High-Fidelity Simulations for Advanced Engine Combustion Research

Presented by

Joseph C. Oefelein (PI)
Guilhem Lacaze and Rainer Dahms

Combustion Research Facility
Sandia National Laboratories

Ramanan Sankaran

Scientific Computing Liaison
Oak Ridge National Laboratory

Large Eddy Simulation (LES)

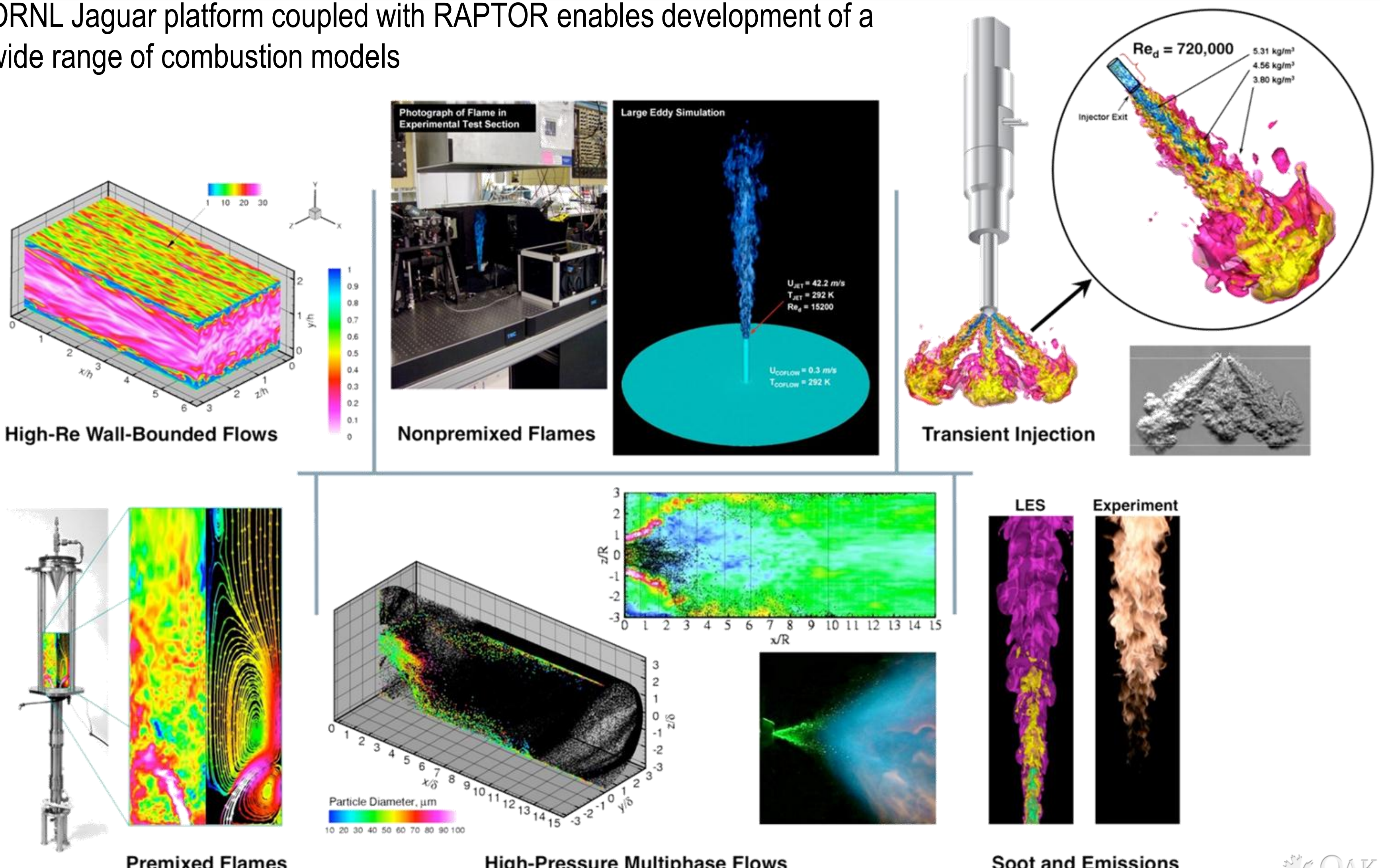
- Turbulent combustion involves interactions over wide ranges of length and time scales
- LES provides mathematical formalism to treat full range of multidimensional scales in a turbulent reacting flow
  - Large energetic scales are resolved directly
  - Small "subgrid scales" are modeled
- Used when 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

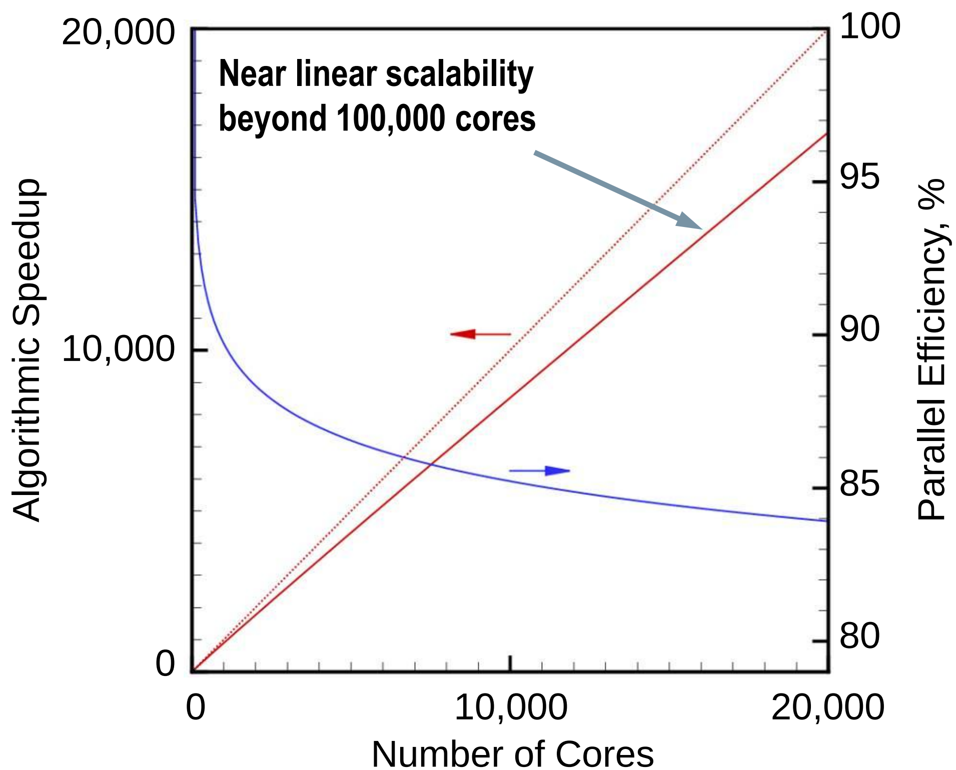
- Fuel streams are rapidly evolving
  - Heavy hydrocarbons
    - Oil sands
    - Oil shale
    - Coal
  - New renewable fuel sources
    - Ethanol
    - Biodiesel
    - Hydrogen
- New engine technologies require analysis at actual operating conditions, in actual geometries
  - Various direct injection (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

