Detailed Chemistry LES-CMC Simulations of Kerosene Swirling Spray Flames

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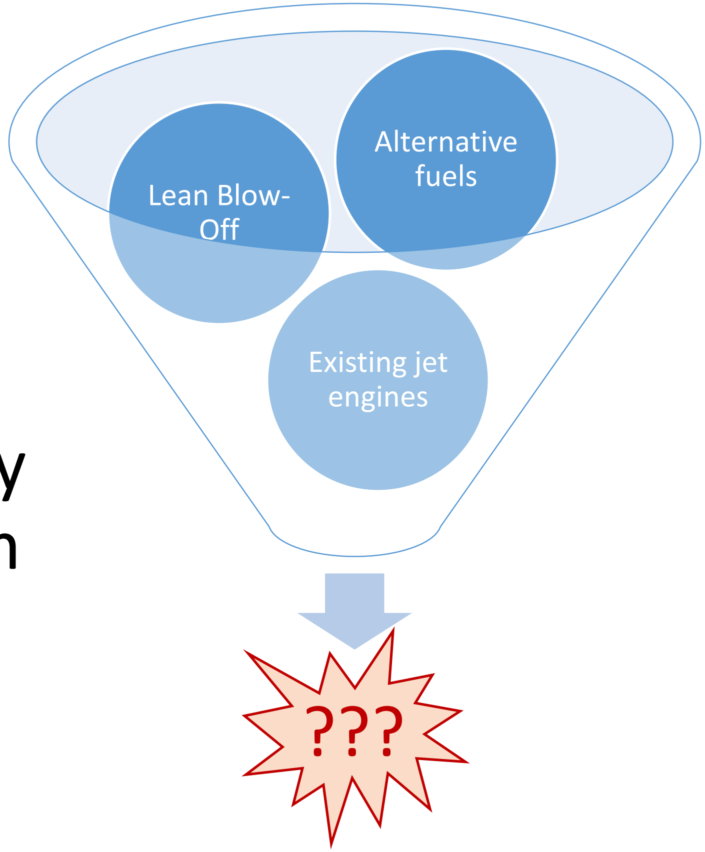
Context

- Alternative and petroleum-derived kerosenes under study in the National Jet Fuels Combustion Program (NJFCP)[1]

- Effect of fuel composition/chemistry on lean blow-off (LBO) of petroleum kerosene spray flames is still not well-understood



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[1] M. Colket et al. AIAA Journal 55.4 (2017)

Burner Setup

- University of Cambridge bluff body non-premixed swirl-stabilized burner at near blow-off condition
- Hollow cone kerosene spray was injected from centre of bluff body at 60° with SMD of 60 µm based on experiments [1]

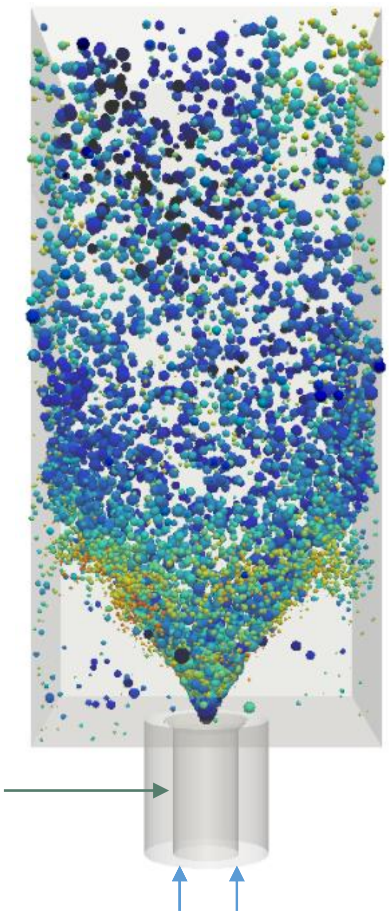
Kerosene Fuels:
- A2: conventional Jet A, $C_{11}H_{22}$
- C1: alcohol-to-jet-fuel, $C_{13}H_{28}$

