CFD Combustion Models for IC Engines

Rolf D. Reitz

Engine Research Center
University of Wisconsin-Madison

ERC Symposium, June 7, 2007

http://www.cae.wisc.edu/~reitz
1. Characteristic Time Combustion Model (KIVA-CTC)
   • Auto-ignition model (SHELL) – ignition with 8 reaction steps
   • Combustion model (CTC) – turbulence mixing timescales

2. Representative Interactive Flamelet Model (KIVA-RIF)
   • Flamelet equations/detailed chemistry coupled with CFD (Peters et al.)
   • Effect of turbulence is modeled with average scalar dissipation rate

3. Direct Integration of CFD with Chemistry (KIVA-CHEMKIN)
   • Each computational cell treated as well stirred reactor
   • ERC reduced mechanism for n-heptane – chemistry timescales

4. KIVA-CHEMKIN-G Model
   • Explicit modeling of turbulent flame propagation combined with detailed chemistry
Auto-ignition and Detailed Chemistry Models

Skeletal Chemistry Mechanism for Multi-Surrogate Fuels

- **Gasoline**
  - Iso-octane
  - 857 species
  - 8586 reactions

- **Diesel**
  - N-heptane
  - 570 species
  - 2580 reactions

- **Bio-diesel**
  - Methyl butanoate
  - 264 species
  - 1219 reactions

- **Aromatic**
  - Toluene

- **Alcohol**
  - Ethanol

**Multi-fuel Mechanism**
- 25 species
- 51 reactions
- 30 species
- 65 reactions
- 41 species
- 150 reactions

**Comprehensive mechanism**
**Skeletal mechanism**

Dr. Youngchul Ra
Jessica Brakora
Validation - Auto-ignition Model

n-heptane-iso-octane/air mixtures, stoichiometric, P=40 Bar)

Shock tube measurements
(Fieweger et al. 1997)

SAE 2007-01-0165
Validation – Cat HD engine

rpm = 1737
eq_ratio = 0.23
c_ratio = 16.1
inj_timing = -113 ca

rpm = 700
eq_ratio = 0.27
c_ratio = 16.1
inj_timing = -274.5 ca

Gasoline HCCI

SAE 2002-01-0418, SAE 2007-01-0190
Validation - GM Light-duty Diesel Engine

KIVA-CHEMKIN

SOIC = -39, -32 and -23

GM 1.9L 4-cylinder
Bore × Stroke  82×90.4 mm
Compression Ratio  16.6: 1
Engine Speed  2000 rev/min
IMEP 5.5 Bar
EGR 67% PCCI

SAE 2007-01-0193
Advances in SI Engine Combustion Modeling

G-equation Combustion Model with Detailed Chemical Kinetics

\[
\frac{\partial \tilde{G}}{\partial t} + (\tilde{v}_f - \tilde{v}_{\text{vertex}}) \cdot \nabla \tilde{G} = \frac{\bar{\rho}_u}{\bar{\rho}} S_T^0 \left| \nabla \tilde{G} \right| - D_T \tilde{k} \left| \nabla \tilde{G} \right|
\]

SAE 2000-01-2809

Discrete particle ignition model

End Gas

Burnt Gas

G-Equation Flame propagation

Auto-ignition (detailed kinetics)

CA = -90.0 ATDC

SAE 2000-01-2809

SAE 2003-01-0722

SAE 2007-01-0165
Validation – Ford SI Engine

KIVA-CHEMKIN-G

PFI mode
-32 °ATDC

PFI Spark sweep

Ford DISI
Bore × Stroke 89×79.5 mm
Compression Ratio 12 : 1
Engine Speed 1500 rev/min

DI Spark sweep

DI MAP sweep

SAE 2007-01-0165
Validation - Sandia Cummins Diesel

High-T, long-ID Condition (Premixed Combustion)

$O_2 = 21\%$

$SOI = -5$

Experiment  
KIVA-CHEMKIN  
KIVA-CHEMKIN-G

SAE 2006-01-0055

Green: OH  
Red: Soot
Validation - Cummins Dual-Fuel Engine

Experimental Measurements

AHRR (J/deg)

Pressure (MPa)

Case 1
Case 2
Case 3
Case 4
Case 5

Model Predictions

AHRR (J/deg)

Pressure (MPa)

