Incorporation of Flamelet Generated Manifold Combustion Closure to OpenFOAM and Lib-ICE
Contents:

- Introduction to Chemistry Reduction Methods
- FGM Implementation to OpenFOAM and Lib-ICE
- Case Study
  - Constant Volume Vessel | ECN Spray A
  - Light Duty Diesel Engine | ECN Spray B
  - Heavy Duty Diesel Engine | Sandia Engine
- Conclusions
Contents:

➤ Introduction to Chemistry Reduction Methods
➤ FGM Implementation to OpenFOAM and Lib-ICE
➤ Case Study
  • Constant Volume Vessel | ECN Spray A
  • Light Duty Diesel Engine | ECN Spray B
  • Heavy Duty Diesel Engine | Sandia Engine
➤ Conclusions
Introduction to Chemistry Reduction Methods

Chemical Kinetics of Reactive Flows

- Result in system of stiff ODE and solution for reaction rates requires specific mathematical algorithms.
- Hinders prospective CFD simulations of reactive flows.
Introduction to Chemistry Reduction Methods

Chemistry Tabulation vs on-the-fly Chemistry

- No integration for Chemistry
- Look up routines for updating sources

- Direct integration for chemistry
- Sources update after chemistry integration

Progress Variable approach

Flame Types:

- **Perfectly Stirred Reactor**
- **Approximated Diffusion Flamelet**
- **Flamelet Generated Manifolds**

Developed at TU/e
Contents:

- Introduction to Chemistry Reduction Methods
- FGM Implementation to OpenFOAM and Lib-ICE
- Case Study
  - Constant Volume Vessel | ECN Spray A
  - Light Duty Diesel Engine | ECN Spray B
  - Heavy Duty Diesel Engine | Sandia Engine
- Conclusions
Flamelet Generated Manifolds

CHEM1D: 1D flamelet solver code:

- Adaptive gridding
- Implicit solver
- Timestepper (real /false)
- Flexible inlet composition
- CHEMKIN III compatible
- Thermal diffusion
- Transport modelling
- Unity Lewis numbers
- Constant Lewis numbers
- Different Flame Types
- Mixture average

www.fgm-combustion.org

The Simulation of Flat Flames with Detailed and Reduced Chemical Models, Bart Somers
FGM Implementation to OpenFOAM and Lib-ICE

Tabulation of counter flow flamelets for Reacting Sprays

Reaction Space – flamelet solver

- CHEM1D solver code was used for flamelet generation.

\[
\frac{\partial \rho}{\partial t} + \rho \frac{\partial u}{\partial x} = -\rho K \\
\frac{\partial \rho Y_n}{\partial t} + \rho \frac{\partial u Y_n}{\partial x} = \frac{\partial}{\partial x} \left( \rho D \frac{\partial Y_n}{\partial x} \right) + \omega_n - \rho K Y_n \\
\frac{\partial \rho h}{\partial t} + \rho \frac{\partial u h}{\partial x} = \frac{\partial}{\partial x} \left( \lambda \frac{\partial h}{\partial x} \right) - \rho Kh
\]

- CHEM1D:
  Includes different Flame Types:
  FREE, BURNERSTABILIZED, COUNTERFLOW, BIO, and …

Transport:
UNITY LEWIS, CONSTANT/VARIABLE LEWIS
FGM Implementation to OpenFOAM and Lib-ICE

Reaction Space

1D flamelets

Temperature [K]

bash script for parallel flamelet generation

Frozen Flamelet Method, FFM for IC Engine applications

CFD

CHEM1D

MATLAB scripts

FGM table

Needed format for table data

Table dimensions parametrization & interpolation

Variable definition & calculation

Unsteady flamelets
Equilibrium lines
Mixing line

Flame
Oxidizer
Fuel
FGM Implementation to OpenFOAM and Lib-ICE

Lib-ICE:
- Flamelet CFD solver for reacting spray and IC engine
- Source code for table dimensions and data handling

Dimensions for tabulation of chemistry can be:

- **Progress variable**
- **Mixture fraction**
- **Unburned Temperature**
- **Pressure**
- **Segregated Mixture Fraction**
- **Segregated Progress variable**
- **Scalar Dissipation Rate**

4D Tables for IC Engines:

