Project ID: ACE007

Large Eddy Simulation (LES) Applied to Advanced Engine Combustion Research

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Office of Energy Efficiency and Renewable Energy
Vehicle Technologies Program
is Gratefully Acknowledged

Overview

Timeline

- Project provides fundamental research that supports advanced engine development
- Focused on next generation simulation capabilities using Large Eddy Simulation (LES)
- Goal is to combine unique code and resources, maximize benefits of DOE "leadership" computers
- Project scope, direction and continuation evaluated annually

Budget

- Total Project Funding
  - FY11 – \$500K
  - FY12 – \$500K

Barriers

- Two sets of barriers addressed
  1 – Development of clean high-efficiency engines using hydrocarbon based fuels (petroleum and non-petroleum)
  – LTC technologies (i.e., understanding effects of fuel-injection, ignition-timing, heat-transfer and engine-geometry on fuel-air mixing, combustion, soot, emissions over broad operating ranges)
  2 – Requirements for efficient and routine use of high-performance computing (HPC), development of both predictive and affordable models for advanced engine combustion research

Partners

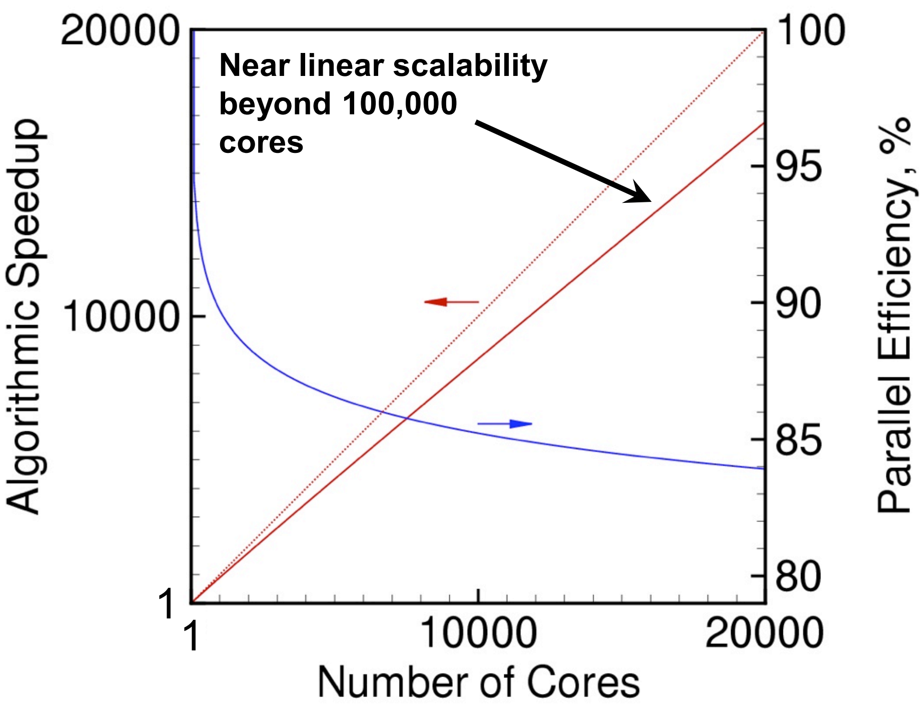
- PI's in the Engine Combustion Group at Sandia, Wisconsin, Penn State, Michigan
- ≈ 50 collaborators and institutions
- Project lead: Joe Oefelein

Objective … combine unique codes, resources to maximize benefits of HPC for AEC research

- **Apply unique high-fidelity simulation capability that complements development of engineering models and codes**
  - Advanced massively-parallel code framework
  - Access to full hierarchy of DOE computers
  - Direct coupling to key experiments
- **Provide strong link between basic and applied research**
  - Synergy between CRF SC-BES and EERE-VT programs
  - Access to DOE Office of Science (SC) supercomputer facilities
    - LBNL NERSC (www.nersc.gov)
    - ORNL NCCS (www.nccs.gov)
    - INCITE program (… Innovative and Novel Computational Impact on Theory and Experiment)
- **Facilitate detailed model development using high-fidelity benchmarks in concert with experiments**
  - Dedicated facilities, resources and collaborative interactions
  - Targeted milestones aimed at priority research directions

