High-fidelity simulation study of microexplosion & puffing of an emulsion fuel droplet

Jun Xia (Brunel University London)
jun.xia@brunel.ac.uk

Spray SIG, University of Brighton
12 June 2017
1. Microexplosion & Puffing EP/J018023/1

- **Microexplosion** *(complete microexplosion)*: rapid disintegration of an emulsion droplet caused by explosive boiling of embedded liquid sub-droplets with a lower boiling point.

- **Puffing** *(partial microexplosion)*: the explosion is limited to a portion of the parent oil droplet.
Benefits & Past findings

• An important secondary breakup mechanism to accelerate spray atomization
  – Can control secondary breakup (atomization)
    • Deeper penetration and more effective mixing
      Large droplet: deep penetration, ineffective mixing
      Small droplet: short penetration, effective mixing
  – Can reduce NO\textsubscript{x} and soot emission
    • Reduced thermal NO\textsubscript{x} by lower flame temperature
    • Added OH radicals

• Spray scale findings
  – Experiments: there are cases but details remain unknown
  – Simulations: rare, and proper modeling is needed

• Droplet scale findings
  – Typically done at enlarged scale (\sim O(1mm))
  – Rarely done at realistic spray scale (\sim O(10\mu m))
Diesel/biodiesel/bioethanol blend

• Diesel is a baseline fossil fuel to be used in existing combustion devices.

• Bioethanol is promising because
  – large amount of production worldwide.
  – It contains oxygen (O) and particulate matter (PM) will be reduced.

• However,
  – Miscibility is not good.
  – Cetane number will be reduced (bad for diesel engines).

• Addition of biodiesel (such as rapeseed oil methyl ester) will
  – Improve the miscibility as emulsion
  – Compensate the reduced cetane number.

• Depending on the blending ratio, the heating and combustion characteristics may vary, including puffing/microexplosion.

*Note:
  bioethanol = ethanol
  biodiesel ≈(but ≠) diesel
**Strategy**

**Step 1: Single droplet dynamics**

- Breakup timing
- Secondary droplet size

**Step 2: Modeling**

- Primary atomization
- High-fidelity simulation based on interface-capturing to directly resolve the dynamics of:
  1. Water-boiling surfaces
  2. Liquid-oil/liquid-water
  3. Non-boiling oil/gas interfaces

**Step 3: Spray simulation**

- Breakup timing
- Secondary droplet size

---

Watanabe & Okazaki (PROCI 2013)
Governing equations

**Navier-Stokes**

\[
\frac{\partial \mathbf{f}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{f} = \mathbf{g}
\]

\[
\mathbf{f} = (\rho, \mathbf{u}, T, Y_i)
\]

\[
\mathbf{g} = \left( -\rho \nabla \cdot \mathbf{u} + S_\rho, -\frac{\nabla P}{\rho} + \mathbf{Q}_u + \mathbf{S}_u, -\frac{P_{TH} \nabla \cdot \mathbf{u}}{\rho c_v} + Q_T + S_T, Q_{Y_i} \right)
\]

\[
P_{TH} = T(\partial p/\partial T)_\rho \quad \mathbf{F}_s = \rho \mathbf{Q}_u = \sigma \kappa \delta \mathbf{n} + \left( \nabla \sigma - (\nabla \sigma \cdot \mathbf{n}) \mathbf{n} \right) \delta
\]

**Level-set**

\[
\partial_t F + (\mathbf{u} \cdot \nabla) F = -|\nabla F| S_L
\]

