Influences of droplet diameter and overall equivalence ratio on the flame structure for spherically expanding flames propagating in fuel droplet-mist: A Direct Numerical Simulation Analysis

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Joint SIG Meeting Spray-Combustion
8th-9th April, 2019
Imperial College London
Introduction: Motivation

Significant practical relevance of:

- Internal Combustion (IC) engines
- Gas turbines
- Industrial furnaces

Includes the critical processes:

- evaporation of liquid droplets
- mixing of fuel vapour with the surrounding air
- interaction of droplets with the flame and flow field

https://www.youtube.com/watch?v=BzgaTDb7E88
Introduction: Objectives

- to demonstrate and explain the influences of droplet size and the overall equivalence ratio on:
  - the flame structure and wrinkling
  - the evolution of flame surface area and
  - the evolution of burned gas volume
  - displacement and consumption speeds in spherically expanding laminar and turbulent n-heptane spray flames.

- to compare the results obtained from spray flames with the corresponding gaseous premixed flames.
Liquid Phase:

**Lagrangian Approach** is used for droplets following the approach proposed by Reveillon & Vervisch.

- Position: \( \frac{d\hat{x}_d}{dt} = \hat{u}_d \)
- Velocity: \( \frac{d\hat{u}_d}{dt} = \frac{\hat{u}(\hat{x}_d,t) - \hat{u}_d}{\tau_d^u} \)
- Diameter: \( \frac{d\hat{a}_d}{dt} = \frac{\hat{a}_d}{\tau_d^p} \)
- Temperature: \( \frac{dT_d}{dt} = \frac{T(\hat{x}_d,t) - T_d - B_d L_v / C_p^g}{\tau_d^T} \)

- \( L_v \) is the latent heat of vaporization
- \( B_d \) is the Spalding mass transfer number
- \( C_p^g \) is the gaseous specific heats at constant pressure

Relaxation time scales associated with droplet:
- Velocity, \( \tau_d^u \)
- Diameter, \( \tau_d^p \)
- Temperature, \( \tau_d^T \)
Mathematical Background

**Gaseous Phase:**

*Eulerian Approach* is used to solve for gas phase combustion.

Coupling between two phases:

\[
\frac{\partial \rho \psi}{\partial t} + \frac{\partial \rho u_j \psi}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \Gamma_\psi \frac{\partial \psi_1}{\partial x_j} \right) + \dot{w}_\psi + \dot{S}_g + \dot{S}_\psi
\]

\(\psi_1 = \{1, u_j, \hat{T}, Y_F, Y_O\}\) for \(\psi = \{1, u_j, e, Y_F, Y_O\}\)

\(\Gamma_\psi = \rho \nu / \sigma_\psi\) for \(\psi = \{1, u_j, Y_F, Y_O\}\) and \(\Gamma_\psi = \lambda\) for \(\psi = e\)

\(\dot{w}_\psi\) is chemical reaction rate,

\(\dot{S}_g\) is an appropriate source/sink term and

\(\dot{S}_\psi\) is *source term due to droplet evaporation*, which is tri-linearly interpolated from the droplet’s sub-grid position, \(\vec{x}_d\), to the eight surrounding nodes.
Mathematical Background

**Code:**

3D, compressible DNS code, SENG A +
- 10th order central difference scheme
- Time advancement: Explicit low-storage 3rd order Runge-Kutta scheme.
- A modified single-step Arrhenius-type irreversible chemical reaction:
- Droplets are treated as sub-grid point sources.

![Graph 1](image1)
![Graph 2](image2)

Variation of the (a) normalised laminar burning velocity $S_b(\phi_g)/\{S_b(\phi_g)\}_{\text{max}}$ and (b) normalised adiabatic flame temperature $T_{b(\phi_g)} = (T_{ad(\phi_g)} - T_0)/(T_{ad(\phi_g=1)} - T_0)$ with equivalence ratio $\phi_g$ for n-heptane obtained from modified single step chemistry (Tarrazo et al., 2006), detailed chemical mechanism (Chaos et al., 2007) and experimental (Kumar et al., 2007) data.

Reacting flow field initialisation:

1D steady-state laminar spray flame, COSILAB

- Generated according to the droplet diameter and overall equivalence ratio
- 1D profiles are then specified in the radial direction from the centre of the domain.
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Mathematical Background

Reacting flow field initialisation:

1D steady-state laminar spray flame, COSILAB

- Generated according to the droplet diameter and overall equivalence ratio
- 1D profiles are then specified in the radial direction from the centre of the domain.