Theoretical-Numerical Framework
(RAPTOR: A general solver optimized for LES)

- **Theoretical framework … (Comprehensive physics)**
  - Fully-coupled, compressible conservation equations
  - Real-fluid equation of state (high-pressure phenomena)
  - Detailed thermodynamics, transport and chemistry
  - Multiphase flow, spray
  - Dynamic SGS modeling (no tuned constants)
- **Numerical framework … (High-quality numeric's)**
  - Dual-time stepping with generalized preconditioning (all-Mach-number formulation)
  - Staggered finite-volume differencing (non-dissipative, discretely conservative)
  - Massively-parallel
- **Extensively validated, ported to all major platforms**



- **Strong (fine-grain) scaling attributes exhibited on the ORNL OLCF CRAY XT system (Jaguar)**
  - Single block, 1.28-million cells
  - 20,000 blocks with 4^3 cells
- **Weak (coarse-grain) scaling on 150,000 cores benchmarked as part of DOE 2009 Joule Code Metric**

Supporting resources

- Combustion Research and Computational Visualization Facility
  - 2000 sq-ft computer room, visualization suite, office/visitor space
  - Mid-scale clusters and file-systems
- Lawrence Berkeley National Laboratory
  - NERSC platforms (BES research)
- Oak Ridge National Laboratory
  - OLCF platforms (VTP research)
- INCITE Grant (3-years, renewable)
  - Innovative and Novel Computational Impact on Theory and Experiment
  - High-Fidelity Simulations for Advanced Engine Combustion Research
    - 60-million CPU-HRS on Jaguar in 2011
    - 65-million in 2012

BES midscale computer upgrade (50 TF, 600 TB storage)

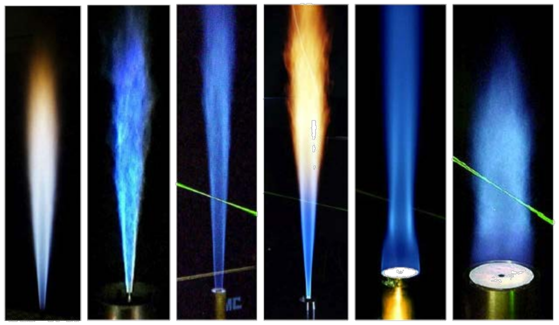
Image courtesy of Oak Ridge National Laboratory

(2.33 PF, 224,256 cores)

Approach … bridge gap between basic and applied research

Basic — Unified Code Framework (RAPTOR) → **Applied**

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

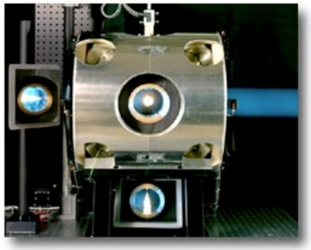


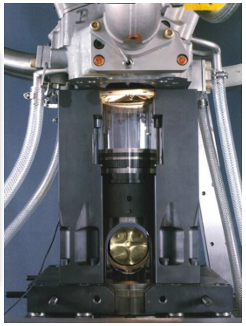
TNF Workshop
www.ca.sandia.gov/TNF

Detailed jet flame data for model development but low Reynolds number and simple fuels

Extensive device relevant measurements but limited due to complex geometry, flow and fuels

LES Applied to Low-Temperature and Diesel Engine Combustion Research
DOE Vehicle Technologies Program





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

- Direct coupling of LES to key target experiments (anchor)
  - High-fidelity simulations that match geometry, operating conditions
  - Validation, then joint analysis …
    - Fundamental insights not available from experiments alone
    - Data reduction aimed at affordable models for engineering
- Work toward predictive models at device relevant conditions
  - High-pressure, low-temperature, multiphase flow and combustion, …

Milestones … have been synchronized with DOE INCITE grants

- Primary focal point … detailed simulation and analysis of direct injection processes with emphasis on ECN experiments
  - Close collaboration with Pickett et al.
  - Target cases: Baseline n-Heptane, Spray-A (n-Dodecane)
  - Fundamentals of liquid-injection at high-pressure conditions
- Additional focal points …
  - Toward LES of combustion processes in HCCI engines at operating conditions identical to the experiment of Dec et al. (August 2012)
    - Development of optimal grid generation capabilities in progress
  - Participate in collaborative activities with industrial consortium on priority research defined in the PreSICE report (Quarterly FY12)
    - Focus on two central issues: 1) the dynamics of fuel injection and sprays, and 2) cycle-to-cycle variation and stochastic nature of in-cylinder flows

Sandia-CRF high-pressure combustion vessel (Pickett et al.)