**Evaporation**

\[
h_i \dot{\omega} = [\lambda \nabla T \cdot \mathbf{n}]
\]

\[
\dot{\omega}(Y_{i,G} - Y_{i,L}) = [\rho D_{\text{diff}} \nabla Y_i \cdot \mathbf{n}]
\]

\[
S_\rho = \rho (\rho_{G}^{-1} - \rho_{L}^{-1}) \dot{\omega} \delta,
\]

\[
S_u = (\rho_{G}^{-1} - \rho_{L}^{-1}) \dot{\omega} (\dot{\omega}/\rho) \delta \mathbf{n},
\]

\[
S_T = -(h_i/\rho c_p) \dot{\omega} \delta.
\]
Numerical methods

- **Eulerian-Eulerian two-phase flow**
  - 3D Navier-Stokes equations
  - Advection by CIP scheme
  - Speed of sound: CCUP (CIP-Combined and Unified Procedure)
  - Interface capturing by Level-Set method combined with MARS (VOF) method (CLSVOF)
  - Surface tension by CSF method
  - Jump condition at the interface for phase change and evaporation

Level-set: signed distance function

(a) Validation on droplet shape oscillation (Shinjo et al. *Phys. Fluids* 2014)

(b) Turbulent atomization (Shinjo & Umemura, *IJMF* 2010)
MEX (MicroEXplosion simulator)

• Incompressible & Compressible (pressure-based)
• Interface-capturing via coupled level-set and volume of fluid
• Dense spray regime
• MPI parallel algorithms
• Refs:
# Droplet configurations

<table>
<thead>
<tr>
<th>Case</th>
<th>Water sub-droplet radius ($R_2/R_0$)</th>
<th>Water sub-droplet volume fraction (%)</th>
<th>Water sub-droplet surface depth ($d/R_0$)</th>
<th>Bubble center location ($R_b/R_0$)</th>
<th>Bubble inclination angle ($\theta_b$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>0.35</td>
<td>12.3</td>
<td>0.12</td>
<td>0.21</td>
<td>0</td>
</tr>
<tr>
<td>A2</td>
<td>0.30</td>
<td>8.9</td>
<td>0.12</td>
<td>0.16</td>
<td>0</td>
</tr>
<tr>
<td>A3</td>
<td>0.25</td>
<td>6.1</td>
<td>0.12</td>
<td>0.11</td>
<td>0</td>
</tr>
<tr>
<td>A4</td>
<td>0.19</td>
<td>3.7</td>
<td>0.12</td>
<td>0.05</td>
<td>0</td>
</tr>
<tr>
<td>A5</td>
<td>0.14</td>
<td>2.0</td>
<td>0.12</td>
<td>0.02</td>
<td>0</td>
</tr>
<tr>
<td>A6</td>
<td>0.35</td>
<td>12.3</td>
<td>0.12</td>
<td>0.21</td>
<td>0</td>
</tr>
<tr>
<td>A7</td>
<td>0.14</td>
<td>2.0</td>
<td>0.12</td>
<td>0.16</td>
<td>0</td>
</tr>
<tr>
<td>B1</td>
<td>0.35</td>
<td>12.3</td>
<td>0.12</td>
<td>0.21</td>
<td>0</td>
</tr>
<tr>
<td>B2</td>
<td>0.35</td>
<td>12.3</td>
<td>0.12</td>
<td>0.16</td>
<td>0</td>
</tr>
<tr>
<td>B3</td>
<td>0.35</td>
<td>12.3</td>
<td>0.12</td>
<td>0.11</td>
<td>0</td>
</tr>
<tr>
<td>B4</td>
<td>0.35</td>
<td>12.3</td>
<td>0.12</td>
<td>0.05</td>
<td>0</td>
</tr>
<tr>
<td>C0</td>
<td>0.35×2</td>
<td>12.3×2 (1 is active)</td>
<td>0.12</td>
<td>0.21</td>
<td>0</td>
</tr>
<tr>
<td>C1</td>
<td>0.35×2</td>
<td>12.3×2</td>
<td>0.12</td>
<td>0.16</td>
<td>0</td>
</tr>
<tr>
<td>C3-1</td>
<td>0.25×4</td>
<td>6.1×4 (2 are active)</td>
<td>0.12</td>
<td>0.11</td>
<td>0</td>
</tr>
<tr>
<td>C3-2</td>
<td>0.25×4</td>
<td>6.1×4</td>
<td>0.12</td>
<td>0.11</td>
<td>0</td>
</tr>
<tr>
<td>C4</td>
<td>0.19×4</td>
<td>3.7×4</td>
<td>0.12</td>
<td>0.05</td>
<td>0</td>
</tr>
<tr>
<td>A1-3D</td>
<td>0.35</td>
<td>4.3</td>
<td>0.12</td>
<td>0.21</td>
<td>0</td>
</tr>
<tr>
<td>B3-3D</td>
<td>0.35</td>
<td>4.3</td>
<td>0.12</td>
<td>0.16</td>
<td>0</td>
</tr>
<tr>
<td>C3-3D</td>
<td>0.25×6</td>
<td>1.5×6</td>
<td>0.12</td>
<td>0.11</td>
<td>0</td>
</tr>
</tbody>
</table>