- 1D: \( C \)
- 2D: \( Z \)
- 3D: \( T_u \)
- 4D: \( c_2 \)
- 6D: \( Z_2 \)
- 7D: \( \chi \)
FGM Implementation to OpenFOAM and Lib-ICE

Reaction Space

1D flamelets

1

Tabulated Chemistry

4D-FGM

Source term from FGM tables

\[
\frac{\partial \rho C}{\partial t} + \frac{\partial \rho u C}{\partial x} = \frac{\partial}{\partial x} \left( \frac{\mu_t}{Sc_t} \frac{\partial C}{\partial x} \right) + \rho \dot{C}
\]

Variable Pressure & Unburned Temperature

FGMFlameletLibrary class was incorporated to the Lib-ICE source
FGM Implementation to OpenFOAM and Lib-ICE

1. Reaction Space
   1D flamelets

2. Transport of \( c \) and \( Z \) Fields

3. \( c, Z, P, \) Tu from CFD to Table

4. cdot from Table to Update CFD
Contents:

- Introduction to Chemistry Reduction Methods
- FGM Implementation to OpenFOAM and Lib-ICE
- Case Study
  - Constant Volume Vessel | ECN Spray A
  - Light Duty Diesel Engine | ECN Spray B
  - Heavy Duty Diesel Engine | Sandia Engine
- Conclusions
Case Study: Constant Volume Vessel  |  ECN Spray A

Experimental configuration

Specifications for Spray A of the ECN

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel injector</td>
<td>Bosch</td>
</tr>
<tr>
<td>Orifice diameter</td>
<td>0.090 mm</td>
</tr>
<tr>
<td>Nozzle K factor</td>
<td>K = 1.5</td>
</tr>
<tr>
<td>Nozzle shaping</td>
<td>Smoothed</td>
</tr>
<tr>
<td>Mini-sac volume</td>
<td>0.2 mm³</td>
</tr>
<tr>
<td>Discharge coefficient</td>
<td>C_d = 0.86</td>
</tr>
<tr>
<td>Number of holes</td>
<td>single hole</td>
</tr>
<tr>
<td>Orifice orientation</td>
<td>Axial</td>
</tr>
</tbody>
</table>

Non-reacting: Liquid/vapor pen. and Mixture Fraction distribution

Reacting: Ignition delay and Flame Lift-off

Large set of experimental and numerical data for non-reacting and reacting operating conditions
Case Study: Constant Volume Vessel | ECN Spray A

Non-reacting: Liquid/vapor penetration and Mixture Fraction distribution

Baseline operating condition

<table>
<thead>
<tr>
<th>2D computational mesh</th>
</tr>
</thead>
<tbody>
<tr>
<td>CFD setup</td>
</tr>
<tr>
<td>• Injection: blob</td>
</tr>
<tr>
<td>• Breakup: KHRT</td>
</tr>
<tr>
<td>• Evaporation: Spalding</td>
</tr>
<tr>
<td>• Turbulence model: standard k-ε with modified C₁</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Test conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Fuel n-dodecane</td>
</tr>
<tr>
<td>• Nozzle diameter: 90 μm</td>
</tr>
<tr>
<td>• $p_{\text{inj}}$: 150 MPa</td>
</tr>
<tr>
<td>• $T_{\text{amb}}$: 900 K</td>
</tr>
<tr>
<td>• $\rho_{\text{amb}}$: 22.8 kg/m³</td>
</tr>
</tbody>
</table>

Non-reacting: Liquid/vapor penetration and Mixture Fraction distribution (RANS)

Vapor & Liquid penetration [m]

Distance from axis [mm]

Time after SOI [s]

Mixture Fraction

Sim. | Exp.
Case Study: Constant Volume Vessel | ECN Spray A

n-dodecane Chemistry:

Mechanism of Yao et al. was used.