<u>Peak Injection Conditions</u>

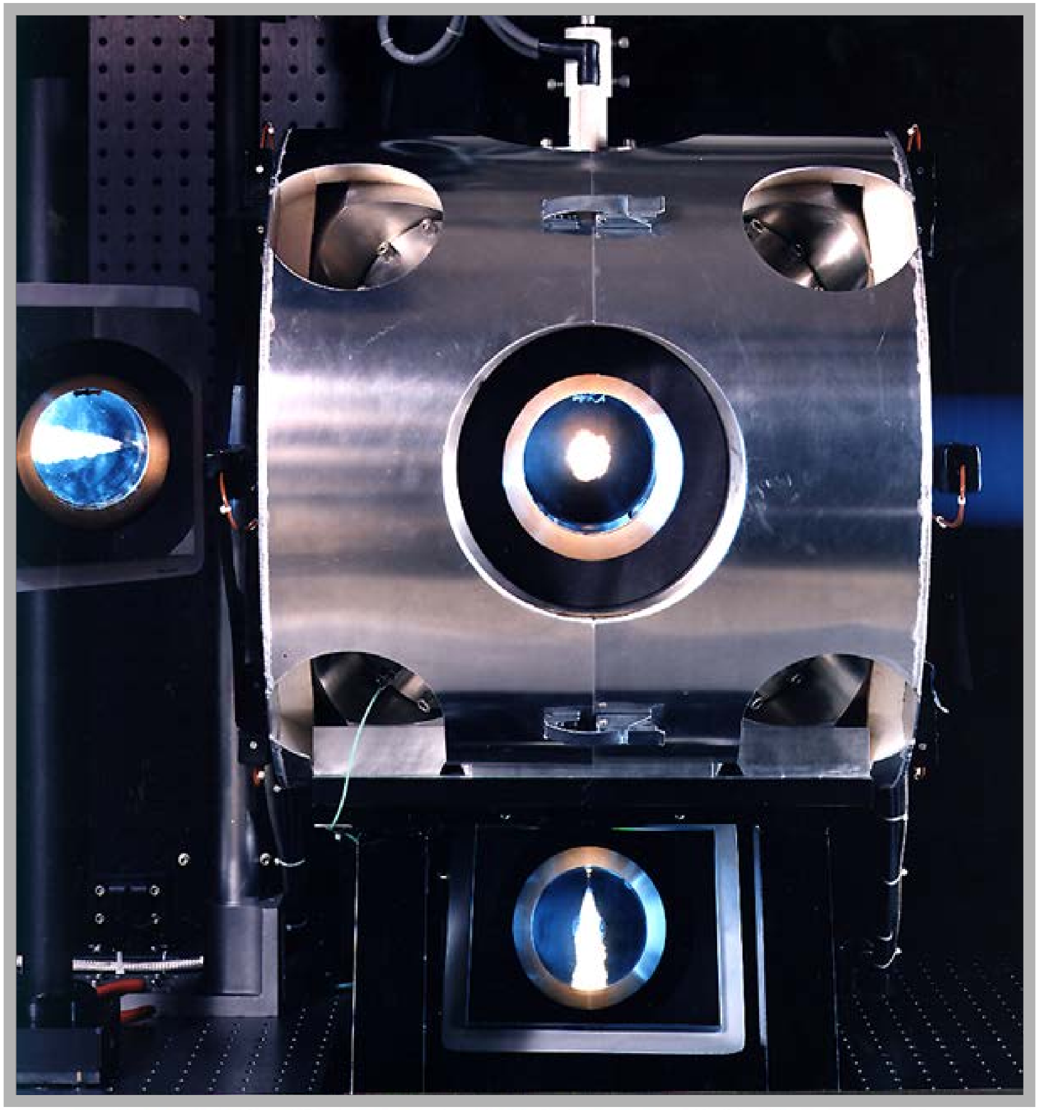
Fuel pressure: 2000 *bar*
(diesel, gasoline, biofuels)

