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

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, \(C_{13}H_{28}\)

<table>
<thead>
<tr>
<th>Flow conditions</th>
<th>(\Phi_{\text{overall}})</th>
<th>(U_b) Air ([\text{m/s}])</th>
<th>(m_{\text{fuel}}) ([\text{g/s}])</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.29</td>
<td>20.15</td>
<td>0.27</td>
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</table>

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

Numerical Methods

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

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

CMC
- In-house unstructured CMC code with spray terms
- Amplitude Mapping Closure model for scalar dissipation rate $\overline{\theta | \eta}$
- Presumed $\beta$-PDF used with reacting scalar $Q_{\alpha}$ to obtain unconditional filtered values

\[ \tilde{Y}_{\alpha}(x, t) = \int_{0}^{1} Q_{\alpha}(|\eta|, x, t) \tilde{P}(|\eta|, x, t) d|\eta| \]

Chemical Mechanisms
- Hybrid Chemistry “HyChem”
- 119 species, 843 reactions (each fuel)

\[ \frac{\partial Q_{\alpha}}{\partial t} + \frac{\partial}{\partial x_i} (Q_{\alpha} \overline{\left[ u_i | \eta \right]} ) - Q_{\alpha} \frac{\partial}{\partial x_i} (\overline{\left[ u_i | \eta \right]} ) = \overline{N | \eta} \frac{\partial^2 Q_{\alpha}}{\partial \eta^2} + \omega_{\alpha} |\eta| + e_{\alpha} + S_{\alpha} (\overline{\Pi | \eta}) \]

$\eta = $ sample space mixture fraction

Numerical Methods - Chemistry

- HyChem mechanism \(^\text{[1]}\): 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)

<table>
<thead>
<tr>
<th>Fuel A2(^\text{[1]})</th>
<th>Fuel C1(^\text{[2]})</th>
</tr>
</thead>
<tbody>
<tr>
<td>POSF10325 =&gt;</td>
<td>POSF11498 =&gt;</td>
</tr>
<tr>
<td>POSF10325+H =&gt;</td>
<td>POSF11498+H =&gt;</td>
</tr>
<tr>
<td>POSF10325+CH3 =&gt;</td>
<td>POSF11498+CH3 =&gt;</td>
</tr>
<tr>
<td>POSF10325+OH =&gt;</td>
<td>POSF11498+OH =&gt;</td>
</tr>
<tr>
<td>POSF10325+H02 =&gt;</td>
<td>POSF11498+H02 =&gt;</td>
</tr>
<tr>
<td>POSF10325+0 =&gt;</td>
<td>POSF11498+0 =&gt;</td>
</tr>
</tbody>
</table>

A2 semi-global steps include \(\text{CH}_4\), \(\text{C}_4\text{H}_8\)-1, \(\text{C}_6\text{H}_6\) and \(\text{C}_6\text{H}_5\text{CH}_3\), unlike fuel C1!

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

Instantaneous stoichiometric iso-contours ($\eta = 0.0637$) for the two kerosenes, coloured with temperature (K), OH mass fraction, CH$_2$O mass 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 ($\xi = 0.0637$) contours shown in white
Preliminary Comparison with Experiments

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

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

Total kAU Consumption: ~10,000 kAU

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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Wed. 11/09/2019
LES-CMC of a sooting ethylene jet flame

Test case – Adelaide jet flame 1 (ISF4)

Fuel: 63.4% C₂H₄ / 4.7% H₂ / 31.9% N₂ % (m/m)

<table>
<thead>
<tr>
<th>Inner jet diameter (mm)</th>
<th>Flow rate (l/min)</th>
<th>Mean exit velocity (m/s)</th>
<th>Exit strain rate (1/s)</th>
<th>Exit Reynolds number</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.4</td>
<td>51.8</td>
<td>56.8</td>
<td>12,900</td>
<td>15,000</td>
</tr>
</tbody>
</table>

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, O₂/OH oxidation, O₂-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)

Acknowledgements

We would like to thank the following for their support with this work:

Thank you for listening!