Flow conditions

$\Phi_{overall}$	U_b Air [m/s]	$\dot{m}_{fuel}$ [g/s]
0.29	20.15	0.27

Burner dimensions
- Enclosure height: 150 mm
- Enclosure side length: 97 mm

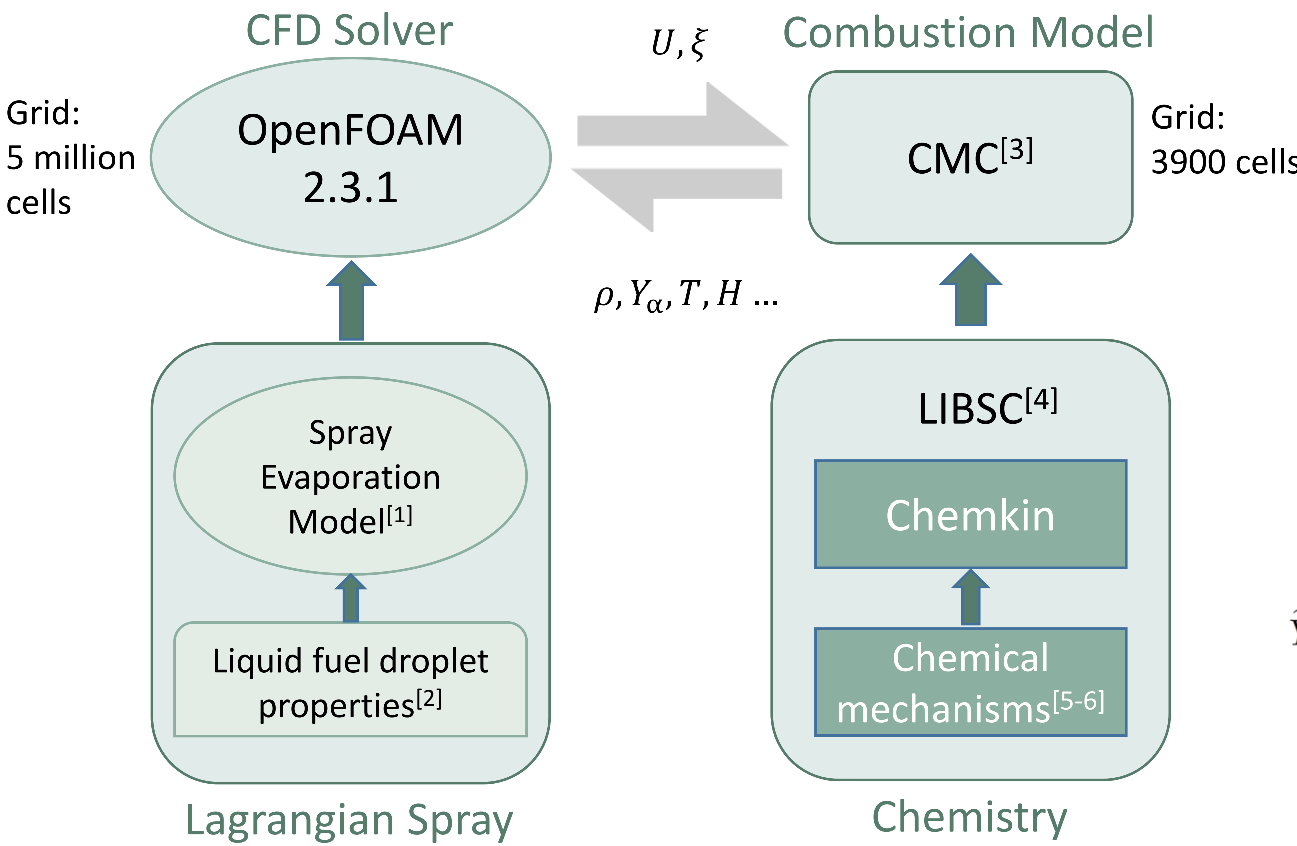
Domain



[1] Sidey, J.A.M. et al., 2017, 55th AIAA Aerospace Sciences Meeting.

Numerical Methods

Large Eddy Simulation (LES) - Conditional Moment Closure (CMC)



$$\frac{\partial Q_\alpha}{\partial t} + \frac{\partial}{\partial x_i}(Q_\alpha \widetilde{\mathbf{u}_i|\eta}) - Q_\alpha \frac{\partial}{\partial x_i}(\widetilde{\mathbf{u}_i|\eta}) = \widetilde{N|\eta}\frac{\partial^2 Q_\alpha}{\partial \eta^2} + \widetilde{\omega_\alpha|\eta} + e_\alpha + S_\alpha(\widetilde{\Pi|\eta})$$

LES

- Mixture fraction $\tilde{\xi}$ and sub-grid scale $\widetilde{\xi''^2}$ transport equations