Turbulent flow field initialisation:

- Incompressible homogeneous isotropic velocity field is superimposed on the laminar spherical flames with \( r_0 / \delta_{st} = 2.0 \)
Simulation parameters

- Domain: $(84.49\delta_z)^3$ (where $\delta_z = \alpha_{T_0}/S_{b(\phi_g=1)}$ is the Zel’dovich flame thickness)
- Grid number: $(512)^3$
- Initial kernel radius: $r_0/\delta_{st} = 2.0$
- Equivalence ratio: $\phi_{ov} = 0.8, 1.0$ and $1.2$

$$\phi_{ov} = \phi_{gas} + \phi_{liq}$$

Equivalence ratio:
$$\phi = \frac{FAR}{FAR_{st}}$$

Stability criterion:
$$\delta_{st} = \frac{(T_{ad(\phi_g=1)} - T_0)}{\max |\nabla T|_L}$$
Simulation parameters:

- Initial rms: \( u' / S_b(\phi_g=1) = 0.0 \) and 4.0
- Longitudinal integral length-scale: \( L_{11} / \delta_{st} = 2.5 \)
- Droplet diameter: \( a_d / \delta_{st} = 0.04, 0.05 \) and 0.06
- Number density: \( 1.28 \leq (\rho_N)^{1/3} \delta_{st} \leq 2.18 \)
- Heat release parameter:
  \[ \tau = \frac{(T_{ad}(\phi_g=1)-T_0)}{T_0} = 6.54 \]

Reaction progress variable, \( c \):
\[
c = \frac{(1 - \xi)Y_{\infty} - Y_0}{(1 - \xi)Y_{\infty} - \max(0, [\xi_{st} - \xi]/\xi_{st})Y_{\infty}}
\]

\[
\xi = \frac{(Y_F - Y_0/s + Y_{\infty}/s)}{(Y_{F\infty} - Y_{\infty}/s)}
\]
Results: Flame-droplet-turbulence interaction

\[ \phi_{ov} = 0.8, 1.0 \text{ and } 1.12 \quad a_d/\delta_{st} = 0.04, 0.05 \text{ and } 0.06 \]

Distribution of $Y_F/Y_{st}$ (magenta lines show $c = 0.1, 0.5, 0.9$ contours from outer to inner periphery) on the central $x$-$y$ mid-plane for laminar flames with $\phi_{ov} = 0.8, 1.0$ and $1.2$. All figures correspond to $t = 2.52\alpha_{T0}/S_b^2(\phi_g=1)$. 
Results: Flame-droplet-turbulence interaction

\[ \phi_{ov} = 0.8, 1.0 \text{ and } 1.2 \quad a_d / \delta_{st} = 0.04, 0.05 \text{ and } 0.06 \]

Distribution of \( Y_F / Y_{st} \) (magenta lines show \( c = 0.1, 0.5, 0.9 \) contours from outer to inner periphery) on the central \( x-y \) mid-plane for turbulent flames with \( \phi_{ov} = 0.8, 1.0 \) and 1.2. All figures correspond to \( t = 2.52 \alpha T_0 / S_b(\phi_g=1) \).
Results: Droplet induced wrinkling

\[ \phi_{ov} = 0.8, 1.0, 1.2 \text{ and } a_d/\delta_{st} = 0.04, 0.05, 0.06 \]

Flame normal vector:
\[ \vec{N} = -\nabla c / |\nabla c| \]

Local curvature:
\[ \kappa_m = \nabla \cdot \vec{N} / 2 \]

A positive curvature → convex to the reactants
A negative curvature → concave to the reactants

- The droplet case with initial \( a_d/\delta_{st} = 0.04 \) for \( \phi_{ov} = 0.8 \) does not show dimples but laminar flame also does not remain spherical.
- Evaporation of clustered droplets creates large distributed dimples for the \( \phi_{ov} = 1.2 \) cases in contrast to small densely packed dimples in the \( \phi_{ov} = 1.0 \) cases.