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



Strong scaling attributes exhibited by RAPTOR for typical IC-engine calculation

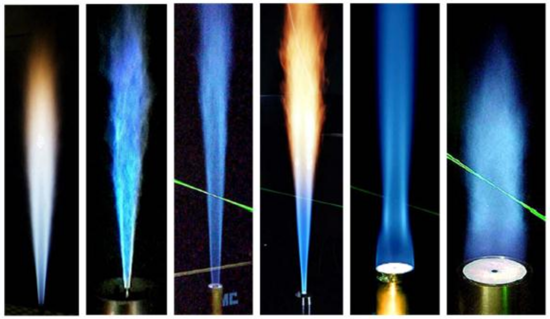


One of the first "capability-class" codes that handles relevant physics and geometry for ICE applications

Application of science-based LES bridges gap between science and applications

Basic — Unified Code Framework (RAPTOR) → Applied

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

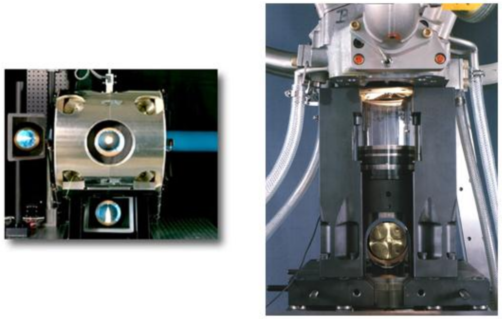


TNF Workshop
www.ca.sandia.gov/TNF

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

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



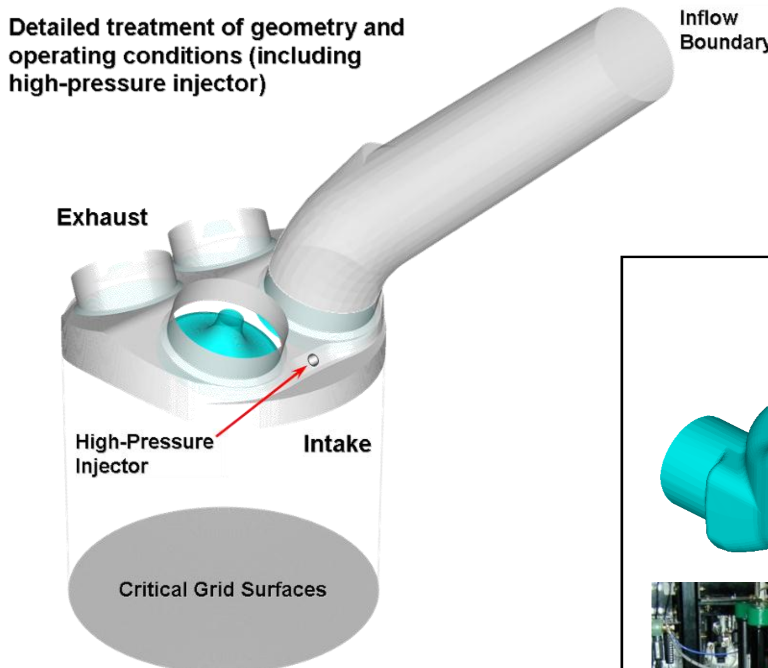
Engine Combustion Network
www.ca.sandia.gov/ECN

- **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 …

DOE Office of Vehicle Technologies funded research focuses on model development for IC engines

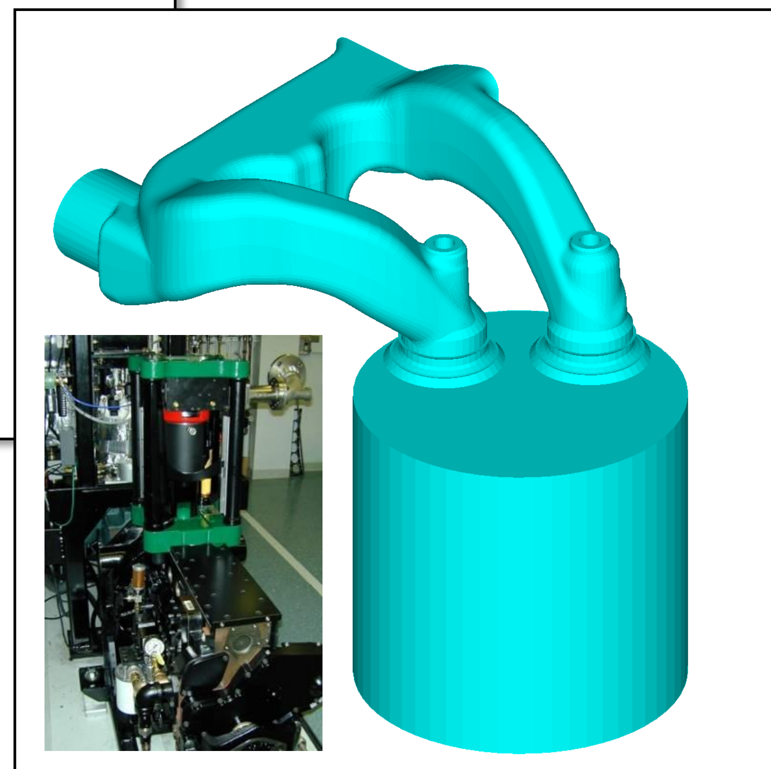
Engine Specifications

Compression Ratio	9 – 12
Bore	92 *mm*
Stroke	85 *mm*
Peak Turbulence Intensity	2.85 *m/s*
Integral Length Scale	2 *mm*
Thermal Layer Thickness	6.3 μm
Kolmogorov Length Scale	5.6 μm
Reaction Zone Thickness	3.9 μm
Turbulent Reynolds Number	2550

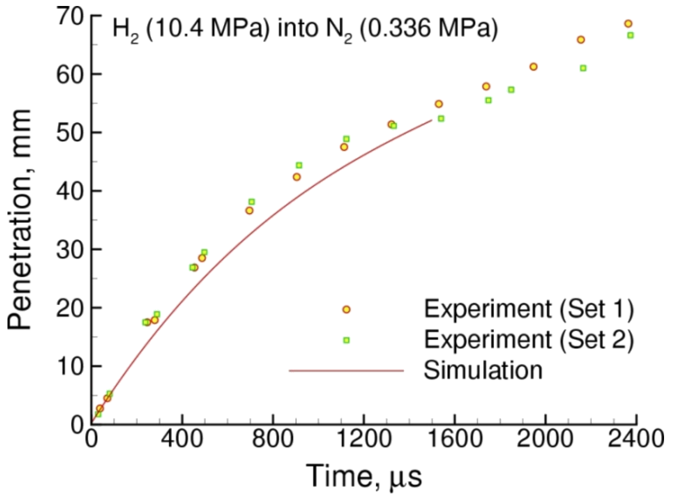


CRF Direct-Injection Hydrogen-Fueled IC Engine (Kaiser et al.)

