Direct Numerical Simulation of High Pressure, Mixed Mode Turbulent Combustion

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Research Objectives

• **Overarching Objectives:**
  – Perform DNS with detailed kinetics to couple high pressure, low temperature kinetics with turbulent transport
  – Investigate ‘turbulence-chemistry’ interactions at ambient and high pressure in mixed modes of combustion relevant to the utilization of transportation fuels.

• **Short-Term Objectives:**
  – Lifted flame stabilization in heated coflow (relevant to diesel lift-off stabilization)
  – Homogeneous charge compression ignition (HCCI) with thermal and concentration stratification (multi-stage ignition fuels: n-heptane and di-methyl ether)
Direct Numerical Simulation Code – S3D

- Used to perform first-principles-based DNS of reacting flows
- Solves compressible reacting Navier-Stokes equations
- High-fidelity numerical methods
- Detailed reaction kinetics and molecular transport models
- Multi-physics: sprays, radiation and soot
- Ported to all major platforms, scales well up to 200,000+ CrayXT5 cores
- Particle tracking capability

DNS provides unique fundamental insight into the chemistry-turbulence interaction

**DNS** ↔ **Physical models** ↔ **Engineering CFD codes (RANS, LES)**
Role of DNS - Case Studies

- Lifted Turbulent Jet Flames in Heated Coflow
- Homogeneous Charge Compression Ignition Combustion
Motivation: Understanding Stabilization of Lifted Flames in Heated Coflow

What is the role of ignition in lifted flame stabilization?

Chemiluminescence from diesel lift-off stabilization for #2 diesel, ambient 21% $O_2$, 850K, 35 bar courtesy of Lyle Pickett, SNL
DNS of Lifted Ethylene-air Jet Flame in a Heated Coflow

- 3D slot burner configuration: $L_x \times L_y \times L_z = 30 \times 40 \times 6 \text{ mm}^3$ with
  - 1.28 billion grid points
  - High fuel jet velocity (204 m/s); coflow velocity (20 m/s)
  - Nozzle size for fuel jet, $H = 2.0$ mm
  - $Re_{jet} = 10,000$
  - Cold fuel jet ($18\% \text{ C}_2\text{H}_4 + 82\% \text{ N}_2$) at $550K$, $\eta_{st} \approx 0.27$
  - Detailed $\text{C}_2\text{H}_4$/air chemistry, 22 species 18 global reactions, 201 steps
  - Hot coflow air at 1,550K

Scalar Dissipation Rate $\chi$, Species Mass Fractions, and Mixture Fraction $\xi$
Conceptual stabilization mechanism

Temporal evolution of OH mass fraction isocontour at $t/\tau_j = 0.227 \sim 1.160$

a) Ignition occurs in lean mixtures with low $\chi$
b) Stabilization point is advected downstream by high convective velocity
c) Ignition occurs in another coherent jet structure

Convective velocity greater than displacement speed for $\eta_{st} = 0.27$
Temporal Tracking of Stabilization Point

Graphs showing the time evolution of various parameters related to stability, such as $x/H$, $y/H$, and velocity in m/s. Arrows indicate changes over time.
Chemical Explosive Mode Analysis, Da, Weighted Explosion Index


\[
\text{sign}(\lambda_{\text{exp}}) \times \log_{10}(\max(1, |\lambda_{\text{exp}}|), 1/s)
\]

(a) (b) (c)

Weighted EI

1. OH
2. OH
3. HO2
4. T
5. CO
6. CH3CHO
Universal auto-ignition underpredicts lift-off;
Steady burning over-predicts lift-off
Multi-regime approach promising for efficiently describing turbulent ignition
Continuing work: using DNS to understand model shortcomings
Future Work

• Model Evaluation:
  – A posteriori comparison with LES/PDF (Pope)
  – A posteriori comparison with LES/Multi-regime Flamelets (Knudsen, Richardson, Pitsch)

• DNS:
  – Effect of DME additive to regulate lift-off height in DME/methane/air jet flames in hot coflow
  – High-pressure Lifted Diesel Jet Stabilization with DME. N-heptane, and butanol (pending mechanism reduction)
Role of DNS - Case Studies

- Lifted Turbulent Jet Flames in Heated Coflow

- Homogeneous Charge Compression Ignition Combustion
  - Thermal and composition stratification with DME
  - Thermal stratification with N-heptane
Motivating example: HCCI Combustion

Overall lean and dilute
High diesel efficiencies without soot and NO$_x$
Challenge is to control ignition timing and rate of heat release rate
Combustion is by spontaneous ignition or mixed mode combustion
Sensitive to ignition kinetics and mixture and thermal stratification
Conditions in DNS are relevant for realistic HCCI engines

Non reacting simulations:

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Initial time

After one integral time

Optical Engine

From J.E. Dec et al (2009)

Integral time = 1 ms

\[
\tau_t = 1 \ \text{msec} \\
\tau_c = 2 \ \text{msec} \\
T' = 15 \text{K}
\]

\[
2\alpha |\nabla T|^2 = \frac{cT}{\tau_t} T''^2
\]

\[
|\nabla T|_{\text{engine}} \approx |\nabla T|_{\text{DNS}}
\]

⇒ Heat release modes in DNS comparable to those in realistic HCCI engines
Reacting cases: (a) 0D, (b) thermally stratified, (c) thermally and compositionally stratified. Three-staged ignition is observed in DME/air mixtures.

I. LTC ignition, $\text{CH}_3\text{CH}_2\text{O}_2$ key intermediate (low T)
II. $\text{H}_2\text{O}_2$ dissociation (intermediate T)
III. $\text{H}+\text{O}_2 = \text{OH} + \text{O}$ (high T)

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Case (b) Thermally Stratified Mixture
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HRR fields (colormap inverted)

1.4 ms  
“Cool flames”

2.075 ms

2.135 ms

“IInd and IIIrd stage “ignition waves” are simultaneously present

IIIrd stage is predominantly a deflagration wave
Close proximity of II\textsuperscript{nd} and III\textsuperscript{rd} stage waves – inter-diffusion of heat and radicals II\textsuperscript{nd} stage is chemistry driven spontaneous front; III\textsuperscript{rd} stage is a deflagration wave.

A twin-ring structure of heat release.

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Isocontour of normalized heat release rate for $T_0 = 934K$, $T' = 15, 30, 60, 100K$ (from left to right) at $t/\tau_{0,ig} = 1.0, 0.96, 0.88, \text{ and } 0.60$, respectively.

C. S. Yoo et al. 2010 submitted to Comb. Flame
Mean Front Speed Evolution

C. S. Yoo et al. 2010 submitted to Comb. Flame

• Temporal evolution of the mean front speed $S^*_d/S_L$ for $T_0 = 850\, K$, 934K, 1008 K and $T' = 30$, 60, and 100 K.

• Combustion is advanced with increasing $T'$ for $T_0 = 934\, K$ and 1008K, but retarded for 850K.

• Duration of deflagration is increased with increasing $T'$. 
Future Work

• 3D DNS HCCI
• Validation of models – flamelet, pdf, CMC
• Hybrid operation – spark assisted HCCI