LES of Spray Combustion using Flamelet Generated Manifolds

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Part I: Non-reacting spray study

Objectives

1. Mesh resolution effects in Large Eddy Simulation
2. Influence of droplet breakup modeling on the local and global flow characteristics

Spray case

Non-reacting Spray A baseline:
\[ P_{\text{inj}} = 150 \text{ MPa} \quad T = 900 \text{ K} \]
\[ P_{\text{amb}} = 6 \text{ MPa} \quad 0\% \text{ O}_2 \]

Reference

Computational Methods

Gas phase
- Large Eddy Simulation (LES)
- Turbulence modeling based on the implicit LES approach [2]
  ⇒ No explicit subgrid scale model
- Finite Volume, open source CFD code OpenFOAM 2.0.x
  (2nd order accurate in space and time)

Liquid phase
- Lagrangian Particle Tracking (LPT)
- No explicit primary break-up model
  ⇒ Initial droplet size distribution (Rosin-Rammler)
- Secondary break-up models:
  1. Enhance Taylor Analogy Breakup (ETAB)
  2. Kelvin-Helmholtz Rayleigh-Taylor (KHRT)
Computational mesh

- Fully hexahedral
- Refinement in the spray region by 2:1 cell splitting
- Applied cell sizes:
  \[
  \begin{array}{cc}
  dx \, [\mu m] & N_{cells} [-] \\
  250 & 0.8M \\
  125 & 1.2M \\
  62.5 & 4.8M \\
  41.67 & 16.2M \\
  \end{array}
  \]
- Constant time step:
  \[\Delta t = 1 \times 10^{-8} \text{ s}\]
Results

Liquid length

- Poor results for 250 µm cell size meshes, regardless of breakup model
- 125 µm cell size:
  - ETAB: Good agreement with experiments
  - KHRT: Significantly over-predicted
- Good results for 62.5 and 41.67 µm cell size meshes, regardless of breakup model
Results

Mixture fraction distribution (KHRT model)

- 250 µm cell size mesh not able to capture the turbulent motion correctly
- 125 µm cell size mesh able to capture a significant part of the turbulent motion
- Increasing level of detail for 62.5 and 41.67 µm cell size meshes
Results

Vapor penetration
(KHRT: ○, ETAB: no marker)
- Slight under-prediction for all cell sizes and both breakup models

Radial mixture fraction profile
(KHRT: ○, ETAB: no marker; \( z = 25 \) mm)
- 125 and 62.5 µm mesh: Values in the center is under- and spreading over-predict
- 41.67 µm mesh: Good agreement with experiments
Results

PDF of droplet diameter

ETAB model

- Uniform distribution
- SMD = 0.3 µm ... 0.4 µm

KHRT model

- Broad range of droplet sizes
- SMD = 1.1 µm ... 1.4 µm

Probability density function of droplet diameter at $t = 1.4$ ms
Part II: Non-reacting spray study

Objectives:
Investigate the ignition characteristics and early flame structure using Large Eddy Simulation and Flamelet Generated Manifold (FGM)

Spray case
Reacting Spray A cases:
\[ P_{\text{inj}} = 150 \text{ MPa} \quad T = 900 \text{ K} \]
\[ P_{\text{amb}} \approx 6 \text{ MPa} \quad \rho_{\text{amb}} = 22.8 \text{ kg/m}^3 \]
15\% O\textsubscript{2}
Computational Methods

Flow solver
- Implicit Large Eddy Simulation
- Lagrangian Particle Tracking (Secondary breakup: ETAB)
- OpenFOAM 2.2.x
- Advanced thermodynamic/transport models (i.e. Wilke/Mathur mixture models)

Flamelet Generated Manifolds (FGM) [3]
- Tabulated chemistry model
- State of combustion is parametrized by a few control variables (here, mixture fraction and a reaction progress variable)
- Chemistry data obtained from 1D igniting/steady counterflow diffusion flames (i.e. flamelets)
- Detailed chemical kinetics (253 species, 1437 reactions [4])
FGM tables

Figure: Temperature

Figure: CO mass fraction

Chemistry parametrized by mixture fraction $Z$ and reaction progress variable $C$
Results

Spray penetration

- Calculation are carried out on the 62.5 µm mesh
- Simulated liquid length matches the experimental data
- Vapor penetration slightly under-predicted
Results

Ignition delay

- Significant over-prediction compared to experiments
- Consistent ignition delay estimate for both ECN definitions ($\frac{dT}{dt}$ & OH mass fraction)

Flame length

- Lift-off length slightly under-predicted
Results

Spray A combustion
Thank you for your attention!
Appendix
1 References