CRF HCCI Engine (Dec et al.)

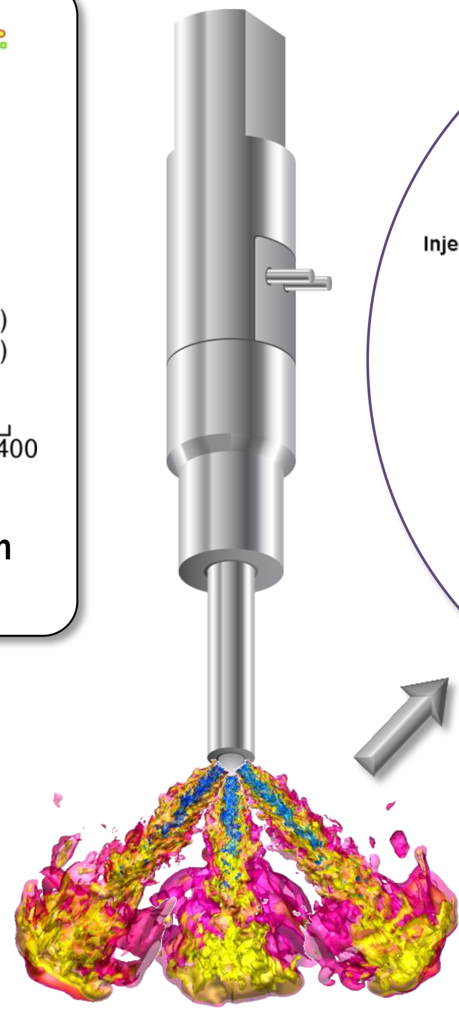


Rigorous validation of high-pressure, high-Reynolds-number fuel injection is prerequisite

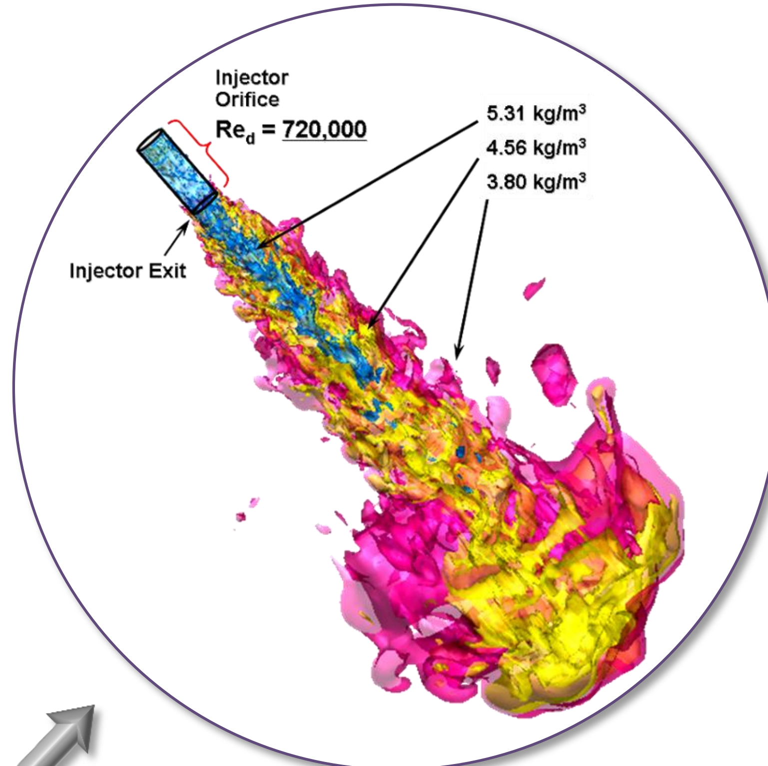


Representative comparison of LES with penetration measurements

Shadowgraph (U. Wisconsin)



