Strategies for Using Detailed Kinetics in Engine Simulations

Ellen Meeks
ERC Symposium: Fuels for Future IC Engines
June 6-7, 2007
Madison, Wisconsin
Outline

● Role of simulation in design
● Importance of chemical kinetics
● Challenges of using detailed kinetics
● Strategies that bridge the gap between design simulation and kinetics
Simulation reduces cost of development

● There is a growing opportunity to:
  – Reduce risk
  – Improve use of testing
  – Speed development
  – Facilitate innovation
How effective can simulation be?

According to our customers, it depends on the accuracy:

- Needs to be predictive to
  * Allow exploration and discovery
  * Guide design and testing

- Must provide deep understanding of dependencies to
  * Manage complexity of tradeoffs
  * Facilitate innovative solutions
Computational fluid dynamics (CFD) is already widely used for engine design.

**Example Goal:**
Maximize uniformity in piston bowl

**CFD Simulation:**
Determine effects of port flow distribution, injector design, injector timing, piston bowl geometry

STAR-CD simulations with simplified chemistry
An engine system is a chemical plant

Fuel
Air
(O₂ + N₂)

Horsepower
CO₂ + H₂O
CO, NOₓ, PM
Unburned HC

Pt / Rh

CO₂ + H₂O
Air
(O₂ + N₂)
There is a gap between CFD simulation and testing requirements

Goal:
Minimize emissions while maximizing efficiency

CFD Simulation:
Determine effects of port flow distribution, injector design, injector timing, piston bowl geometry

Test:
Determine emissions, efficiency, performance

Workflow is incomplete

CFD users cannot predict chemistry effects adequately

Ignition delay, CO, UH, PM, etc.
Detailed chemistry is required to address many important issues

- Ignition timing
  - Diesel
  - HCCI/CAI
- Knock reduction
- Emissions control
  - NO\textsubscript{x}, CO, UHC, PM
- Fuel flexibility
- Exhaust-gas recirculation
- System control
Challenges for using detailed kinetics

- Real fuels are too complex

- *Validated* detailed mechanisms are scarce

- Simulations are too time-consuming

- Companies often lack chemistry expertise
Addressing the challenges...

- Real fuels are too complex
- Validated detailed mechanisms are scarce
- Simulations are too time-consuming
- Companies often lack chemistry expertise
Real fuel components can be categorized

- Classes of chemical compounds have
  - Common molecular structures
  - Similar chemical behavior

- Biofuels have different compositions
  - Methyl-ester structures
  - Contain oxygen

Example: Gasoline*

Surrogate fuel mixtures can be used to represent real fuels in simulations.

- 1 or 2 molecules represent each significant chemical class, e.g.:

<table>
<thead>
<tr>
<th>Real Fuel Component</th>
<th>Surrogate Fuel Candidate</th>
</tr>
</thead>
<tbody>
<tr>
<td>iso-paraffins</td>
<td>iso-octane, hepta-methyl nonane</td>
</tr>
<tr>
<td>normal paraffins</td>
<td>n-heptane, n-hexadecane</td>
</tr>
<tr>
<td>single ring aromatics</td>
<td>toluene</td>
</tr>
<tr>
<td>cyclo-paraffins</td>
<td>methylcyclohexane</td>
</tr>
<tr>
<td>olefinic species</td>
<td>1-pentene</td>
</tr>
<tr>
<td>multi-ring aromatics</td>
<td>alpha-methyl naphthalene</td>
</tr>
<tr>
<td>oxygenates</td>
<td>methyl stearate, methyl linoleate</td>
</tr>
</tbody>
</table>

- Detailed chemistry models are built for each molecule
  - Use elementary reactions
  - Allow merging to form mixtures
Different model fuels can be assembled for different applications

- Tailor to prediction of desired combustion and physical properties:
  - Ignition delay
  - Knocking tendency
  - Flame speeds
  - Pollutant emissions
  - Sooting tendency & particle size distributions
Example shows prediction of ignition delay with 5-component mixture

- Surrogate mixture compositions defined to match class composition or RON #*
  - All do reasonably well in capturing ignition behavior with idealized model of engine, detailed kinetics

*Reported by: C. V. Naik, et al
SAE 2005-01-3742
With a database of molecules, we can assemble an appropriate surrogate

Real Fuel Characteristics
- Class composition
- Heat-release rate
- Octane / Cetane #
- H/C ratio, O content

Match Properties
- Select Molecules
- Set Composition

Merge Mechanisms
- Species
- Reactions

Surrogate Fuel Composition

U.S. E15 Gasoline

Chemical Model for Simulation
Addressing the challenges...

