High-Fidelity Simulations for Clean and Efficient Combustion of Alternative Fuels
Application of the Large Eddy Simulation Technique

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Large Eddy Simulation (LES)

- Turbulent combustion involves interactions over wide ranges of length and time scales
- LES provides mathematical formalism to treat full range of multidimensional scales in a turbulent reacting flow
  - Large energetic scales are resolved directly
  - Small “subgrid scales” are modeled
- Used when direct numerical simulations are not feasible
  - Inhomogeneous turbulence characteristics induced by complex geometries
  - High-Reynolds-number turbulence-chemistry interactions at high pressures
  - Device-scale geometries, operating conditions, and run times
- Our focus is on propulsion and power devices (e.g., gas turbines, IC engines, liquid rockets)
Motivation: Changing world of fuels and engines

• Fuel streams are rapidly evolving
  – Heavy hydrocarbons
    • Oil sands
    • Oil shale
    • Coal
  – New renewable fuel sources
    • Ethanol
    • Biodiesel
    • Hydrogen

• New engine technologies require analysis at actual operating conditions, in actual geometries
  – Various direct injection (DI) concepts
  – Low-temperature combustion

• Mixed modes of turbulent combustion, complex mixture preparation strategies

• Advanced scientific understanding is necessary to develop next-generation predictive models
Example: If optimized, homogeneous charged compression ignition (HCCI) engines can deliver both high efficiency and low emissions.

Low Temperature Combustion (LTC)
- Diesel-like efficiency
- Low NO\textsubscript{X}, soot, hydrocarbon emissions
- Challenges: Operation limited to low loads. Controlling combustion difficult
- Detailed analysis of in-cylinder processes is required

HCCI
- A form of LTC that is mostly premixed
- Lean or dilute with EGR

Diesel Combustion
- Controlled timing and HRR
- High efficiency (relative to SI)
- High NO\textsubscript{X} and soot

Spark-Ignition Combustion
- Controlled timing and HRR
- Low NO\textsubscript{X}, hydrocarbon emissions
- Low efficiency (relative to diesel)

Adiabatic flame temperature in air

CO to CO\textsubscript{2} conversion diminishes

Akihama et. al 2001, SAE2001-01-0655
Theoretical-numerical framework “RAPTOR” (a general solver optimized for LES)

ORNL Jaguar platform coupled with RAPTOR enables development of a wide range of combustion models.
**Application of science-based LES bridges gap between science and applications**

**Objective:** Combine state-of-the-art LES with key experiments
- High-fidelity simulations that match geometry, BCs, ...
- Validation, then joint analysis of results ...
  - Fundamental insights not available from experiments alone
  - Scientific foundation for advanced model development

**Goal:** Predictive models at device-relevant conditions
- High-pressure combustion, multiphase flow, clean, efficient, stable combustion ...

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**Basic**

LES of Turbulence-Chemistry Interactions in Reacting Flows  
DOE Office of Basic Energy Sciences  

 TNF Workshop  
[www.ca.sandia.gov/TNF](http://www.ca.sandia.gov/TNF)

**Unified Code Framework (RAPTOR)**

- Detailed measurements for model development but low Reynolds number and simple fuels
- Detailed measurements for engine development at high Re with complex geometry and fuels

**Applied**

LES of High-Pressure, Low-Temperature Engine Combustion Processes  
DOE Office of Vehicle Technologies  

[Engine Combustion Network](http://www.ca.sandia.gov/ECN)
Experiments funded by DOE Basic Energy Sciences provide basic foundation for model development

**DLR-A Flame**: $Re_d = 15,200$

- **Fuel**: 22.1% CH$_4$, 33.2% H$_2$, 44.7% N$_2$
- **Coflow**: 99.2% Air, 0.8% H$_2$O
- **Detailed Chemistry and Transport**: 12-Step Mechanism (J.-Y. Chen, UC Berkeley)

Comparisons with 1D Raman/Rayleigh/CO-LIF line images complete (Barlow et al.)

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Mean</th>
<th>RMS</th>
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<tbody>
<tr>
<td>Temperature</td>
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<tr>
<td>Mixture Fraction</td>
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<tr>
<td>$H_2O$ Mass Fraction</td>
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**Comparisons with 1D Raman/Rayleigh/CO-LIF line images complete (Barlow et al.)**

**Experiment**

- **Mean**
- **RMS**

**Temperature**

**Mixture Fraction**

**$H_2O$ Mass Fraction**

**CO Mass Fraction**
DOE Office of Vehicle Technologies funded research focuses on model development for IC engines

<table>
<thead>
<tr>
<th>Engine Specifications</th>
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<tbody>
<tr>
<td>Compression Ratio</td>
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<tr>
<td>Bore</td>
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<tr>
<td>Stroke</td>
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<tr>
<td>Peak Turbulence Intensity</td>
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<tr>
<td>Integral Length Scale</td>
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<td>Thermal Layer Thickness</td>
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<tr>
<td>Kolmogorov Length Scale</td>
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<tr>
<td>Reaction Zone Thickness</td>
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<tr>
<td>Turbulent Reynolds Number</td>
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</tbody>
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CRF Direct-Injection Hydrogen-Fueled IC Engine (Kaiser et al.)

CRF HCCI Engine (Dec et al.)
Rigorous validation of high-pressure, high-Reynolds-number fuel injection is prerequisite

- **Iso-Contours of Density (H₂ – N₂)**
  - Injector Orifice
  - \( \text{Re}_d = 720,000 \)
  - \( 5.31 \text{ kg/m}^3 \)
  - \( 4.56 \text{ kg/m}^3 \)
  - \( 3.80 \text{ kg/m}^3 \)
  - Injector Exit

- **Values**
  - Orifice diameter: 0.8 mm
  - Injection pressure: 10.4 MPa
  - Injection temperature: 298 K
  - Chamber pressure: 0.336 MPa
  - Chamber temperature: 298 K

- **Graph**
  - \( H_2 (10.4 \text{ MPa}) \) into \( N_2 (0.336 \text{ MPa}) \)
  - Penetration, mm vs. Time, \( \mu \text{s} \)
  - Experiment (Set 1), Experiment (Set 2), Simulation

- **Images**
  - Shadowgraph (U. Wisconsin)
  - Large Eddy Simulation

- **Representative comparison of LES with penetration measurements**
Strong scaling attributes associated with high-pressure injector calculations

One of the first “capability-class” codes that handles relevant physics and geometry for ICE applications
Full engine calculations in geometry shown here are currently in progress

Multiscale simulations of turbulent combustion will provide the foundational science required to develop a validated, predictive combustion modeling capability to optimize the design and operation of evolving fuels in advanced engines for transportation applications. This will enable transportation technology breakthroughs, ensuring American competitiveness and U.S. energy security and minimizing harmful environmental emissions.

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