Instantaneous view of \( c = 0.5 \) isosurface coloured with local values of \( \kappa_m \times \delta_{st} \) for the cases with \( \phi_{ov} = 0.8, \phi_{ov} = 1.0 \) and \( \phi_{ov} = 1.2 \) at \( t = 2.52 \alpha_{T0} / S_d^2(\phi_b=1) \).
Results: PDF of gaseous equivalence ratio

<table>
<thead>
<tr>
<th>Premixed Gas</th>
<th>Droplet Cases</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \phi_{ov} = 0.8 )</td>
<td>( \phi_{ov} = 0.8 )</td>
</tr>
<tr>
<td>( \phi_{ov} = 1.0 )</td>
<td>( \phi_{ov} = 1.0 )</td>
</tr>
<tr>
<td>( \phi_{ov} = 1.2 )</td>
<td>( \phi_{ov} = 1.2 )</td>
</tr>
</tbody>
</table>

- A peak of the \( \phi_g \)-PDF at \( \phi_g \approx \phi_{ov} \)
- The probability of finding \( \phi_g < \phi_{ov} \) supersedes the availability of \( \phi_g > \phi_{ov} \)
- Localised fuel-rich pockets are more frequent for large droplets and \( \phi_{ov} = 1.2 \)
Results: The evolution of flame surface area

A, flame surface area: \[ A = \int |\nabla c|dV \]

\[ S_A \] is a flame speed which can be defined based on the flame surface area.

\[ r_A = \sqrt{A/4\pi} \]

\[ S_A = d r_A/dt \]

<table>
<thead>
<tr>
<th>( \phi_{ov} )</th>
<th>( \phi_{ov} = 0.8 )</th>
<th>( \phi_{ov} = 1.0 )</th>
<th>( \phi_{ov} = 1.2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a_d/\delta_{st} )</td>
<td>( \text{Laminar} )</td>
<td>( u'/S_b(\phi_{g}=1) = 4 )</td>
<td>( \text{Laminar} )</td>
</tr>
<tr>
<td>0.04</td>
<td>3.30</td>
<td>3.48</td>
<td>5.46</td>
</tr>
<tr>
<td>0.05</td>
<td>3.90</td>
<td>5.30</td>
<td>4.87</td>
</tr>
<tr>
<td>0.06</td>
<td>4.57</td>
<td>5.97</td>
<td>4.69</td>
</tr>
<tr>
<td>( \text{Premixed} )</td>
<td>3.18</td>
<td>4.10</td>
<td>5.42</td>
</tr>
</tbody>
</table>

Normalised flame speed \( S_A/S_b(\phi_{ov}) \), which quantifies the growth rate of flame surface area \( A \).

- The presence of droplets enhances \( S_A/S_b(\phi_{ov}) \) for \( \phi_{ov} = 0.8 \) except for the initial \( a_d/\delta_{st} = 0.04 \).
- For \( \phi_{ov} = 1.0 \) and 1.2, only the small droplets with initial \( a_d/\delta_{st} = 0.04 \) under laminar conditions demonstrate higher \( S_A/S_b(\phi_{ov}) \) than the corresponding laminar premixed flame.
- \( S_A/S_b(\phi_{ov}) \) increases with increasing droplet diameter for \( \phi_{ov} = 0.8 \), whereas it shows just the opposite behaviour for \( \phi_{ov} = 1.0 \) and 1.2.
Results: The evolution of burned gas volume

<table>
<thead>
<tr>
<th>$a_d/\delta_{st}$</th>
<th>$\phi_{ov} = 0.8$</th>
<th>$\phi_{ov} = 1.0$</th>
<th>$\phi_{ov} = 1.2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laminar</td>
<td>$u'/S_{b(\phi_g=1)} = 4$</td>
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</tr>
<tr>
<td>0.04</td>
<td>3.03</td>
<td>5.34</td>
<td>6.43</td>
</tr>
<tr>
<td>0.05</td>
<td>2.97</td>
<td>4.90</td>
<td>5.21</td>
</tr>
<tr>
<td>0.06</td>
<td>4.07</td>
<td>4.91</td>
<td>5.12</td>
</tr>
<tr>
<td>Premixed</td>
<td>3.55</td>
<td>5.5</td>
<td>5.25</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Normalised flame speed $S_V/S_{b(\phi_{ov})}$, which quantifies the growth rate of burned gas volume $V_b$.