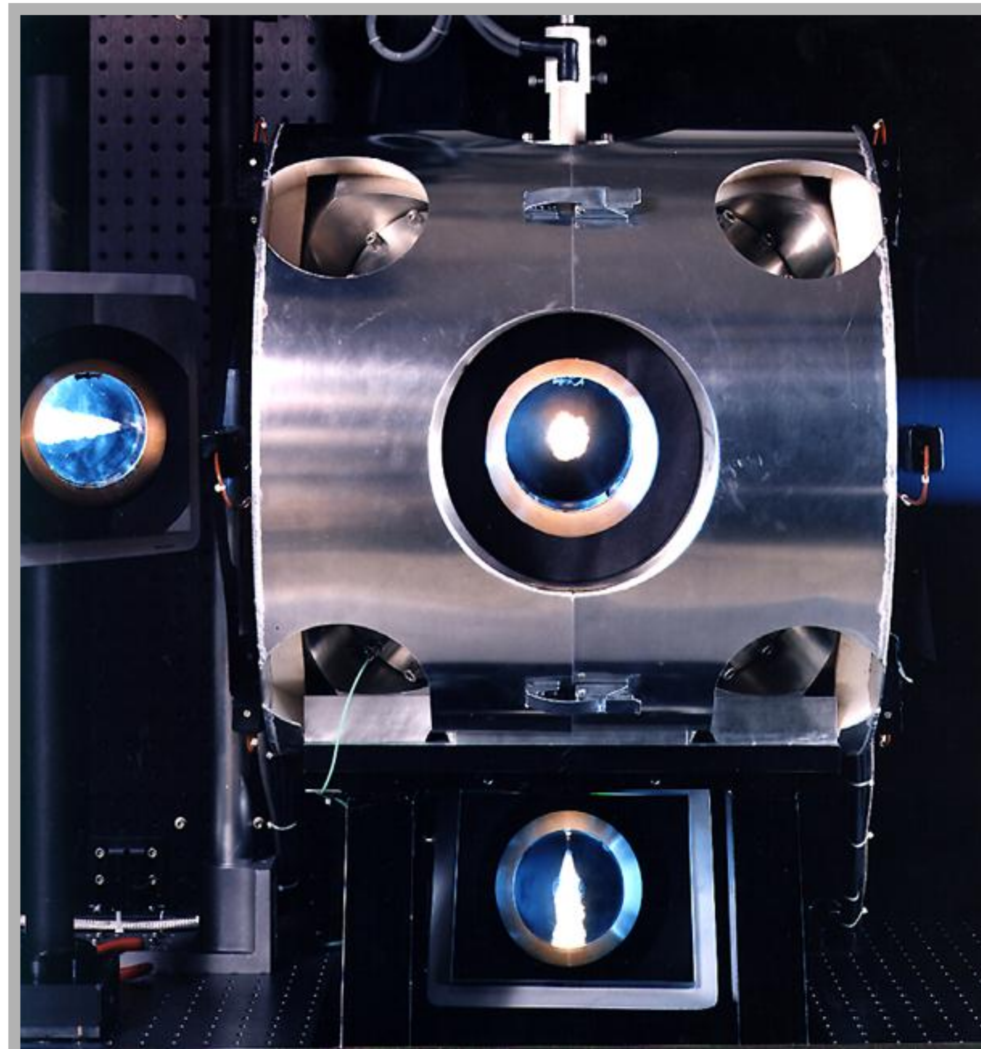
Large Eddy Simulation



Iso-Contours of Density ($H_2 - N_2$)	
Orifice diameter	0.8 mm
Injection pressure	10.4 MPa
Injection temperature	298 K
Chamber pressure	0.336 MPa
Chamber temperature	298 K

Sandia high-pressure combustion vessel provides experimental data

Designed to emulate engine conditions (diesel, gasoline)



Peak Injection Conditions

Fuel pressure: 2000 *bar*
(diesel, gasoline, biofuels)

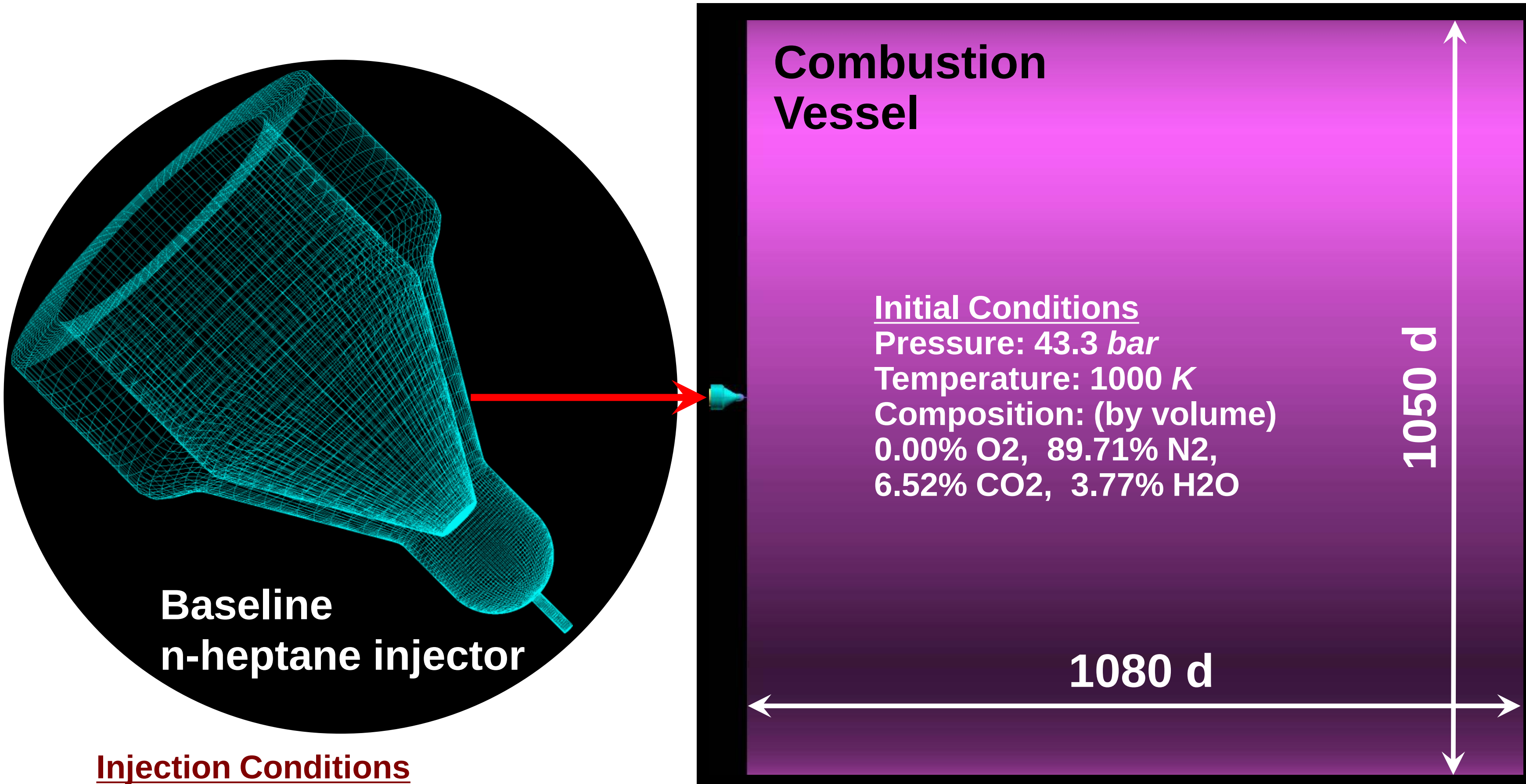
Peak Chamber Conditions

Pressure: 350 *bar*
Temperature: 1300 *K*
Composition: 0 – 21% O_2

Available Data

Internal injector geometry
Rate of injection
Liquid length versus time
Vapor penetration versus time
Rayleigh scattering images
Schlieren movies

