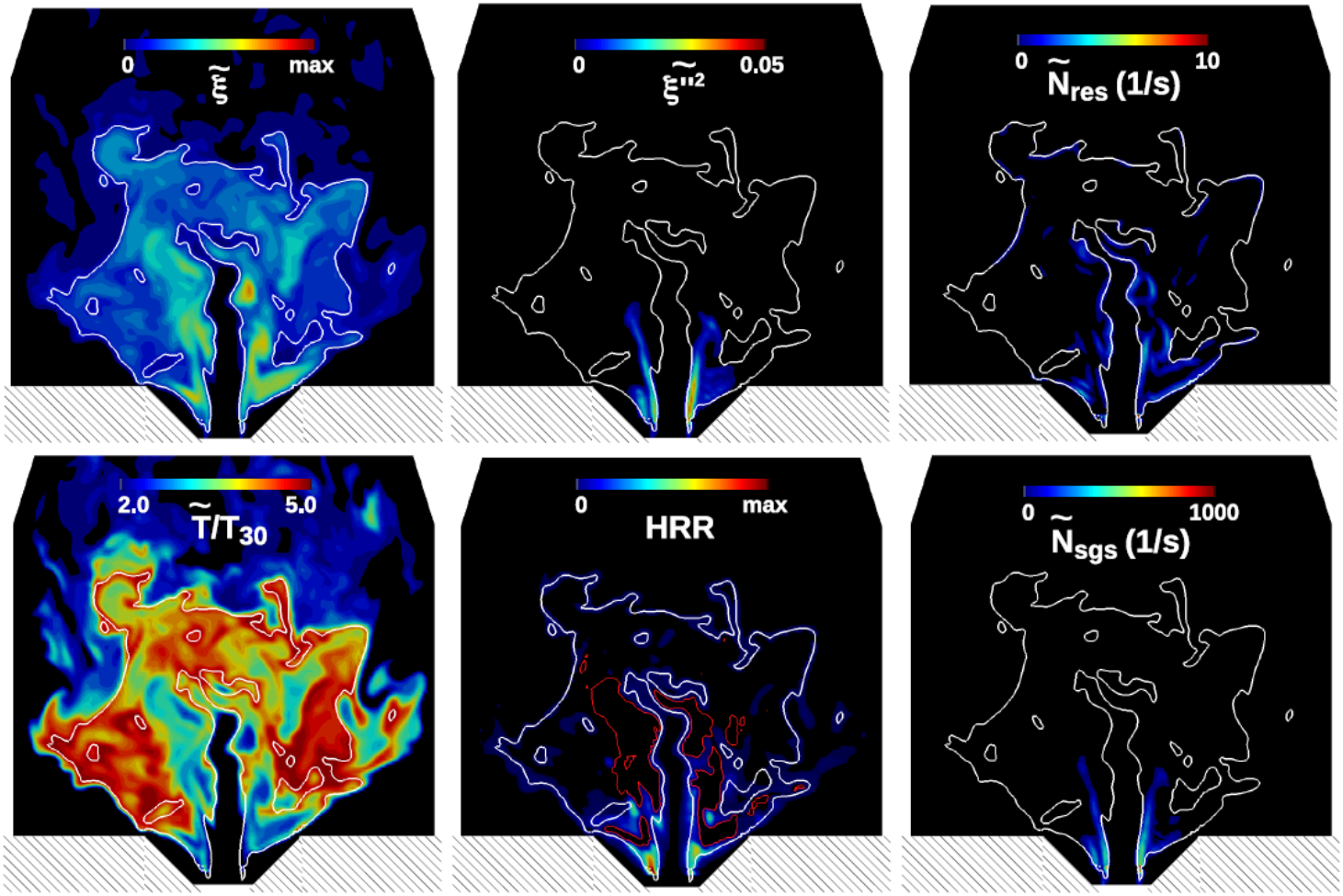
Mean temperature



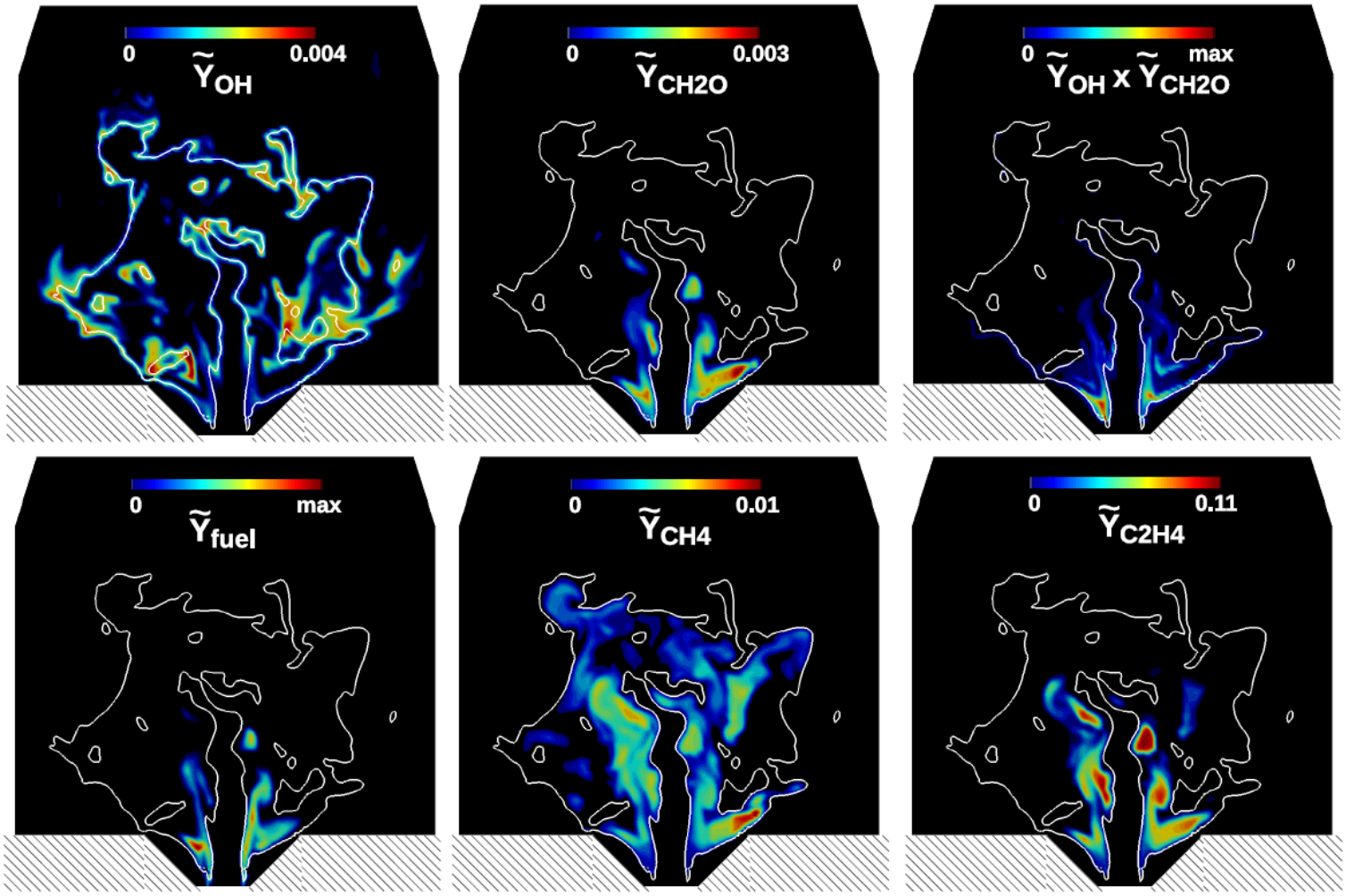


Underprediction of the flame temperature in the pilot flow region. Experiments over-predict the temperature there since super-equilibrium behavior is expected

