Direct Numerical Simulation of Turbulent Combustion: Fundamental Science towards Predictive Models

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Motivation: Changing World of Fuels and Engines

- Fuel streams are rapidly evolving
  - Heavy hydrocarbons from oil sands and oil shale
  - New renewable fuel sources like ethanol and biodiesel
- National goals:
  - Reduce greenhouse gas emissions by 80% by 2050
  - Reduce petroleum usage by 25% by 2020
- New engine technologies
  - Direct Injection (DI)
  - Homogeneous Charge Compression Ignition (HCCI)
  - Low-temperature combustion
- Mixed modes of combustion
  - Dilute, higher-pressure and lower-temperature
- Sound scientific understanding is necessary to develop predictive, validated multi-scale models!
Combustion is a Complex, Multi-physics, Multi-scale Problem

- Stiffness: wide range of length and time scales
  - In-cylinder geometry (cm)
  - Turbulence-chemistry (mm)
  - Soot inception (nm)
- Chemical complexity
  - Large number of species and reactions (100's of species, thousands of reactions)
- Multi-Physics complexity
  - Multiphase (liquid spray, gas phase, soot, surface)
  - Thermal radiation
  - Acoustics ...
- All these are tightly coupled
DNS / LES / RANS of Combustion

• Reynolds Averaged Navier Stokes (RANS)
  – No attempt to resolve any scales
  – Inexpensive. Empirical models

• Large Eddy Simulation (LES)
  – Energetic scales are resolved
  – Presumed universal behavior at unresolved scales. Closure used for scalar flux, combustion source terms

• Direct Numerical Simulation (DNS)
  – All continuum scales are resolved
  – Provides fundamental insight, causality and benchmark data
  – Extremely expensive
**Direct Numerical Simulation (DNS)**

- First-principles simulation of reacting flows
  - Flame and dissipative flow scales are fully resolved
  - Chemistry and molecular transport terms are modeled
- Solves compressible reacting Navier-Stokes equations with detailed reaction kinetics
- High-fidelity numerical methods
- Multi-physics: sprays, radiation and soot
- Lagrangian tracer particles

DNS provides unique fundamental insight into the chemistry-turbulence interaction
Fundamental Insights on Turbulent Combustion

• DNS is a tool for fundamental studies of the micro-physics of turbulent reacting flows
  – Full access to time resolved 3D fields
  – Study turbulence-chemistry interaction
  – Limited to canonical geometries

• Develop and validate reduced model descriptions used in macro-scale simulations of engineering-level systems
  – “LES faces the same closure problem as RANS based approaches” (Bilger et al. 2005)
Role of Direct Numerical Simulation

- DNS is a numerical microscope to study the microphysics of combustion
  - Study flow-flame interaction under controlled variation of parameters

Picture of a medieval English Bakery
From Fort Vancouver Bakery by John A. Hussey
Growth of DNS

Homogeneous Charge Compression Ignition (HCCI) Engines

- Potential for high diesel-like efficiencies with low soot and NOx emissions
- Fuel-lean and low temperature combustion
- Challenges:
  - Hard to control ignition timing
  - Sensitive to fuel chemistry
  - High load burn rate needs to be moderated
- Need to better understand ignition of fuel blends and oxygenated hydrocarbon fuels in biomass derived fuels
Homogeneous charge compression ignition engine-out emissions—does flame propagation occur in homogeneous charge compression ignition?