<u>Peak Chamber Conditions</u>

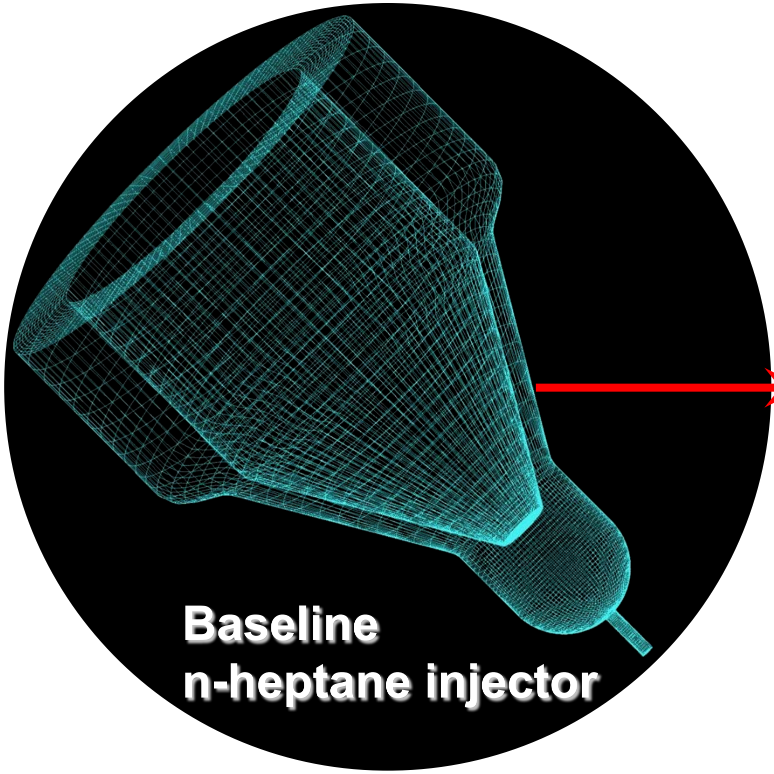
Pressure: 350 *bar*
Temperature: 1300 *K*
Composition: 0 – 21% O_2