CMC

- In-house unstructured CMC code with spray terms [3]
- Amplitude Mapping Closure model for scalar dissipation rate $\widetilde{N|\eta}$
- Presumed β-PDF used with reacting scalar Q_α to obtain unconditional filtered values

$$\widetilde{Y}_\alpha(x,t) = \int_0^1 Q_\alpha(\eta,x,t)\widetilde{P}(\eta,x,t)d\eta$$

Chemical Mechanisms

- Hybrid Chemistry “HyChem”
- 119 species, 843 reactions (each fuel)[5-6]

η = sample space mixture fraction

[1] Abramzon, B., & Sirignano, W. Int. J. Heat Mass Transfer, 32, (1989).
[2] Esclapez, L. et al., Combust. Flame, 181, (2017).
[3] Giusti, A. and Mastorakos, E., Proc. Combust. Inst., 36, (2017).
[4] Perini, F. et al., Energy and Fuels, 26, (2012)
[5] Wang, H. et al. Combust. and Flame, 193 (2018).
[6] Wang, K. et al., Combust. Flame, 198, (2018).

Numerical Methods - Chemistry

- HyChem mechanism [1]: lumped pyrolysis, single-component fuel
    - ➢ Pyrolysis lumped into 7 semi-global reaction steps
    - ➢ Main products of pyrolysis are: ethylene, propene, iso-butene, 1-butene, benzene, toluene, hydrogen and the methyl radical
    - ➢ Oxidized with detailed mechanism USC-Mech II (not pictured)

Fuel cracking step

Fuel A2[1]

```
POSF10325    =>            1.7426762C2H4 + 0.8190578C3H6 + 0.0871338iC4H8 + 0.2614014C4H81 + 0.1700C6H6 + 0.1633333C6H5CH3 + 0.5H + 1.5CH3
POSF10325+H  =>   H2 + 0.45CH4 + 1.5945764C2H4 + 0.7494509C3H6 + 0.0797288iC4H8 + 0.2391865C4H81 + 0.2465C6H6 + 0.2368333C6H5CH3 + 0.3H + 0.7CH3
POSF10325+CH3=>        1.45CH4 + 1.5945764C2H4 + 0.7494509C3H6 + 0.0797288iC4H8 + 0.2391865C4H81 + 0.2465C6H6 + 0.2368333C6H5CH3 + 0.3H + 0.7CH3
POSF10325+OH =>  H2O + 0.45CH4 + 1.5945764C2H4 + 0.7494509C3H6 + 0.0797288iC4H8 + 0.2391865C4H81 + 0.2465C6H6 + 0.2368333C6H5CH3 + 0.3H + 0.7CH3
POSF10325+O2 =>  HO2 + 0.45CH4 + 1.5945764C2H4 + 0.7494509C3H6 + 0.0797288iC4H8 + 0.2391865C4H81 + 0.2465C6H6 + 0.2368333C6H5CH3 + 0.3H + 0.7CH3
POSF10325+HO2=> H2O2 + 0.45CH4 + 1.5945764C2H4 + 0.7494509C3H6 + 0.0797288iC4H8 + 0.2391865C4H81 + 0.2465C6H6 + 0.2368333C6H5CH3 + 0.3H + 0.7CH3
POSF10325+O  =>   OH + 0.45CH4 + 1.5945764C2H4 + 0.7494509C3H6 + 0.0797288iC4H8 + 0.2391865C4H81 + 0.2465C6H6 + 0.2368333C6H5CH3 + 0.3H + 0.7CH3
```

Fuel C1[2]