E W Kaiser, J Yang, T Culp, N Xu and M M Maricq
Research Laboratory, Ford Motor Company, Dearborn, Michigan, USA

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The results in this paper present data from a limited set of experiments on one engine and are in no way comprehensive. However, the observations made herein suggest that it is important to examine the combustion processes in HCCI engines in more detail. While the data may be able to be explained by models based on purely homogeneous reactions, the occurrence of ordinary flame propagation between isolated ignition sites over distances short relative to the cylinder diameter should not be dismissed, and the existence of exhaust particulates must be carefully evaluated in the light of particulate regulations.
Fuel chemistry and mixing control the rate of combustion in HCCI engines

- Inhomogeneities (thermal or composition) lead to sequential ignition front propagation down the gradient
- Combustion modes range from homogeneous explosion to propagating flames
- New modes operate far from equilibrium with highly transient intermittent ignition occurring at multiple sites
- Better understanding needed to predict behavior of alternative fuels in HCCI engines

Optical engine experiments show front-like propagation.

S. Walton, M. S. Wooldridge et al. (Univ of Michigan)
DNS of DME HCCI Autoignition (G. Bansal et al. 2011)

- Turbulence and scalars initialized using an energy spectrum
- Initial turbulence integral time-scale and scalar RMS values – guided from practical engine experiments
- Reduced DME chemistry – 30 species
- Initially homogeneous composition
- \( \phi = 0.3 \) with Gaussian temperature distribution, \( T' = 25K \)
- Isentropic compression simulates HCCI engine operation from 36 CAD to TDC
Simultaneous Existence of Flames and Spontaneous Ignition

A twin-ring structure of heat release

- Close proximity of IIInd and IIIird stage waves – inter-diffusion of heat and radicals
- IIInd stage is chemistry driven spontaneous front. IIIird stage is a deflagration wave
Transported PDF Modeling of Molecular Mixing in Flames with Differential Diffusion

• Differential diffusion of species influences flame dynamics, pollution, and radiation.

• DNS is currently the ONLY tool that gives resolved 3D information on differential diffusion physics in turbulent flow.
  – unprecedented opportunities to validate and refine predictive models.

• Transported PDF methods handle mixed mode combustion – provides exact closure for chemical source terms

• But multi-scalar molecular mixing requires modeling in both RANS and LES

• Can we model differential diffusion in a PDF mixing model that satisfies conservation of means, localness, and realizability?
PDF Modeling of Molecular Mixing in Flames with Differential Diffusion

- Mixing rates controlled by species diffusivities and flame structure.
- Predictions of the state-of-the-art EMST model accounts for flame structure but not differential diffusion.
- New PDF modeling developed by Richardson and Chen (Combustion and Flame, 2012) includes species diffusivities in a rigorous manner and correctly predicts the physics observed in the DNS.

Variation of normalised species mixing rates versus time

Richardson, Bansal and Chen (2012)
Stabilization of Turbulent Lifted Jets in Heated Air Coflow

Chemiluminescence from diesel lift-off stabilization for #2 diesel, ambient 21% O₂, 850K, 35 bar courtesy of Lyle Pickett, SNL

What is the role of ignition in lifted flame stabilization?
DNS of Lifted Ethylene-Air Flame in a Hot Coflow

• Slot burner configuration
  – $L_x \times L_y \times L_z = 30 \times 40 \times 6$ mm$^3$
  – 1.28 billion grid points
  – Fuel jet nozzle size = 2.0mm
  – Jet Reynolds number = 10,000

• Detailed ethylene/air chemistry
  – 22 species and 201 elementary reaction steps


Ethylene-air lifted jet flame at Re=10000
Temporal Evolution of OH at Stabilization Point
Conceptual Stabilization Mechanism

- 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

Su & Mungal
Reactive Jets in Crossflow

- Relevant to stationary gas turbines
  - Fuel injection in premixer section

- Understanding of flame stabilization mechanism important to ensure intrinsic flash back safety

- DNS of jet in cross flow to study flame stabilization
  - Parametric study varying nozzle geometry, injection angle and fuel composition
Flame anchors on leeward side due to low velocity region induced by cross-flow wrapping around around the perceived obstruction due to the jet, resulting in an opposed flow at the symmetry plane on the jet lee. (Grout et al., *Proc. Combust. Inst.*, 2011, vol. 33.)
Thank You!