54 species and 269 reactions

Yao et al. 9th U. S. National Combustion Meeting
Case Study: Constant Volume Vessel | ECN Spray A

FGM: Table dimensions and progress variable definition

Spray A ambient composition

\[ C = Y_{HO_2} + Y_{CH_2O} + Y_{H_2O} + Y_{CO_2} + Y_{CO} \]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Range</th>
<th>No. of discretization points</th>
</tr>
</thead>
<tbody>
<tr>
<td>Progress Variable</td>
<td>(0 &lt; c &lt; 1)</td>
<td>500</td>
</tr>
<tr>
<td>Mixture Fraction</td>
<td>(0 &lt; Z &lt; 1)</td>
<td>500</td>
</tr>
<tr>
<td>Unburned Temperature [K]</td>
<td>(750 &lt; T_u &lt; 1100)</td>
<td>6</td>
</tr>
<tr>
<td>Pressure [bar]</td>
<td>(50 &lt; p &lt; 80)</td>
<td>3</td>
</tr>
</tbody>
</table>

![Graphs showing C vs Z at different temperatures]
Case Study: Constant Volume Vessel | ECN Spray A

Reacting: Ignition Delay, PRR, Flame Lift-off

<table>
<thead>
<tr>
<th>Ambient temperature [K]</th>
<th>800</th>
<th>900</th>
<th>1000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ignition delay [ms] Simulation</td>
<td>0.91</td>
<td>0.45</td>
<td>0.25</td>
</tr>
<tr>
<td>Experiment</td>
<td>0.85</td>
<td>0.41</td>
<td>0.24</td>
</tr>
<tr>
<td>Flame lift-off [mm] Simulation</td>
<td>25.1</td>
<td>16.5</td>
<td>11.7</td>
</tr>
<tr>
<td>Experiment</td>
<td>26.2</td>
<td>16.7</td>
<td>12.2</td>
</tr>
</tbody>
</table>

- **800 K**
- **900 K**
- **1000 K**
Case Study: Constant Volume Vessel | ECN Spray A

Reacting: Ignition Delay, PRR, Flame Lift-off at 3 CAD ATDC

800 K

900 K

1000 K

<table>
<thead>
<tr>
<th>Temperature [K]</th>
<th>OH</th>
<th>Pressure rise rate [bar/ms]</th>
</tr>
</thead>
<tbody>
<tr>
<td>800 K</td>
<td>0.00107</td>
<td>0.5</td>
</tr>
<tr>
<td>900 K</td>
<td>0.001211</td>
<td>0.5</td>
</tr>
<tr>
<td>1000 K</td>
<td>0.001276</td>
<td>0.5</td>
</tr>
</tbody>
</table>

End of Inj.→
Contents:

- Introduction to Chemistry Reduction Methods
- FGM Implementation to OpenFOAM and Lib-ICE
- Case Study
  - Constant Volume Vessel | ECN Spray A
  - Light Duty Diesel Engine | ECN Spray B
  - Heavy Duty Diesel Engine | Sandia Engine
- Conclusions
**Case Study: Light Duty Diesel Engine | ECN Spray B**

Experimental configuration

### Spray B – Bosch injector

- **Injector type:** #211199 Bosch Spray B
- **Hole sizes:** #1, 2, 3, 90.9 μm, 91.7 μm, 90.9 μm
- **Nominal included angle:** 145°
- **Nozzle shaping:** Smoothed
- **Discharge coefficient:** C_d = 0.86
- **Hole angular position:** 
  - #1 36.4°, #2 -62.3°, #3 180°

### Sandia Optical Engine

<table>
<thead>
<tr>
<th>Component</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intake valves</td>
<td>2</td>
</tr>
<tr>
<td>Exhaust valves</td>
<td>1</td>
</tr>
<tr>
<td>Swirl ratio</td>
<td>0.5</td>
</tr>
<tr>
<td>Bore x Stroke</td>
<td>13.97 x 15.24 cm</td>
</tr>
<tr>
<td>Bowl width x depth</td>
<td>9.78 x 1.55 cm</td>
</tr>
<tr>
<td>Displacement</td>
<td>2.34 L</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>11.22 : 1</td>
</tr>
<tr>
<td>Connecting rod length</td>
<td>30.48 cm</td>
</tr>
</tbody>
</table>

### Mie scattering

- **Color Phantom v611**
- **Frame rate:** 67kHz
- **Exposure:** 14us
- **Lens:** =85mm f/1.4

### Schlieren

- **Phantom v71**
- **Frame rate:** 25kHz
- **Exposure:** 19us
- **Lens:** 105mm f/2.5