LES performed at identical conditions



Injection Conditions

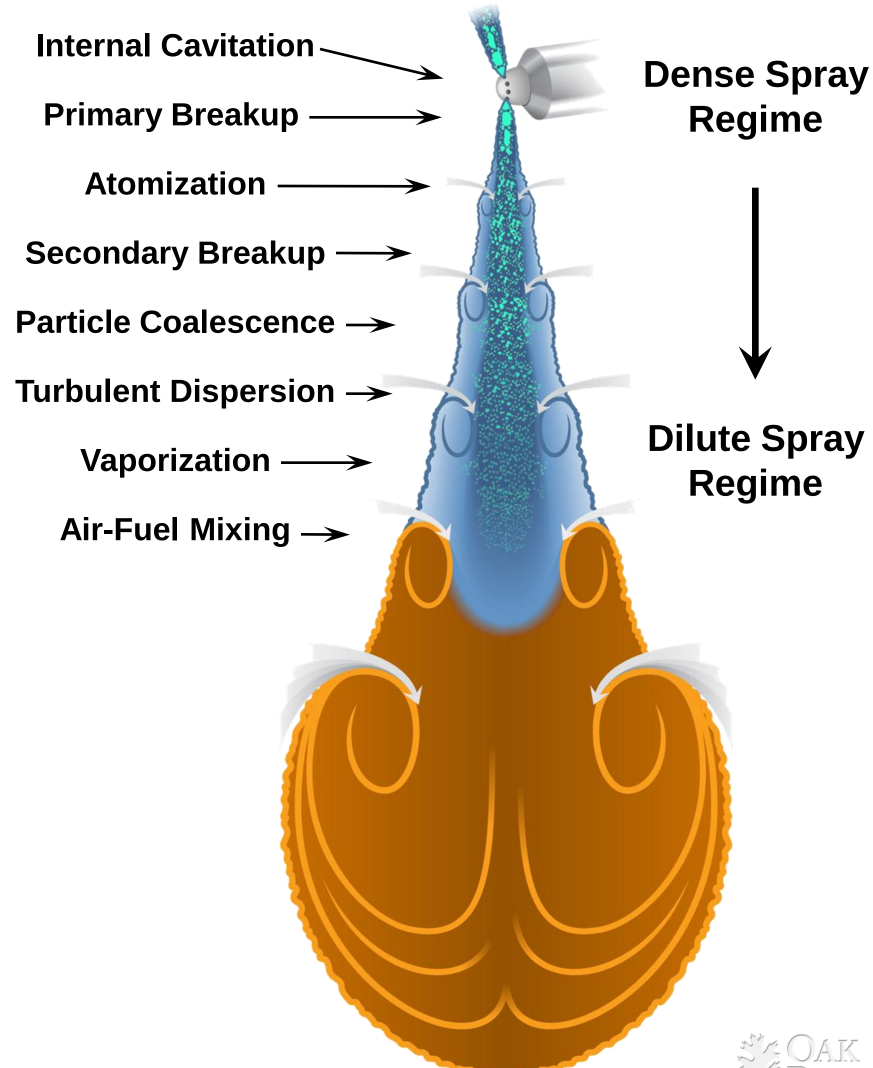
Density:	**620** kg/m^3
Temperature:	**373** K
Peak Velocity:	**554** m/s
Orifice Diameter:	**0.1** mm
Peak Re_d**:**	**150,000**

Computational Domain

- **Coupled effects of high-Reynolds number, high-pressure, and geometry**
- **12-million cells, 2 ns time-step, 10 ms duration**

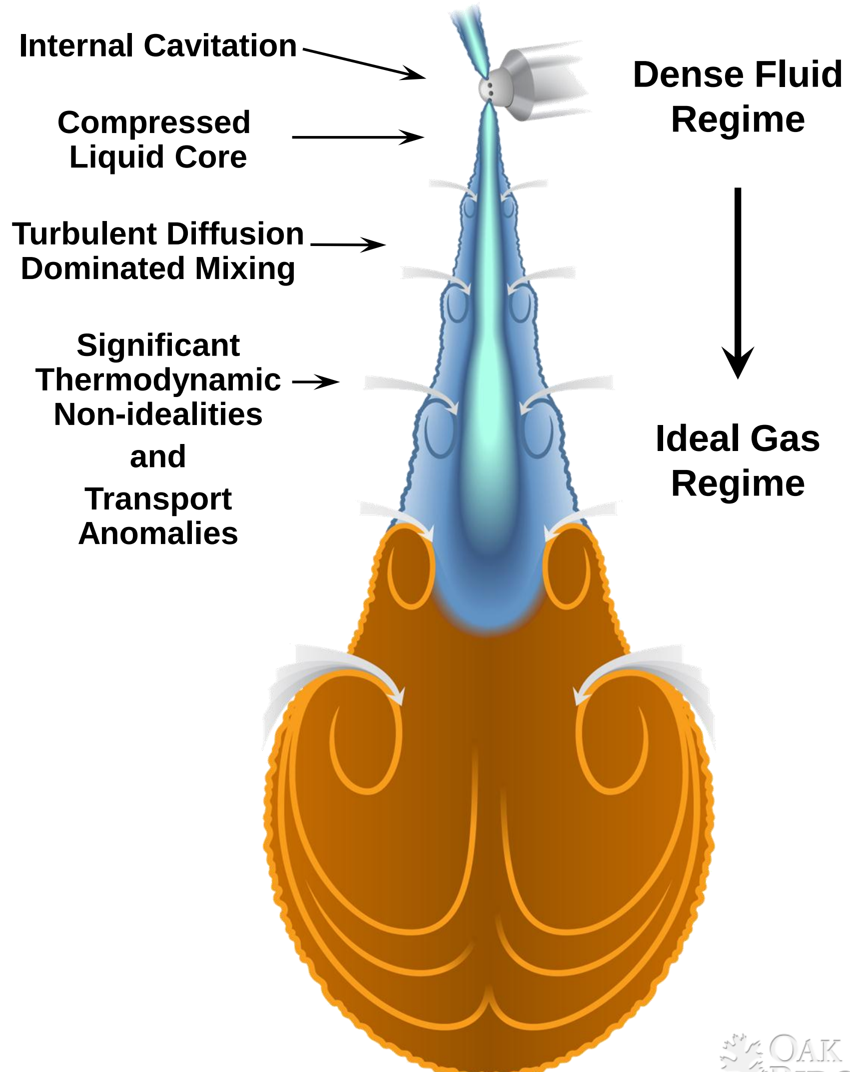
Injected liquid jets can exhibit different physics at high-pressures

- Subcritical Chamber Pressures (Diesel Engine Conditions)
  - Well defined interface separates the injected liquid from ambient gases due to the presence of surface tension
  - Dynamic shear forces and surface tension promote primary atomization and secondary breakup processes
  - Heterogeneous spray evolves from dense state (where liquid exists as sheets, filaments or lattices) to dilute state (where drop-drop interactions are negligible)