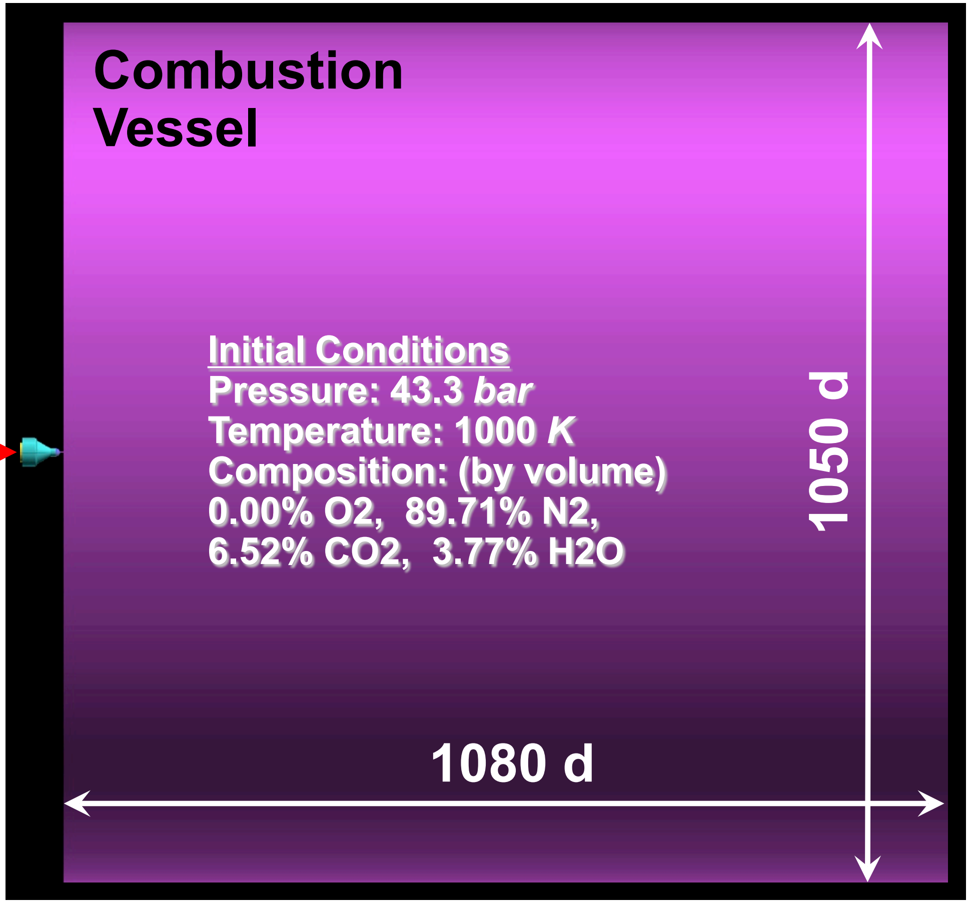
<u>Available Data</u>

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



LES at identical conditions …



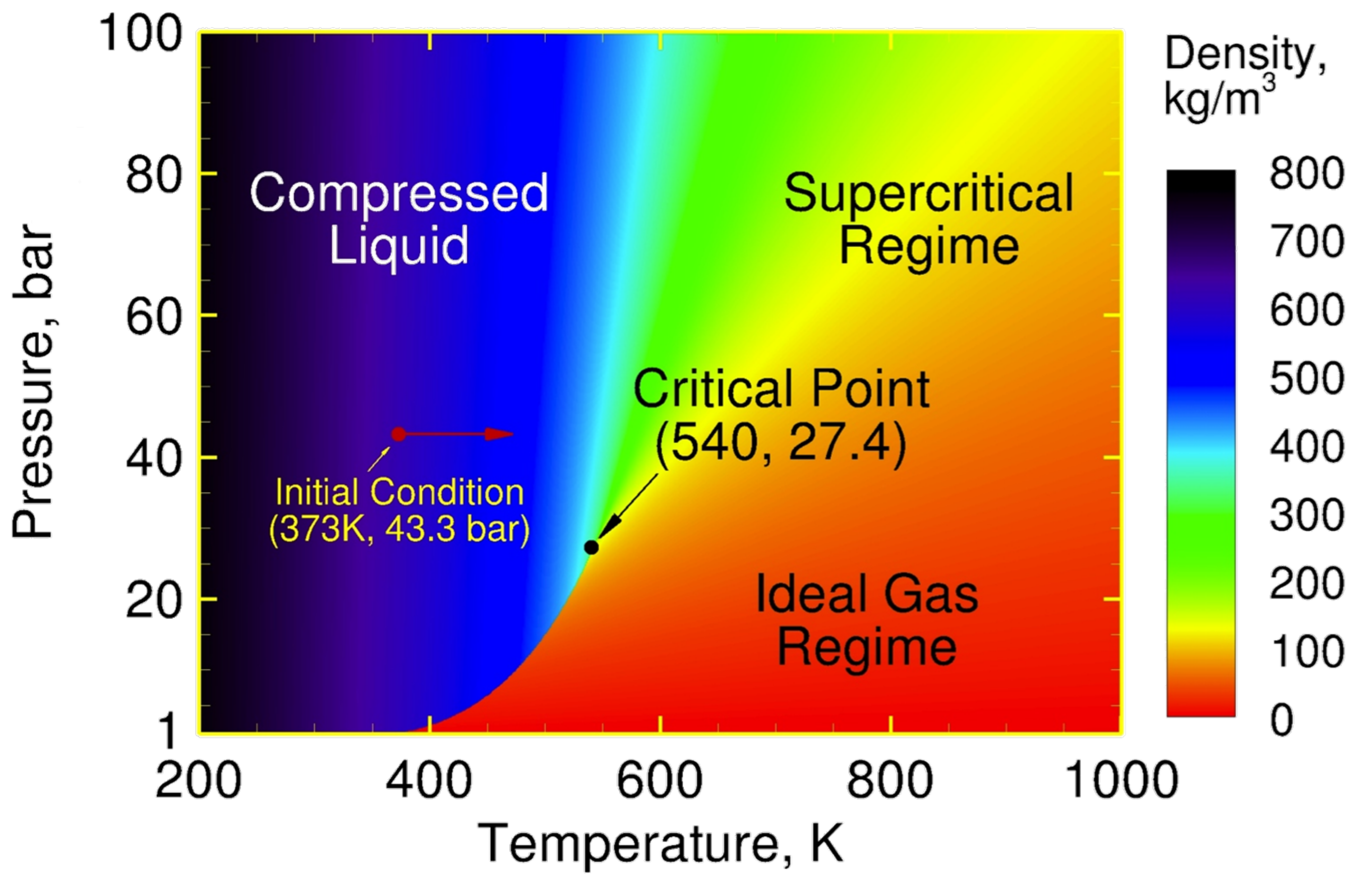