- Real fuels are too complex
- *Validated* detailed mechanisms are scarce
- Simulations are too time-consuming
- Companies often lack chemistry expertise
Mechanism generation for a molecule can be fully automated

Based on work in collaboration with the Dow Chemical Company
Validation focused on mechanism-generation rules is key to building database

- Well studied molecules used to refine rules
- Assures consistency between surrogate fuel component mechanisms
- Allows easy assembly of mixtures
Get full benefit from molecules that have been well studied experimentally

- For example: n-heptane
  - Shock-tube, JSR, Flames, RCM, and Engine data

![Graph showing ignition delay time vs. 1000/Temperature (1/K)]

Shock-tube and RCM Data
Pressure Range: 0.07 to 60 atm
Stoichiometry: $\phi = 0.1$ to 4
Validation involves simulations of well controlled experiments with full chemistry

- CHEMKIN simulation of shock-tube show detailed kinetics ability to predict ignition
Improvement of rules creates solid foundation for mechanism generation

- Enables full power of mechanism generation
- Assures consistency in mixtures

Example: Improvement of MCH mechanism involved updated reaction rate rules for RO₂ chemistry

Work performed in collaboration with C. Westbrook and W. Pitz, et al., LLNL
Addressing the challenges...

● Real fuels are too complex

● *Validated* detailed mechanisms are scarce

● Simulations are too time-consuming

● Companies often lack chemistry expertise
Several methods allow linking to CFD with limited impact on simulation time.

- Automated Zone Mapping
- Multi-zone model
- Detailed Chemistry Model
- Automated Chemistry Reduction
- Single-zone or 1-D flame model

Table look-up vs. Progress variable

+ global chemistry
+ reduced chemistry
+ progress variables
Multi-zone models allow detailed kinetics

- Multiple, homogeneous regions
  - Core, boundary layer, crevice
  - Connected through work/heat
  - Can be auto-extracted from CFD
  - Can include full particle-formation chemistry

- Approach shows good prediction of heat-release, pressure, ignition, emissions

From:
S. M. Aceves, et al., SAE 2001-01-1027
Automated mechanism reduction can be very effective for “skeletalization”

- **Ignition delay example:**
  - 5-component gas. surrogate
  - 60% reduction, ~ 5X Faster
    * Equivalence ratio 0.1 - 2.0
    * T= 600 - 1800K
    * P= 0.5 - 60atm
  - < 4% error

- **Flame-speed example:**
  - n-heptane diesel surrogate
  - 80% reduction, ~ 30X Faster
    * Equivalence ratio 0.7 - 1.7
    * T= 300 - 700K
  - < 2% error
More severe reduction can also be achieved

- **Lumping of species or reactions**
  - Remove requirement of elementary reactions

- **Use of partial equilibrium assumptions**
  - Remove some species from flow equations

- **Identification of “manifolds”**
  - Separate out timescales
Addressing the challenges...

- Real fuels are too complex
- **Validated** detailed mechanisms are scarce
- Simulations are too time-consuming
- Companies often lack chemistry expertise
The Model Fuels Consortium is addressing many of these issues

- Industry funded and Directed
- Built on commercial offerings
- Advised by leading science experts
Overall goal is to bridge gap between chemistry and engine design simulation

- Make better use of expensive tests
- Improve accuracy of design simulations
- Provide bridge between detailed chemistry and design tools
- Build fuel-chemistry knowledge base
Focus is on building a validated database and engineering analysis tools

Knowledge-base

Fuel Mixture Representation

Master Mechanism Assembly

Mechanism Evaluation and Validation

Mechanism Reduction

Fuel Component Mechanisms

Reduced Mechanisms

Software Tools

Development of Mechanism Analysis and Engine Simulation Tools

Development of Mechanism Reduction Tools
MFC Technical Advisory Team

- Dr. Charles Westbrook – Chief Technical Advisor
  - A pioneer in combustion modeling while at the Lawrence Livermore National Laboratory
- Prof. Mitsuo Koshi, Tokyo University
  - Expert in combustion kinetics and mechanism generation
- Prof. Anthony Dean, Colorado School of Mines
  - Expert kineticist; formerly lead scientist at Exxon
- Prof. William Green, Massachusetts Inst. of Technology
  - Expert in numerical methods for model reduction and mechanism generation techniques
- Prof. Ulrich Maas, Universität Karlsruhe
  - Expert in engine combustion simulation and numerical methods
- Prof. Hiromitsu Ando, Fukui University
  - Former deputy general manager of engine research at Mitsubishi Motors
Summary and Conclusions

- There is increasing need for detailed chemistry simulation for engine design
- Advances in technology facilitate use of kinetics in simulation
  - Automation of mechanism generation
  - Automation of mechanism reduction
  - Advanced overlay techniques with CFD
  - More powerful computers
Contributors
C. V. Naik
K. V. Puduppakkam
C. Wang

Thank You