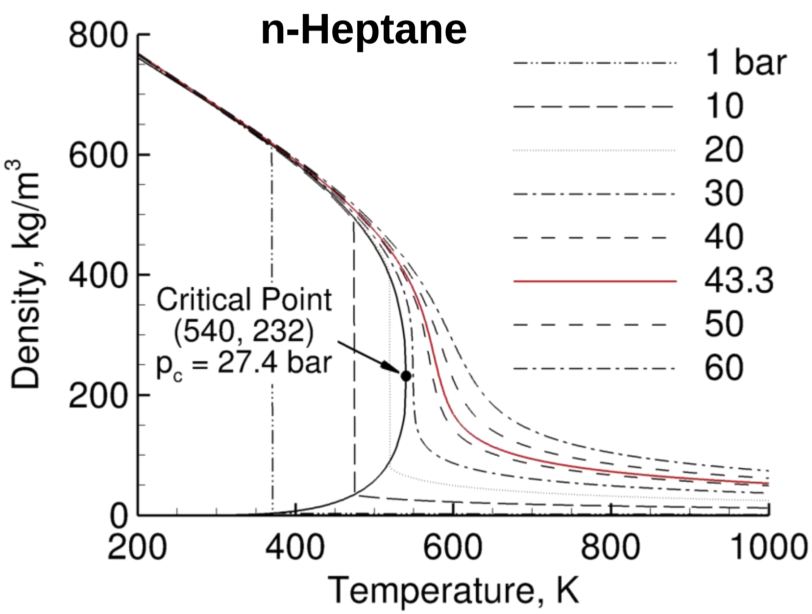


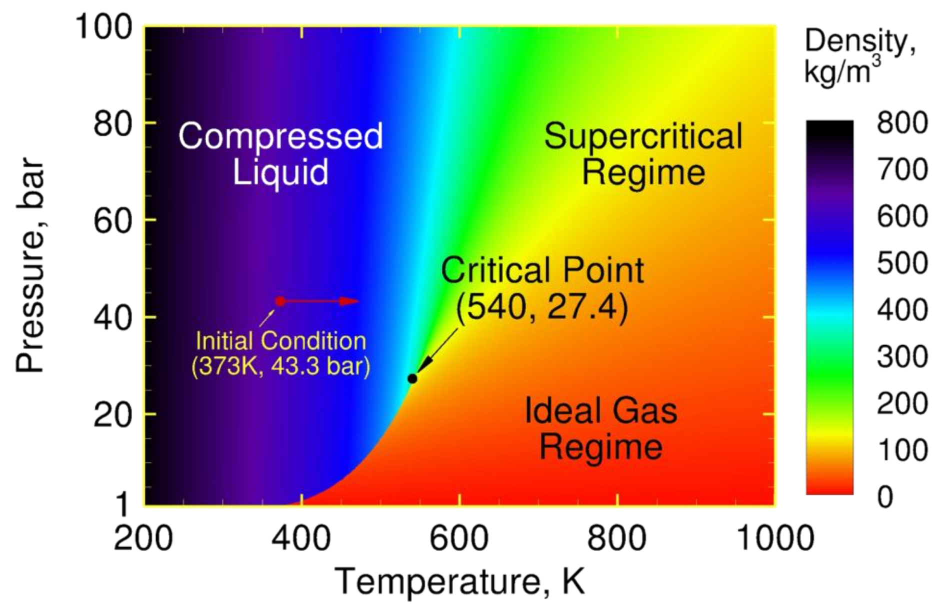
Injected liquid jets can exhibit different physics at high-pressures

- Supercritical Chamber Pressures (Diesel Engine Conditions)
  - Effects of surface tension become diminished and distinct gas-liquid interface does not exist
  - Injected jets undergo transcritical change of state as interfacial fluid temperatures rise above critical temperature
  - Lack of inter-molecular forces promote diffusion dominated mixing processes prior to atomization and jets evolve in the presence of large but continuous gradients



Detailed treatment of thermodynamics and transport required

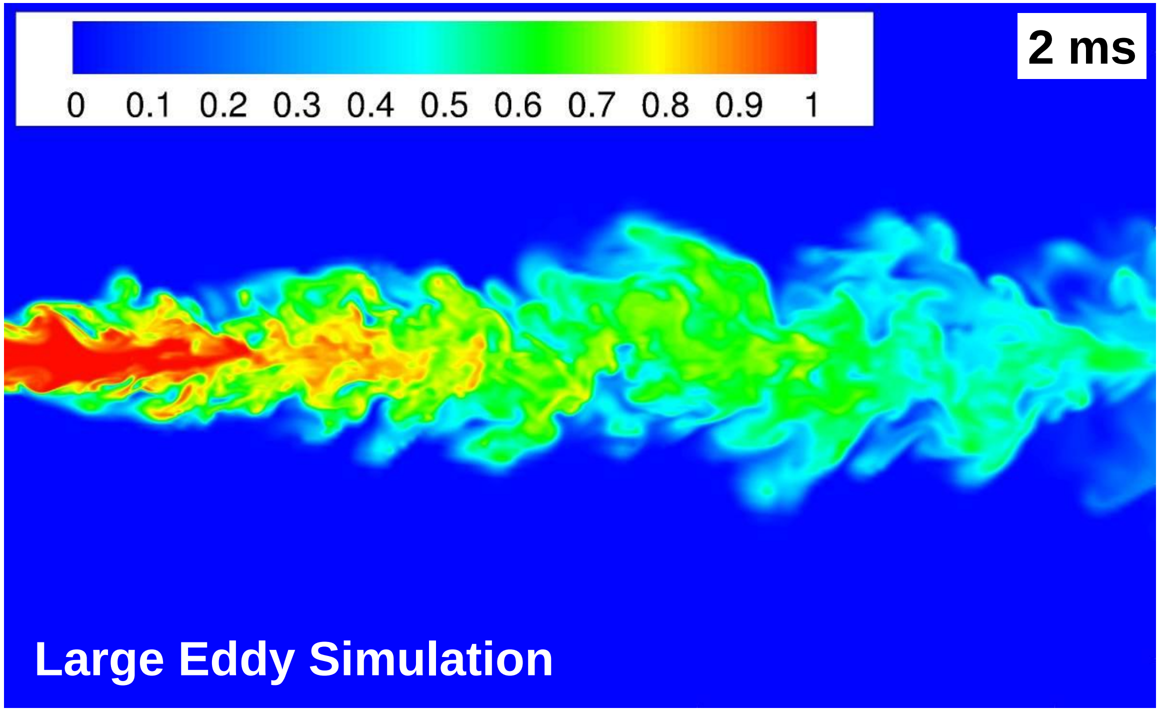


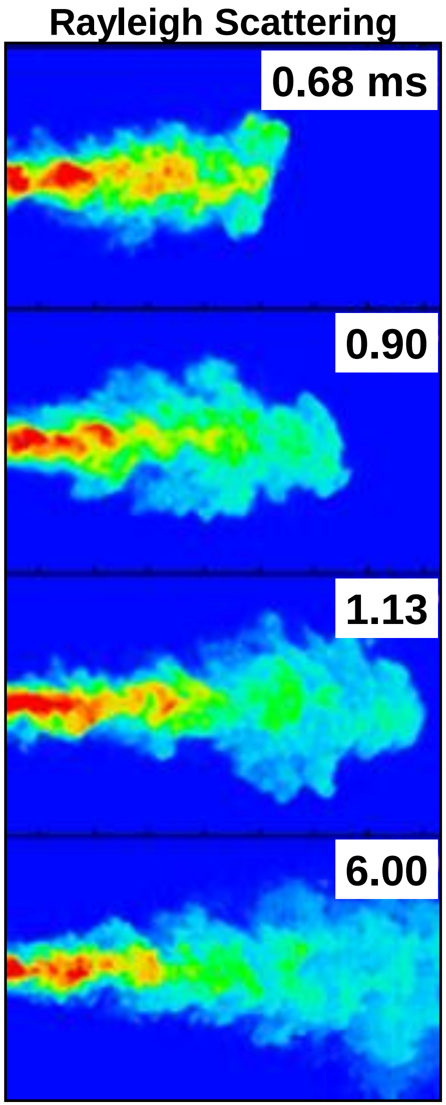


- Real fluid mixture properties obtained using extended corresponding states model
- Designed for arbitrary hydrocarbon mixtures (Fuel/Oxidizer/Products)
- Validated using NIST library, etc.