D0=2R0=30μm
Puffing & After-puffing dynamics

• Fuel spray scale droplets (~O(10 µm)) are targeted.

A. Initial bubble growth and burst due to boiling (puffing)
B. The remaining water sub-droplet pushes the parent oil droplet and its edge regresses

B2. If water sub-droplet shape oscillation is strong, regression is interfered temporarily.
C. And finally, the sub-droplet is detached.

Sub-droplet small
Pulling dominant

And EDGE REGRESSION dynamics

Sub-droplet large
Thrust dominant

Pulling vs. Thrust (& Shape oscillation)

ONE-STAGE DETACHMENT

TWO-STAGE DETACHMENT
Boiling surface instability

– Landau-Darrieus (LD) instability

• Mass flux at the interface bends the streamlines.
• The liquid phase flow may be irrotational, but the mass flux at the interface generates vorticity in the vapor phase.

*Landau-Darrieus instability also emerges at a premixed flame front.


FIG. 1. Qualitative illustration of the mechanism causing the surface instability, seen from a frame of reference in which the undisturbed evaporating surface is at rest. The evaporating mass flux is increased at the (liquid) troughs and decreased at the (liquid) crests. As a consequence the “backpush” of the departing vapor on the liquid is greater at the troughs than at the crests. The associated pressure gradient drives the liquid towards the crests causing their growth and the amplification of the surface deformation.

\[ J' = \rho_L \left( v_L - \frac{\partial \eta}{\partial t} \right) = \rho_G \left( v_G' - \frac{\partial \eta}{\partial t} \right) \]

FIG. 2. Qualitative illustration of the vorticity pattern in the vapor over the surface wave in the unstable case. The liquid motion is irrotational.

• “As a consequence, the rotational velocity component decreases the velocity on crests and increase it on troughs and enhances the instability” [8].
Boiling surface edge regression

This vorticity generation is due to strong bubble burst, not due to LD instability.

At edges, vorticity is generated by mass flux to enhance the regression. Finally, the water sub-droplet is detached.

\[ x \text{-axis} \]
\[ \omega_x > 0 \]
\[ \omega_x < 0 \]
Realistic microexplosion simulation

- Puffing/microexplosion
- Convective heating of emulsion droplet

- 3D
- Flow convection
- Inner-droplet temperature distribution
- Both a single droplet and a droplet group

- Puffing/microexplosion of blended decane/bioethanol droplet under convective heating

Nucleation and boiling
- One bubble
- Two bubbles
- Four bubbles
- ....