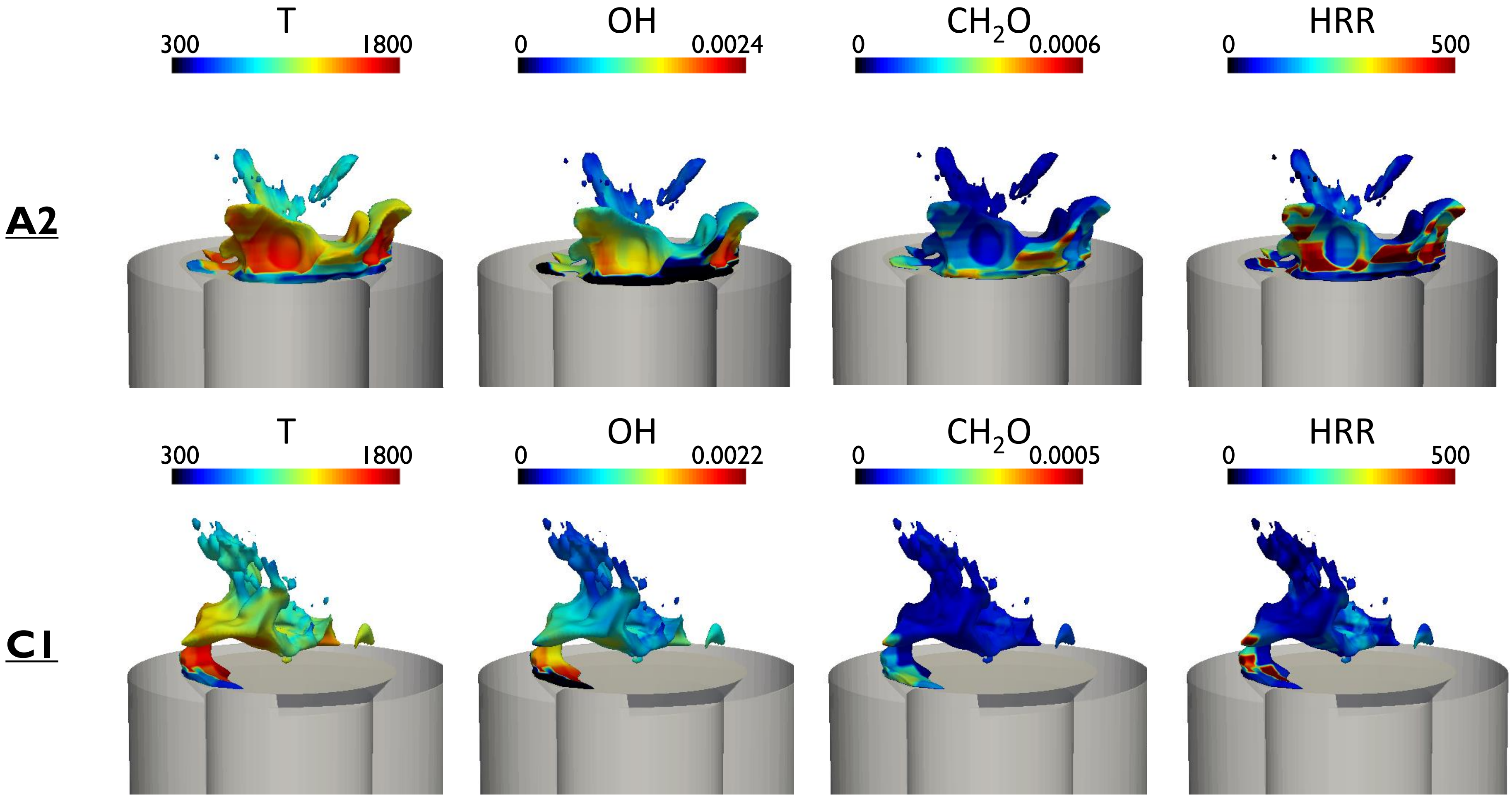
```
POSF11498    =>      2.4625807iC4H8 + 0.5710129C3H6 + 0.2461822C2H4 + 1.055726H + 0.944274CH3
POSF11498+H  => H2  +2.6513789iC4H8 + 0.6147906C3H6 + 0.2650562C2H4 +     0.98H     + 0.02CH3
POSF11498+CH3= >CH4 +2.6513789iC4H8 + 0.6147906C3H6 + 0.2650562C2H4 +     0.98H     + 0.02CH3
POSF11498+OH => H2O +2.6513789iC4H8 + 0.6147906C3H6 + 0.2650562C2H4 +     0.98H     + 0.02CH3
POSF11498+O2 => HO2 +2.6513789iC4H8 + 0.6147906C3H6 + 0.2650562C2H4 +     0.98H     + 0.02CH3
POSF11498+HO2=> H2O2+2.6513789iC4H8 + 0.6147906C3H6 + 0.2650562C2H4 +     0.98H     + 0.02CH3
POSF11498+O  => OH  +2.6513789iC4H8 + 0.6147906C3H6 + 0.2650562C2H4 +     0.98H     + 0.02CH3
```

A2 semi-global steps include CH_4, C_4H_8-1, C_6H_6 and $C_6H_5CH_3$, unlike fuel C1!