Oefelein, J. C. (2011). General package for evaluation of multicomponent real-gas and liquid mixture states at all pressures. SAND Report.

Joint analysis of numerical and experimental data provides revealing insights





<u>Available Data</u>

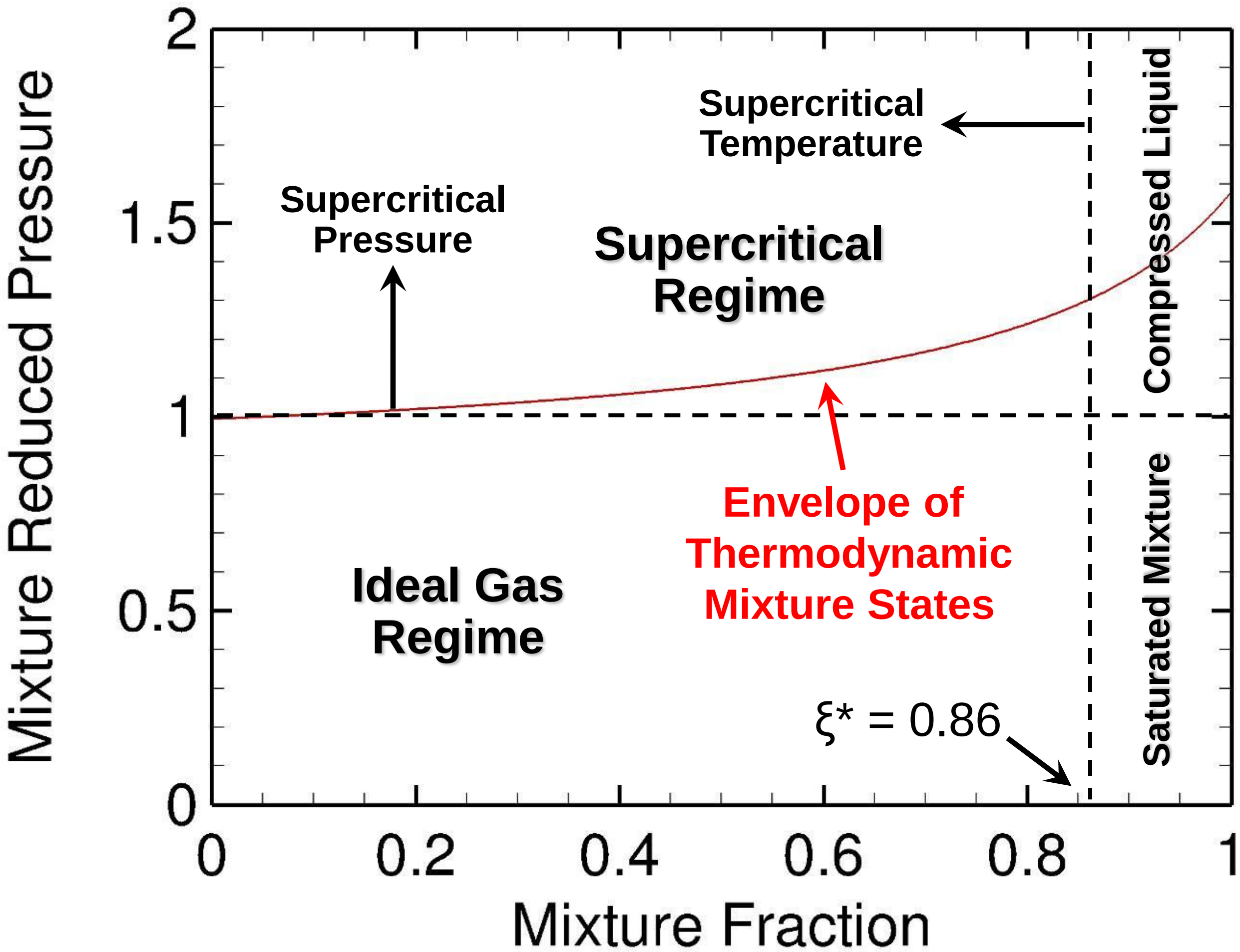
- Internal injector geometry
- Rate of injection
- Liquid length versus time
- Vapor length versus time
- Rayleigh scattering images
- Schlieren movies

Results raise questions regarding what is really being represented by widely used light-scatter measurements