Case 1
Case 2
Case 3
Case 4
Case 5

Validation - Cummins Dual-Fuel Engine

NOx

Measured
Predicted

BMEP 10 bar
SOI -87 BTDC
PIVC 2.1 bar
NG $\phi$ 0.44
CR 14.5

Primary Fuel: Natural Gas
Ignition Source: Diesel Pilot (10%)

Case 1 2 3 4 5
TIVC (K) 392 397.5 403 405 408
Validation - Cummins Dual-Fuel Engine

KIVA-CHEMKIN vs KIVA-CHEMKIN-G

Case 1

Pressure (MPa)

AHRR (J/deg)

CAD ATDC

Without flame-propagation combustion is too slow

Gas Temp. (K)

CA = -1  CA = 4

CA = 9  CA = 14

Ignition kernel

Ignition

Ignition kernels
Summary and Conclusions

• Current CFD models describe important physical and chemical processes of engine flows, but validation experiments are needed for model development and improvement
• CFD combustion models capture engine performance and emissions trends and can be combined with optimization tools for design and evaluation of engine design concepts
• Methodologies are in place for modeling a wide range of combustion regimes:
  HCCI $\rightarrow$ PCCI $\rightarrow$ Diesel $\rightarrow$ SI flame propagation $\rightarrow$ dual-fuel
• Multi-component fuel vaporization models can be coupled with advanced chemical kinetics models
• Surrogate fuel models are under development to represent representative practical fuels (MB, toluene, ethanol…..)
Multi-Component fuel modeling – Dr. Youngchul Ra

**Gasoline**

*Adapted from J. Farrel, Exxon Mobil Corp.*

**Diesel**

<table>
<thead>
<tr>
<th>Component</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aromatics</td>
<td>16</td>
</tr>
<tr>
<td>Sulfur</td>
<td>7.3 ppm</td>
</tr>
<tr>
<td>Paraffins</td>
<td>42</td>
</tr>
<tr>
<td>Napthenes</td>
<td>42</td>
</tr>
<tr>
<td>Olefins</td>
<td>0.3</td>
</tr>
<tr>
<td>C/H ratio</td>
<td>6.393</td>
</tr>
</tbody>
</table>

**Continuous** $f_p(I)$

**Discrete** $g_p(mw_i)$

**Single comp approx**

**Fuel species in fuel model**

**Fuel species in chemistry model**

- $m_1$
- $m_2$
- $m_3$
- $m_4$
- $m_5$
- ...

*Adapted from J. Farrel, Exxon Mobil Corp.*
PRF50: Emissions

LTC regime (EGR=65%)
Injection sweep
Reduced Biodiesel Mechanism – Jessica Brakora

**LLNL methyl butanoate (MB)**
- Surrogate to represent the large methyl esters in biodiesel
- MB chemical formula: $\text{C}_5\text{H}_{10}\text{O}_2$
- 264 species, 1219 reactions

**Mechanism Reduction Method**
- SENKIN constant volume analysis
- Identify key species and reaction paths based on ignition timing
  - Peak concentration: remove species that never exceed specified mole fraction thresholds (-112 species)
  - XSENK PLOT reaction flux analysis: identify key reaction pathways, remove less important paths (-111 species)
- Adjust rate constants for key reactions to optimize ignition timing

Reduced MB Kinetic Mechanism

These species further break down into lower-level carbon species

MB reduced coupled with ERC n-heptane: 41 species, 150 reactions

![Graph showing ignition delay vs. initial temperature for MB reduced and LLNL detailed models at P = 40 bar and Phi = 1.0]
Auto-ignition and Detailed Chemistry Models

ERC n-heptane mechanism SAE 2004-01-0558: 34 species
ERC PRF Reduced Chemistry SAE 2007-01-0190, SAE 2007-01-0165: 47 species
Multi-component Fuel – DMC/PRF Models

**PRF50 fuel**

![Graph showing pressure and heat release rate (HRR) for different injection pressures and fuels](image)

- **n-heptane**
- **iso-octane**

**Axes:**
- Pressure [MPa]
- Heat release rate [J/deg]

**Lines and Colors:**
- P, inj= -45
- P, inj= -42
- P, inj= -39
- P, inj= -33
- P, inj= -27
- P, inj= -21
- P, iC8
- P, nC7
- HRR, inj= -45
- HRR, inj= -42
- HRR, inj= -39
- HRR, inj= -33
- HRR, inj= -27
- HRR, inj= -21
- HRR, iC8
- HRR, nC7