Computational Domain

Injection Conditions

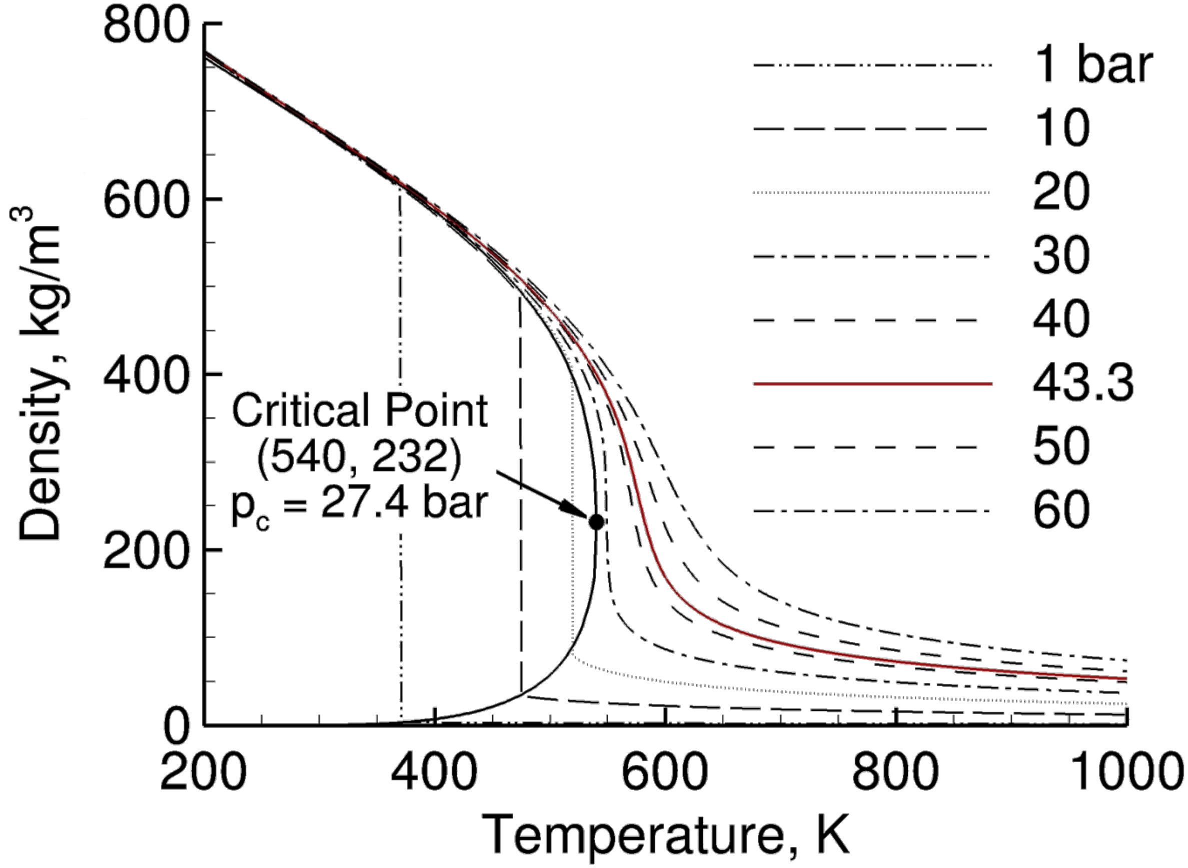
Density:	620 kg/m^3
Temperature:	373 K
Peak Velocity:	554 m/s
Orifice Diameter:	0.1 mm
Peak Re_d:	150,000