Low liquid temperature

High liquid temperature
# Realistic microexplosion simulation

## 3D cases (decane/ethanol)

<table>
<thead>
<tr>
<th>Case</th>
<th>A1</th>
<th>A2</th>
<th>A3</th>
<th>A4</th>
<th>A5</th>
<th>B1</th>
<th>B2</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. of nucleation</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>8</td>
<td>12</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>No. of parent droplets</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>Upstream BC</td>
<td>F</td>
<td>F</td>
<td>F</td>
<td>F</td>
<td>F</td>
<td>F</td>
<td>P</td>
</tr>
</tbody>
</table>

F: fixed upstream air velocity  
P: periodic (=in the wake of preceding droplets)

\[ D=30\mu m, \ U_G=10m/s, \ T_G=900K, \ Re=30 \]

**Series A**: single droplet  
\~243 million grid points

**Series B**: multiple droplets  
\~576 million grid points
Puffing dynamics

The growth of a single bubble can be well understood by the Rayleigh equation

$$R\ddot{R} + \frac{3}{2} \dot{R}^2 = \frac{p_v - p_0}{\rho_L} - \frac{2\sigma}{\rho_L R}$$

Similar behavior in enlarged single-droplet experiment
Puffing and vapor ejection

- **Decane vapor**
- **Evaporation**
- **Ethanol vapor**
- **Boiling**

- 1 explosion
- 2 explosions
- 4 explosions
- 4+4 explosions

- Blue iso-surfaces
- Red iso-surfaces

Liquid surface area

- Decane vapor evaporation
- Ethanol vapor boiling

Secondary breakup

Ejection hole

Graph showing liquid surface area over time:

- A1
- A2
- A3
- A4
- A5
Fuel-vapor/air mixing

Define mixture fractions as

\[ Z_i = \frac{Y_i - Y_{i,0}}{Y_{i,1} - Y_{i,0}} \quad i = 1, 2 \]

- \( Y_{i,0} = 0 \) in the far field
- \( Y_{i,1} = 1 \) at the droplet center

The mixture fractions \( Z_i \) reduce to the fuel mass fractions,

- \( Z_1 = Y_{\text{decane}} \)
- \( Z_2 = Y_{\text{ethanol}} \)

In the physical field,

\[
\frac{\partial}{\partial t} (\rho Z_i) + \frac{\partial}{\partial x_j} (\rho u_j Z_i) = \frac{\partial}{\partial x_j} \left[ \rho D \left( \frac{\partial Z_i}{\partial x_j} \right) \right] + S_{Z_i}
\]

In the \( Z \) field,

\[
\rho \frac{\partial Y_i}{\partial t} - \frac{\rho}{2Le_i} \left( \chi_1 \frac{\partial^2 Y_i}{\partial Z_1^2} + 2\chi_{12} \frac{\partial^2 Y_i}{\partial Z_1 \partial Z_2} + \chi_2 \frac{\partial^2 Y_i}{\partial Z_2^2} \right) = S_{Y_i}
\]

is solved.

**Primary fuel: Decane**

**Secondary fuel: Ethanol (vf: 7.4%)**
Fuel/Air Micromixing:
(1) Decane (primary fuel) vapor +
(2) ethanol (secondary fuel) vapor + (3) air

**Volume fraction of Ethanol: 7.4%**

Scalar dissipation rates

\[
\chi_1 = 2D|\nabla Z_1|^2, \\
\chi_2 = 2D|\nabla Z_2|^2, \\
\chi_{12} = 2D(\nabla Z_1 \cdot \nabla Z_2).
\]

The transport equation for \( \chi_1 \) is

\[
\frac{\partial \chi_1}{\partial t} = -\frac{1}{4}\left(\frac{\partial \chi_1}{\partial Z_1}\right)^2 + 2\alpha \chi_1 + \chi_{12} \left( \frac{\partial^2 \chi_1}{\partial Z_1 \partial Z_2} - \frac{\partial^2 \chi_1}{\partial Z_2^2} \right) + S_{\chi_1}
\]

\( \alpha \): (dominant) compressive strain

*Similar for \( \chi_2 \)
Mixing without puffing

- Before puffing

It is known that droplet vapor region is similar to flame region (Zoby et al. 2011).