[1] H. Wang et al., Combustion and Flame 193, (2018).

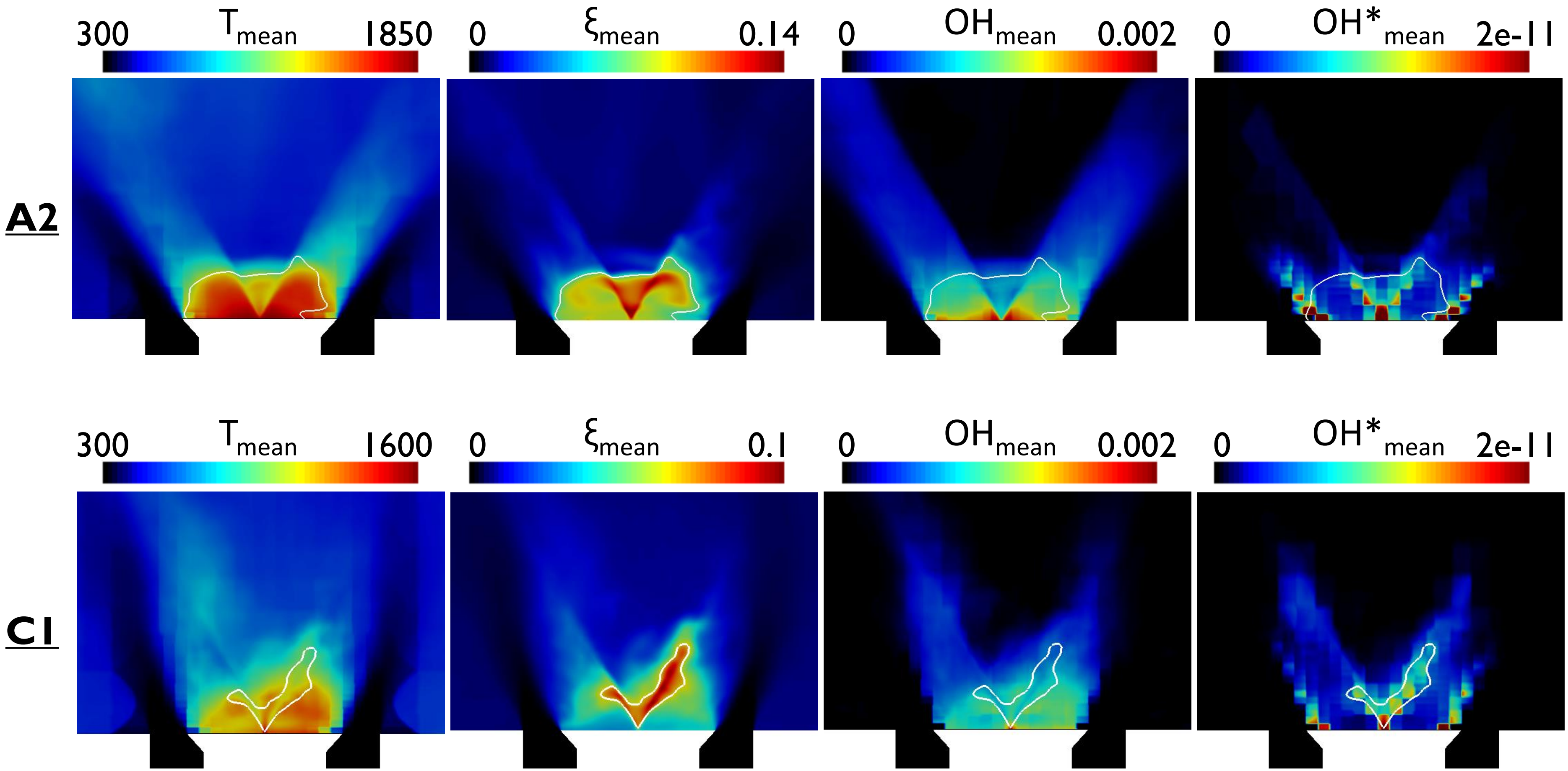
[2] K. Wang et al., Combustion and Flame 198, (2018).