### Chimiluminescence OH*

- **Intensified Phantom v71**
- **Frame rate:** 7.2kHz (1CAD)
- **Exposure:** 55us
- **Lens:** 105mm UV f/4.5

**SAE 2016-01-0743**
Case Study: Light Duty Diesel Engine | ECN Spray B

Operating conditions:

<table>
<thead>
<tr>
<th>Case name</th>
<th>900K</th>
<th>800K</th>
<th>1000K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature at IVC [K]</td>
<td>380</td>
<td>340</td>
<td>454</td>
</tr>
<tr>
<td>Pressure at IVC [bar]</td>
<td>2.25</td>
<td>2.01</td>
<td>2.61</td>
</tr>
<tr>
<td>Temperature at TDC [K]</td>
<td>900</td>
<td>800</td>
<td>1000</td>
</tr>
<tr>
<td>Density at TDC [kg/m³]</td>
<td>22.8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Non-reacting O₂ [%]</td>
<td>7.5</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Reacting O₂ [%]</td>
<td>15</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Injection pressure [bar]</td>
<td>1500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Injected mass [mg/cycle]</td>
<td>3.68</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Engine Speed [rpm]</td>
<td>1200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Inj. start [CAD ATDC]</td>
<td>-2.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Inj. duration [CAD]</td>
<td>11</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Spray oriented grid

45,916 cells at TDC
341,562 cells at BDC
48.7 and 11.2 for maximum and average mesh non-orthogonality
Case Study: Light Duty Diesel Engine | ECN Spray B

Non-reacting: Liquid/vapor penetration
Reacting: In-cylinder Pressure and AHRR

### 800 K
- **In-cylinder pressure [bar]**
- **AHRR [J/CAD]**

### 900 K
- **In-cylinder pressure [bar]**
- **AHRR [J/CAD]**

### 1000 K
- **In-cylinder pressure [bar]**
- **AHRR [J/CAD]**
Case Study: Light Duty Diesel Engine | ECN Spray B

Reacting: Flame Lift-off

![Temperature Maps](image-url)

- **800 K**: Temp [K] 2300, Time: -165 CAD ATDC
- **900 K**: Temp [K] 2300, Time: -165 CAD ATDC
- **1000 K**: Temp [K] 2300, Time: -165 CAD ATDC
Reacting: Flame Lift-off

- Simulation results for 800 K, 900 K, and 1000 K temperatures.
- Experimental data at 800 K, 900 K, and 1000 K temperatures.

Graph showing flame lift-off as a function of CAD ATDC.
Contents:

- Introduction to Chemistry Reduction Methods
- FGM Implementation to OpenFOAM and Lib-ICE
- Case Study
  - Constant Volume Vessel | ECN Spray A
  - Light Duty Diesel Engine | ECN Spray B
  - Heavy Duty Diesel Engine | Sandia Engine
- Conclusions
Case Study: Heavy Duty Diesel Engine  |  Sandia Engine

Experimental configuration

Operating conditions

<table>
<thead>
<tr>
<th>Case</th>
<th>HT-Sh-ID</th>
<th>HT-Lo-ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine Speed [rpm]</td>
<td>1200</td>
<td>1200</td>
</tr>
<tr>
<td>Temperature at IVC [K]</td>
<td>384</td>
<td>320</td>
</tr>
<tr>
<td>Pressure at IVC [bar]</td>
<td>1.2</td>
<td>1.2</td>
</tr>
<tr>
<td>Temperature at TDC [K]</td>
<td>900</td>
<td>800</td>
</tr>
<tr>
<td>Density at TDC [kg/m³]</td>
<td>24</td>
<td>22.3</td>
</tr>
<tr>
<td>Injected mass [mg/cycle]</td>
<td>61</td>
<td>61</td>
</tr>
<tr>
<td>Inj. start [CAD ATDC]</td>
<td>-7</td>
<td>-5</td>
</tr>
<tr>
<td>Inj. duration [CAD]</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>O₂ concentration [% by Vol.]</td>
<td>21</td>
<td>21</td>
</tr>
</tbody>
</table>