Thermodynamic considerations



n-Heptane is being injected as a compressed liquid at supercritical pressure

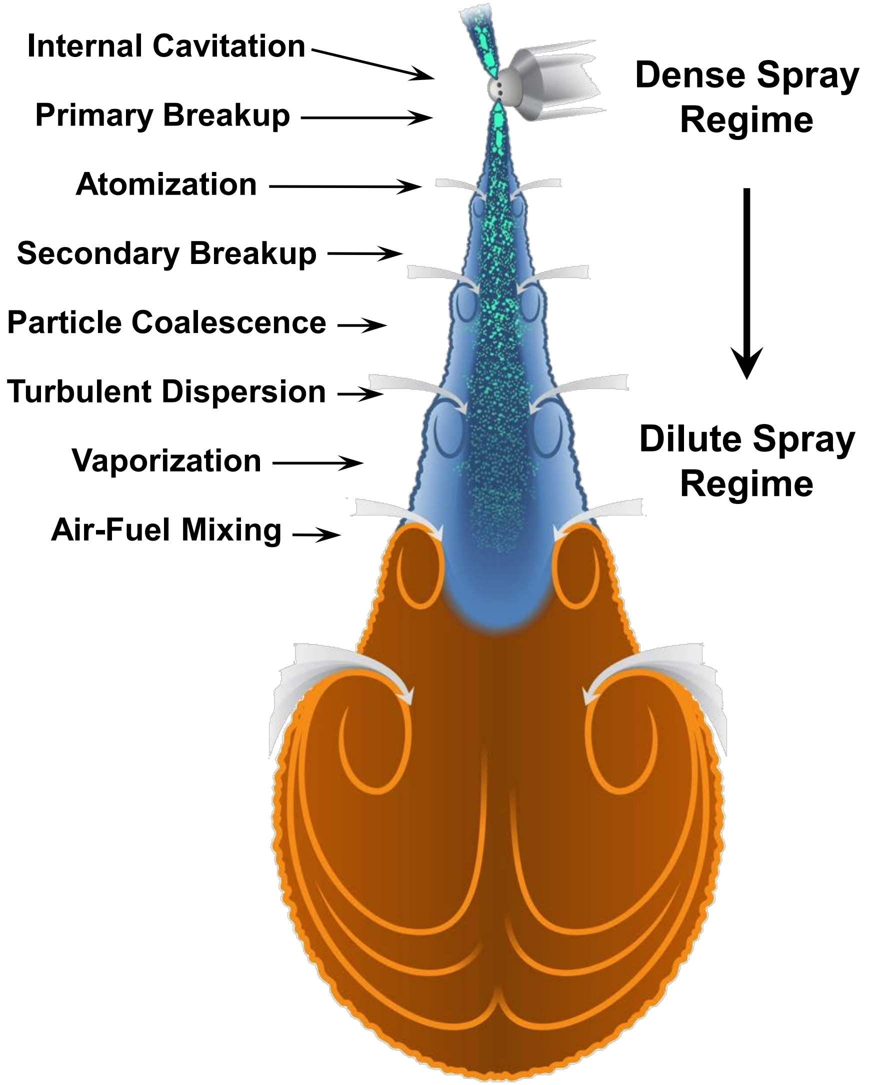
Thermodynamic considerations



n-Heptane is being injected as a compressed liquid at supercritical pressure

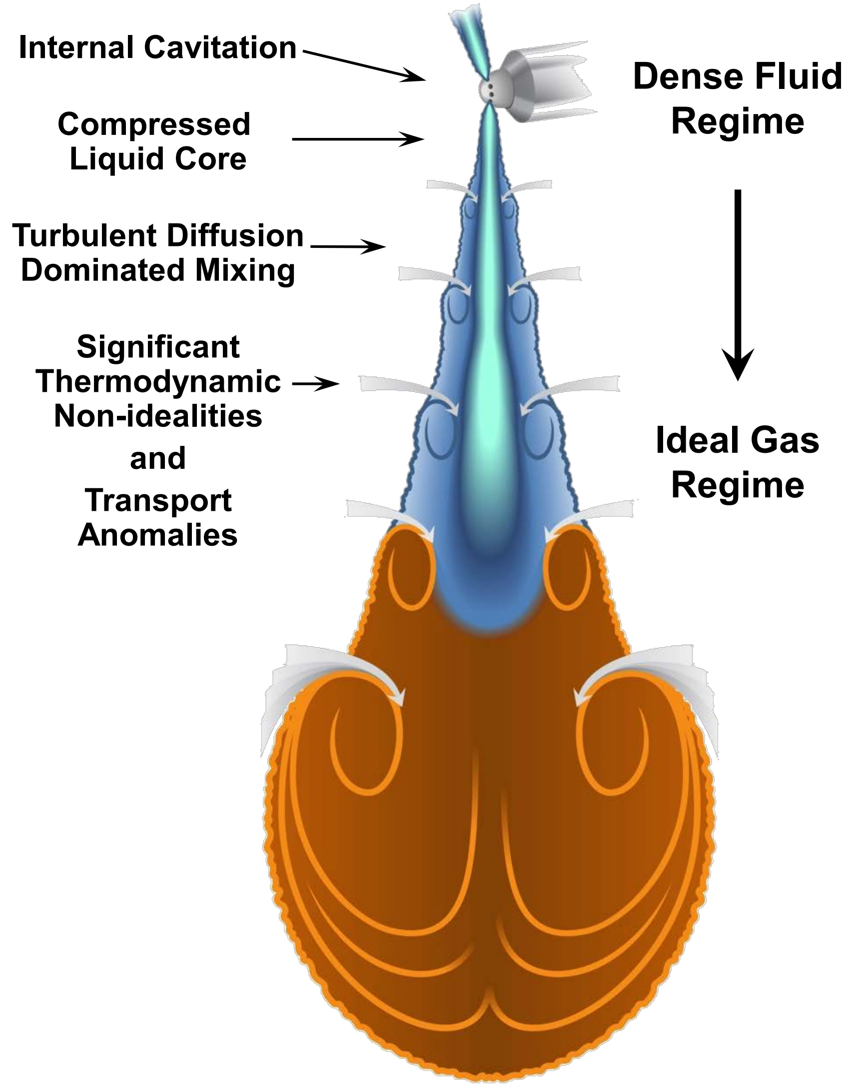
Injection of liquid fuel at high-pressure conditions is not well understood

- **Subcritical Cylinder Pressures**
  - Well-defined molecular interface separates the injected liquid from ambient gases due to the presence of surface tension