Observations …

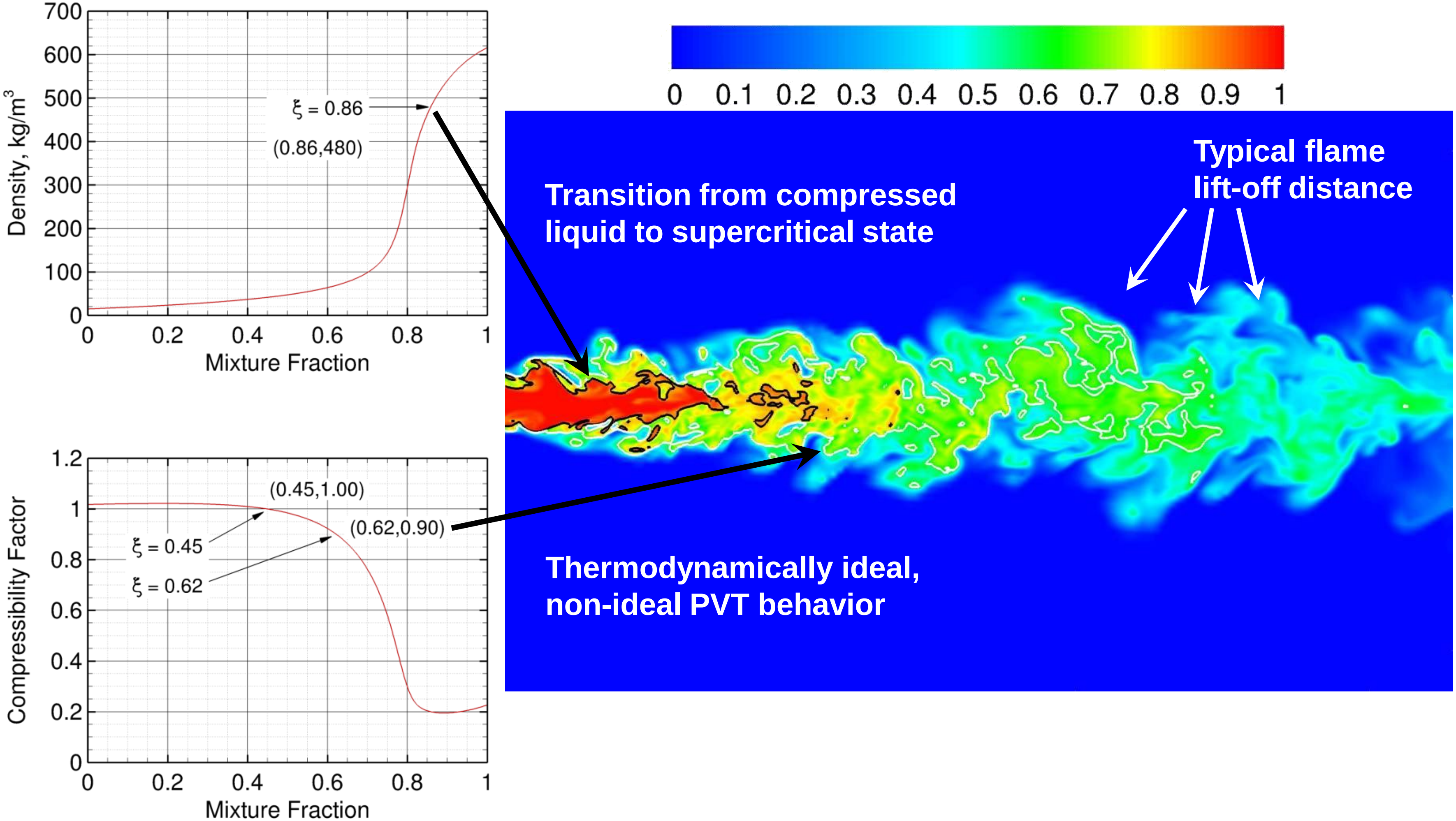
- **Model captures behavior of arbitrary multi-component mixtures at near-critical and supercritical conditions**
  - Data reveals that the envelope of mixture conditions varies from a compressed liquid to supercritical state
  - 1st order vapor-liquid phase transitions do not occur, which implies a distinct gas-liquid interface does not exist
  - Surface tension is diminished, lack of inter-molecular forces promotes diffusion dominated mixing prior to atomization
  - Jets evolve in the presence of exceedingly large but continuous thermo-physical gradients (i.e., 2nd order phase transitions)
- **Classical view of jet atomization and spray as appropriate model for <u>some</u> Diesel engines injection processes is questionable**

Envelope of mixture states mapped to thermodynamic regime diagram

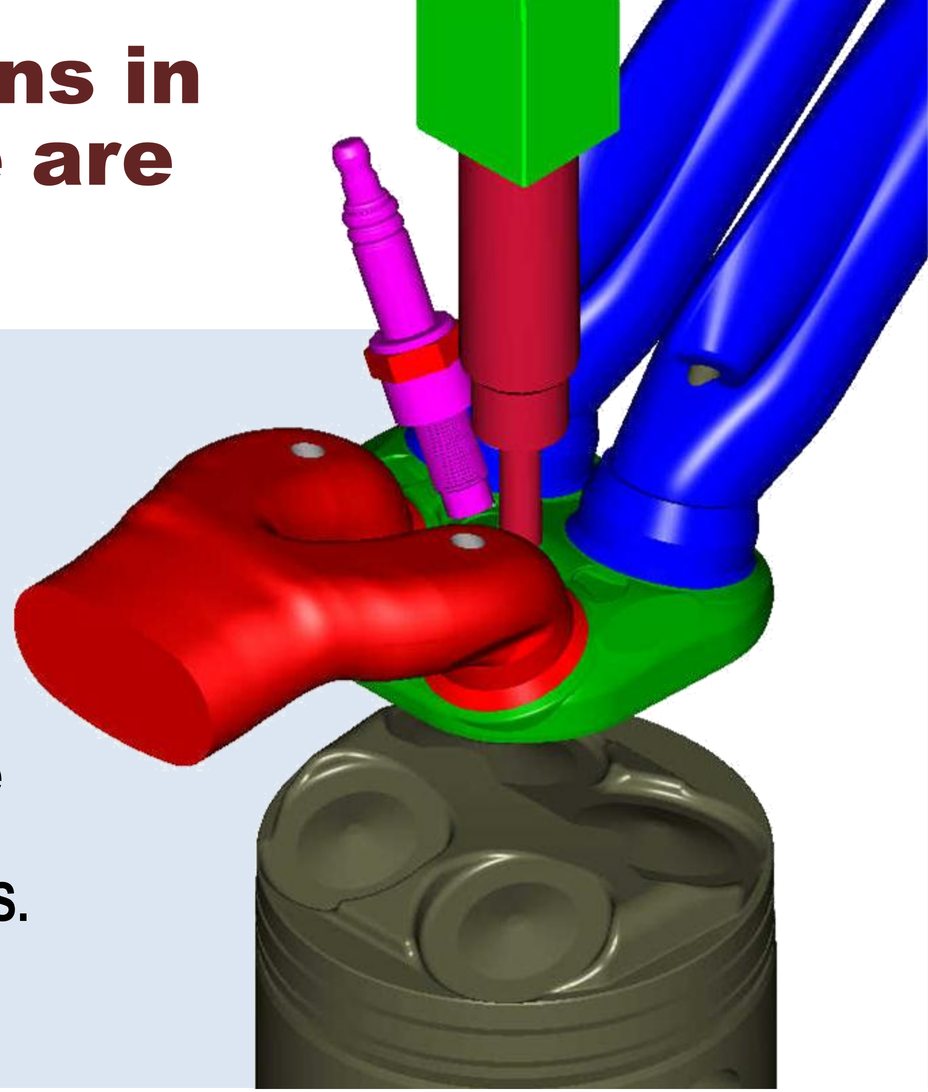


Mixing path never crosses liquid/vapor regime

Significant non-idealities associated with thermodynamics, transport



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

Support provided by the DOE Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program, the Oak Ridge National Laboratory National Center for Computational Sciences (ORNL NCCS), the DOE Office of Basic Energy Sciences, and the DOE Office of Vehicle Technologies is gratefully acknowledged

Contact

Joseph C. Oefelein

Principal Investigator
Combustion Research Facility
Sandia National Laboratories
Livermore, California 94551-9051
oefelei@sandia.gov

Ramanan Sankaran

Scientific Computing Liaison
National Center for Computational Sciences
Oak Ridge National Laboratory
sankaranr@ornl.gov