Injected Mass = $16.2 \times$ Injected Mass

Heavy Duty Spray B

SAE 2006-01-0055
Case Study: Heavy Duty Diesel Engine | Sandia Engine

Non-reacting: Liquid penetration

Operating conditions

<table>
<thead>
<tr>
<th>Case</th>
<th>HT-Sh-ID</th>
<th>HT-Lo-ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine Speed [rpm]</td>
<td>1200</td>
<td>1200</td>
</tr>
<tr>
<td>Temperature at IVC [K]</td>
<td>384</td>
<td>320</td>
</tr>
<tr>
<td>Pressure at IVC [bar]</td>
<td>1.2</td>
<td>1.2</td>
</tr>
<tr>
<td>Temperature at TDC [K]</td>
<td>900</td>
<td>800</td>
</tr>
<tr>
<td>Density at TDC [kg/m³]</td>
<td>24</td>
<td>22.3</td>
</tr>
<tr>
<td>Injected mass [mg/cycle]</td>
<td>61</td>
<td>61</td>
</tr>
<tr>
<td>Inj. start [CAD ATDC]</td>
<td>-7</td>
<td>-5</td>
</tr>
<tr>
<td>Inj. duration [CAD]</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>O₂ concentration [% by Vol.]</td>
<td>21</td>
<td>21</td>
</tr>
</tbody>
</table>

Injected Mass = 16.2 × Injected Mass

Heavy Duty

Spray B

Injected Mass

Liquid length [mm]

CAD ATDC

HT-Sh-ID

HT-Lo-ID

Experiments
Case Study: Heavy Duty Diesel Engine | Sandia Engine

Reacting: In-cylinder Pressure & AHRR

HT-Sh-ID

HT-Lo-ID
Case Study: Heavy Duty Diesel Engine | Sandia Engine

Reacting: Flame Structure at -5 CAD ATDC

HT-Sh-ID
HT-Lo-ID
Case Study: Heavy Duty Diesel Engine | Sandia Engine

Reacting: Flame Structure at -4 CAD ATDC

Graphs showing temperature distribution and in-cylinder pressure and AHRR with injection timing for HT-Sh-ID and HT-Lo-ID cases.
Case Study: Heavy Duty Diesel Engine | Sandia Engine

Reacting: Flame Structure at -1 CAD ATDC
Case Study: Heavy Duty Diesel Engine | Sandia Engine

Reacting: Flame Structure at TDC

In-cylinder pressure (bar) vs. CAD ATDC

HT-Sh-ID

HT-Lo-ID

Injection
Case Study: Heavy Duty Diesel Engine  |  Sandia Engine

Reacting: Flame Structure  at 3 CAD ATDC

---

**Graphs:**

- **HT-Sh-ID:**
  - Temperature and In-cylinder pressure vs. CAD ATDC.
  - Experiment and Simulation curves.
  - Injection point indicated.

- **HT-Lo-ID:**
  - Similar to HT-Sh-ID but with different parameters.

---

**Graph Details:**

- **Axes:**
  - Temperature (K) vs. CAD ATDC for HT-Sh-ID.
  - In-cylinder pressure [bar] vs. CAD ATDC for HT-Sh-ID.
  - In-cylinder pressure [bar] vs. CAD ATDC for HT-Lo-ID.

---

3rd Two-day Meeting on IC Engine Simulations Using OpenFOAM Technology 22-23 Feb 2018 - Milano
Contents:

- Introduction to Chemistry Reduction Methods
- FGM Implementation to OpenFOAM and Lib-ICE
- Case Study
  - Constant Volume Vessel | ECN Spray A
  - Light Duty Diesel Engine | ECN Spray B
  - Heavy Duty Diesel Engine | Sandia Engine
- Conclusions
Conclusions

- FGM combustion closure was incorporated into OpenFOAM and Lib-ICE to model reacting spray and Diesel engine conditions.

- Progress variable source provided by FGM tabulation was capable of accurate predictions for state of thermodynamics of the mixture under non/partially premixed combustion configurations.

- For studied ambient temperature conditions, results of ignition delay, PRR or AHRR as well as flame lift-off was well agreeing with the experiments.

- n-dodecane chemical kinetics still suffers from comprehensive mechanism for low temperature combustion and there is a need for an extensively validated mechanism.
Thanks for your attention!

Amin Maghbouli
contact: amin.maghbouli@gmail.com