LES-CMC 3D Preliminary Instantaneous Results



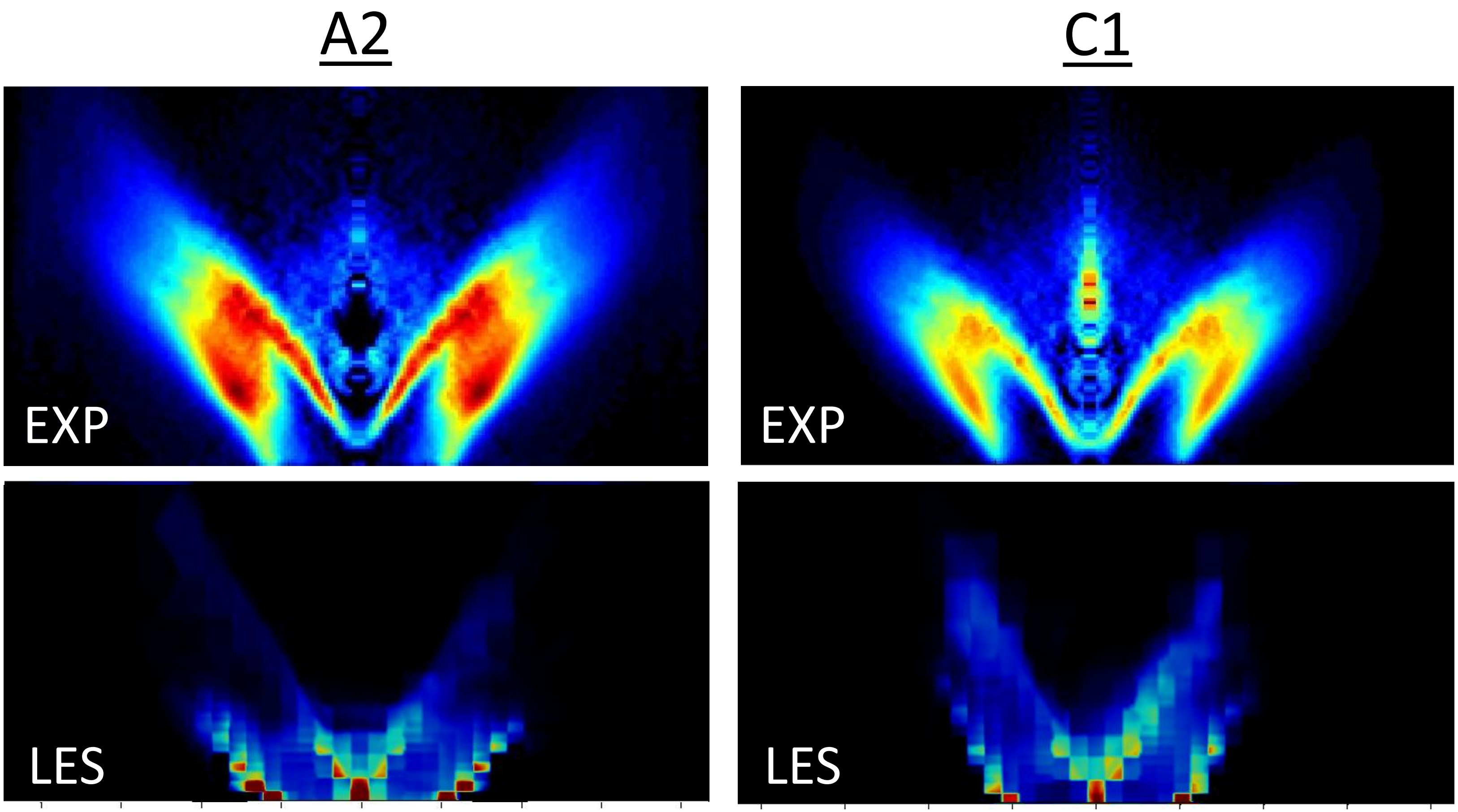
Instantaneous stoichiometric iso-contours (η = 0.0637) for the two kerosenes, coloured with temperature (K), OH mass fraction, CH_2Omass fraction, and heat release rate (MW/m^3)

LES-CMC Preliminary Time-Averaged Results



Temperature (K), mixture fraction, mean OH mass fraction and mean OH* mass fraction, with mean stoichiometric mixture fraction iso-line (ξ = 0.0637) contours shown in white

Preliminary Comparison with Experiments



Mean inverse OH* Abel transformed chemiluminescence images[1] (top) and LES-CMC time-averaged OH* cross-sectional results (bottom)

[1] Sidey, J.A.M. et al., 2017, 55th AIAA Aerospace Sciences Meeting.