$S_V$ is a flame speed which is defined based on the burned gas volume.

\[
S_V = \frac{d r_V}{d \ t}
\]

\[
r_V = \left(\frac{3V_b}{4\pi}\right)^{1/3}
\]

- The presence of droplets enhances $S_V/S_{b(\phi_{ov})}$ for $\phi_{ov} = 0.8$ with the initial $a_d/\delta_{st} = 0.06$ under laminar conditions.
- Turbulence significantly affects $S_V/S_{b(\phi_g)}$ and increases the growth rate of burned gas volume for large droplets with $\phi_{ov} = 0.8$ and for small droplets with $\phi_{ov} = 1.0$ and 1.2.
Results: The evolution of burned gas volume

\[ S_n = \frac{dr}{dt} \]

### Laminar

#### Experiment

- Gaseous
- \( a_d = 12 \mu m \)
- \( a_d = 23 \mu m \)
- \( a_d = 31 \mu m \)

#### DNS

\[ r_V = (3V_b/4\pi)^{1/3} \]

Normalised flame speed \( S_V/S_b(\phi_{ov}) \), which quantifies the growth rate of burned gas volume \( V_b \).

\[ S_V = \frac{dr_V}{dt} \]

### Comparison

Comparison \( S_n \) of for gaseous and aerosol ethanol-air at various \( \phi_{ov} \).

\[ S_{n}(m/s) \]

\[ \phi_{ov} \]

Results: Mean flame speed statistics

\[ S_A^* / S_b(\phi_g=1) \]

Mean values of \( S_c / S_b(\phi_g=1) \) and \( S_d^* / S_b(\phi_g=1) \) on \( c = 0.8 \) isosurface along with alternative flame speeds \( S_A^* / S_b(\phi_g=1) \) and \( S_V^* / S_b(\phi_g=1) \). The value of \( S_b(\phi_g=\phi_{ov}) / S_b(\phi_g=1) \) is shown by the horizontal black dashed line.

\[ S_d = \frac{\nabla \cdot (\rho D \nabla c) + \dot{\omega}_c + S_c + \dot{A}_c}{\rho |\nabla c|} \]

density-weighted displacement speed:

\[ S_A^* = \frac{S_d}{\rho_0} \]

consumption speed:

\[ S_c = \rho_0^{-1} \int \dot{\omega} dn \]

\[ S_V^* = \frac{S_V}{\rho_0} \]

\[ S_A^* = \frac{S_A}{\rho_0} \]
Conclusions and ongoing work

- **Overall equivalence ratio**, **droplet size** and **turbulence** have an important influence on the flame structure.

- The presence of droplets leads to **dimples on the flame surface** for large droplet diameters and large droplet number densities.

- **The gaseous phase mixture** within the flame is predominantly fuel-lean in comparison to the overall equivalence ratio for $\phi_{ov} = 1.0$ and 1.2 droplet cases.

- The **growth rate of flame surface area** increases with increasing droplet diameter under fuel-lean mixture conditions, whereas an opposite behaviour has been observed for $\phi_{ov} = 1.0$ and 1.2.

- **Displacement** and **consumption speeds** can be related with the **rates of flame area generation** and **the burned gas volume** in spherically expanding spray flames.
Conclusions and ongoing work

Planar Spray Flame

Spherical Expanding
Spray Flame

\[
\frac{a_d}{\delta_{th}} = 0.06
\]

\[
\frac{a_d}{\delta_{th}} = 0.06
\]


Conclusions and ongoing work

**Simulation Parameters**

- **Domain**: \((63.3\delta_z)^3\) (where \(\delta_z = \alpha_{T_0}/S_b(\phi_g=1)\) is the Zel’dovich flame thickness)
- **Grid number**: \((384)^3\)
- **Equivalence ratio**: \(\phi_d = 1.0\)
- **Initial rms**: \(u'/S_b(\phi_g=1) = 2.0\)
- **Longitudinal integral length-scale**: \(L_{11}/\delta_{th} = 2.5\)
- **Mean inlet velocity of** \(\bar{u}_{mean}/S_{b, st} = 5\).
- **Holder position** \((x,y)\): \((120\Delta x, 192 \Delta y)\)
- **Heat release parameter**: \(\tau = \frac{T_{ad(\phi_g=1)}-T_0}{T_0} = 6.4\)
- **Droplet diameter**: \(a_d/\delta_{th} = 0.04, 0.05\) and \(0.06\)

Reaction progress variable isosurfaces at \(c = 0.1, 0.5\) and \(0.9\) for \(a_d/\delta_{th} = 0.06\) initial droplet diameter, at \(t = 1.5t_{flow}\).
Publications:

Journal Papers:


Conferences:


THANK YOU

The financial support of the Republic of Turkey Ministry of National Education and EPSRC (EP/K025163/1) and the computational support of Rocket and ARCHER are gratefully acknowledged.