Model 1
\[
< \chi | Z > \sim F(Z) \sim \exp \left( -2 \left[ \text{erfc}^{-1} \left( \frac{2Z}{Z_{\text{max}}} \right) \right]^2 \right)
\]

Model 2
\[
< \chi | Z > \sim S(Z) = 8D\alpha \left[ Z^2 \ln \left( \frac{A}{f} \right) \right]
\]
\[
\alpha = \frac{U}{4Dl}
\]
\[
A = \dot{m}_d (Z_d - Z_{\infty}) / 4\pi \rho Dl
\]

• Comparison Good!
• Model 1 is better.
Weak-Puffing effects on Mixing

2 explosions

Ethanol vapor

Decane vapor

$E_{\text{ejection velocity magnitude}}$

$t = 10.56 \mu s$

$t = 11.88 \mu s$

$t = 12.54 \mu s$

$\langle X | Z_1, Z_2 \rangle$

1 = decane

2 = ethanol
Weak-Puffing effects on Mixing

2 explosions

Mean SDRs and mean rate of change of $\chi_1$ conditioned on $Z_1$ for case A2. Thick lines are profiles at $t=11.88\mu s$ and thin lines at $t=13.20\mu s$.

$$\frac{\partial \chi_1}{\partial t} = -\frac{1}{4} \left( \frac{\partial \chi_1}{\partial Z_1} \right)^2 + \frac{2a\chi_1}{Production} + \left( \frac{\chi_1}{2} \frac{\partial^2 \chi_1}{\partial Z_1^2} \right)_{Diffusion-\chi_1} + \left( \chi_{12} \frac{\partial^2 \chi_1}{\partial Z_1 \partial Z_2} \right)_{Diffusion-\chi_{12}} + \left( \frac{\chi_2}{2} \frac{\partial^2 \chi_1}{\partial Z_2^2} \right)_{Diffusion-\chi_2} + S_{\chi_1}^{Source}$$
Strong-Puffing effects on Mixing

4 explosions

1=decane
2=ethanol

$t=9.24\mu s$

$\chi_1$

$t=10.56\mu s$

$\chi_2$

$t=13.20\mu s$

$\chi_{12}$

Ethanol vapor

$4$ explosions

$\chi_1$

$\chi_2$

$\chi_{12}$

$t=9.24\mu s$

$t=13.20\mu s$

$t=10.56\mu s$
Strong-Mixing of decane and ethanol

Mean SDRs and mean rate of change of $\chi_1$ conditioned on $Z_1$ for case A2. Thick lines are profiles at $t=10.56\mu$s and thin lines at $t=13.20\mu$s.

$$\frac{\partial \chi_1}{\partial t} = -\frac{1}{4} \left( \frac{\partial \chi_1}{\partial Z_1} \right)^2 + 2a\chi_1 + \frac{\chi_1}{2} \frac{\partial^2 \chi_1}{\partial Z_1^2} + \frac{\chi_1}{2} \frac{\partial^2 \chi_1}{\partial Z_1 \partial Z_2} + \chi_{12} \frac{\partial^2 \chi_1}{\partial Z_1^2} + \chi_{12} \frac{\partial^2 \chi_1}{\partial Z_1 \partial Z_2} + \frac{\chi_2}{2} \frac{\partial^2 \chi_1}{\partial Z_2^2} + S_{\chi_1}$$

*DSource is removed.*
Puffing and puffing-induced interaction between ejected ethanol vapour and the decane-droplet wake flame

Summary

• Microexplosion & puffing directly simulated by interface-capturing methods; **Physics unveiled.**
• After-puffing dynamics determined by 3 competing mechanisms: (1) **pulling**, (2) **thrust**, & (3) **shape oscillation**.
  - Pulling dominant → one-stage detachment
  - Thrust dominant → two-stage detachment
• **Edge regression dynamics** plays a key role in after-puffing & water sub-droplet detachment.
• Model proposed for droplet heating.
• Interaction between a droplet wake flame and puffing.