Key Findings

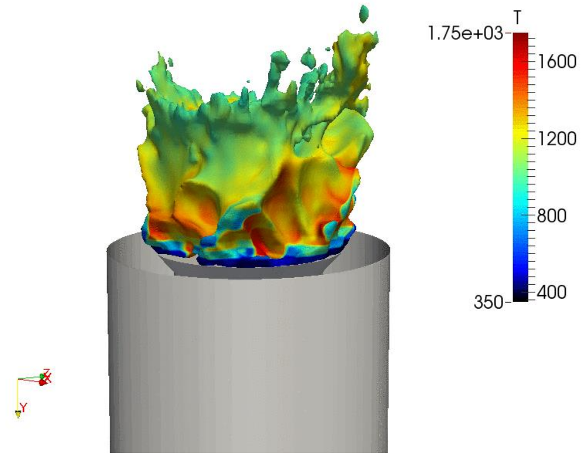
- LES-CMC is capable of capturing LBO phenomena (local extinction and flame lift-off) of real fuels at near blow-off conditions
- Flame shape produced by LES-CMC is similar to shapes seen in experiments

To Do:

- Need to explore why we are not capturing the flame lobes observed experimentally
- Add interpolation between CMC cells

Other Ongoing Work

- Another synthetic kerosene fuel, C5, currently being simulated at near blow-off condition
- Same flames at higher equivalence ratio (lower air flow rate)
- Analysis in mixture fraction space, observing local extinction in cells around the shear layer



C5 flame

Total kAU Consumption: ~10,000 kAUs

How all this work contributes to the field

- Simulations solve for combustion using very recently developed detailed chemical mechanisms (HyChem) modelling real fuels
- Lagrangian parcel spray modelling including evaporation and fuel-specific liquid properties
- Model capability capturing flame lift-off and local extinction phenomena

Comprehensive soot particle size distribution modelling of a turbulent ethylene jet flame

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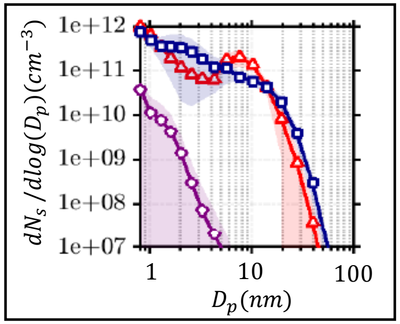
LES-CMC of a sooting ethylene jet flame

Test case – Adelaide jet flame 1 (ISF4)

Fuel: 63.4% C_2H_4 / 4.7% H_2 / 31.9% N_2 % (m/m)

Inner jet diameter (mm)	Flow rate (l/min)	Mean exit velocity (m/s)	Exit strain rate (1/s)	Exit Reynolds number
4.4	51.8	56.8	12,900	15,000

Example of PSDs [*]



Modelling – a comprehensive approach

★ LES-CMC without/with large-scale differential diffusion of soot particles

★ Radiation

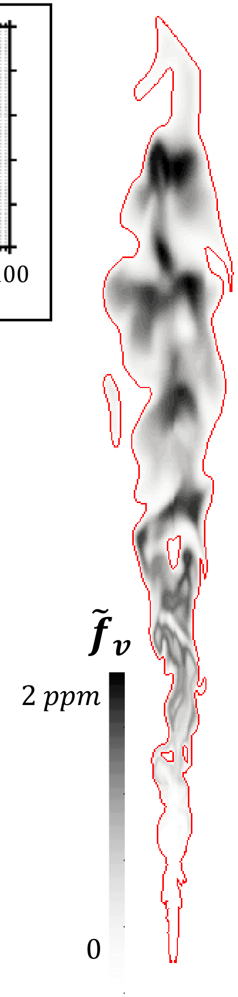
★ Detailed chemistry with PAH up to pyrene (67 species)

★ Sectional soot model by D'Anna and co-workers (22 stable + 22 radical soot bins)
Reaction classes: Nucleation (PAH dimerization), HACA growth, PAH condensation, coalescence/agglomeration, O_2/OH oxidation, O_2-induced fragmentation

Objectives

★ Investigate the hierarchy of reaction pathways during soot evolution in a jet flame

★ Study the effects of soot particles transport to particle size distribution (PSD)



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[*] Gkantonas, S., Sirignano, M., Giusti, A., D'Anna, A., Mastorakos, E., 2019. MCS, Tenerife, Spain.

Acknowledgements

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Thank you for listening!