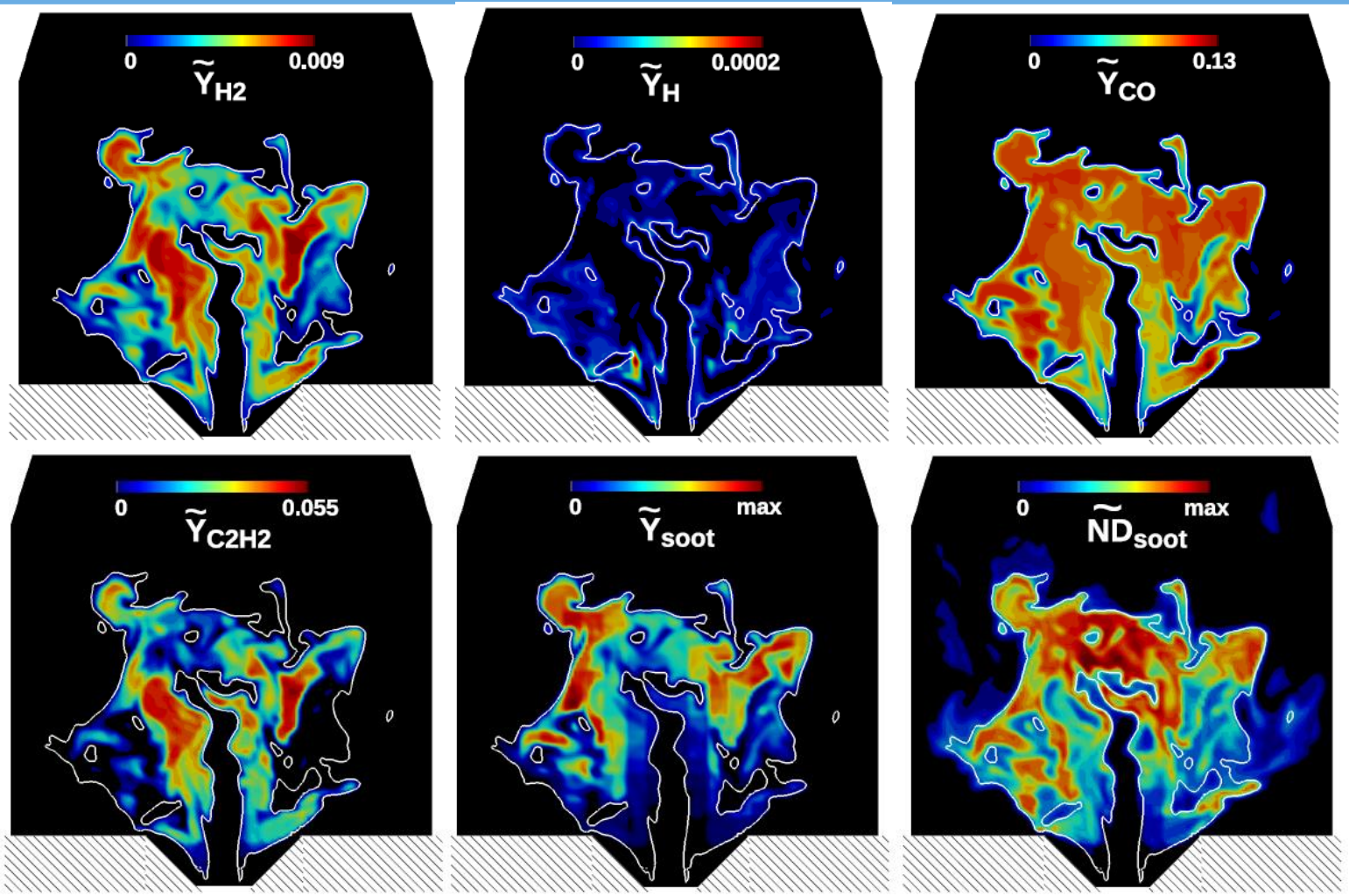
Instantaneous flow field quantities



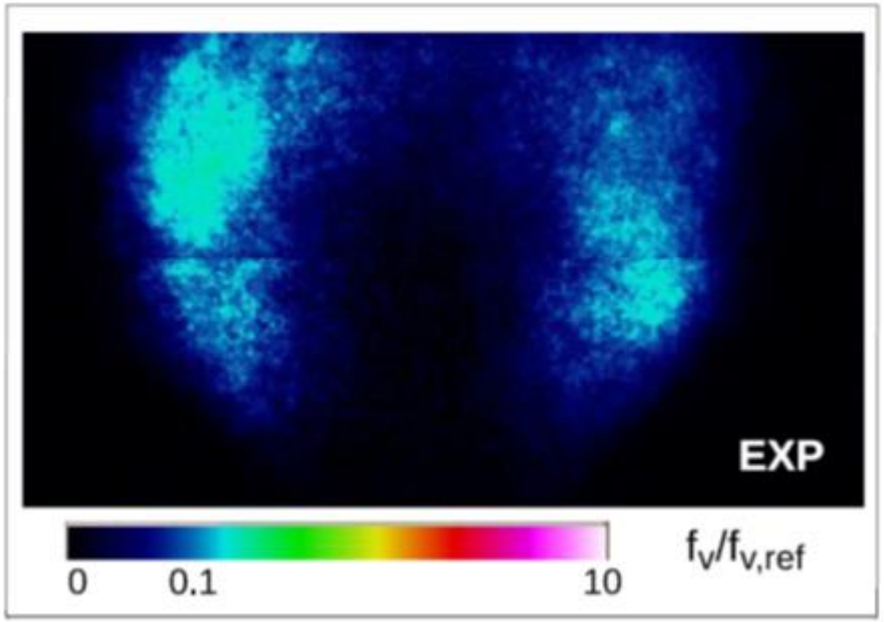
Pyrolysis and reacting region

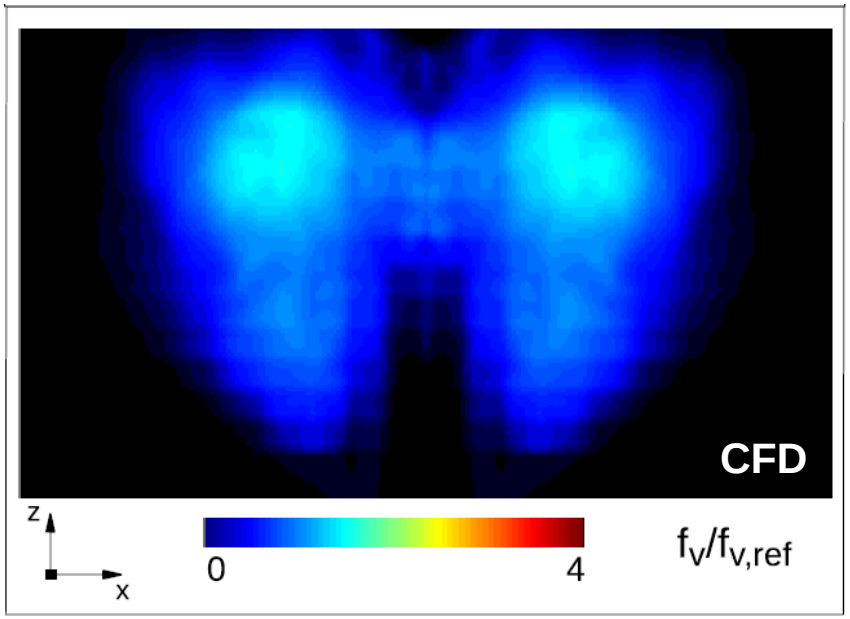


Pyrolisis and reacting region



CMC results: soot formation and location





LES/CMC shows a promising capability of capturing the soot location

Concluding remarks

- A LES/CMC simulation of a model combustor has been performed including:
  - Interaction between the flame structure and evaporation
  - Detailed chemical mechanism
  - Soot model

- The LES/CMC showed a promising capability in capturing the soot location

Ongoing work:

- Further development of CMC+soot models
- Application of the LES/CMC to the simulation of RQL combustors

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