  - Interactions between dynamic shear forces and surface tension promote primary atomization and secondary breakup processes
  - Resultant spray evolves from a dense state, where the liquid exists as sheets filaments or lattices; to a dilute state, where drop-drop interactions are negligible and dilute particle theory applies



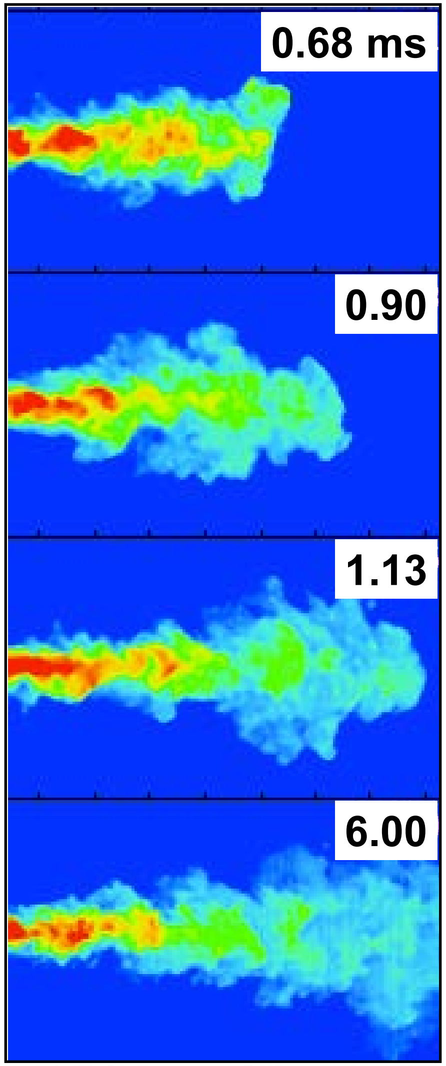
Injection of liquid fuel at high-pressure conditions is not well understood

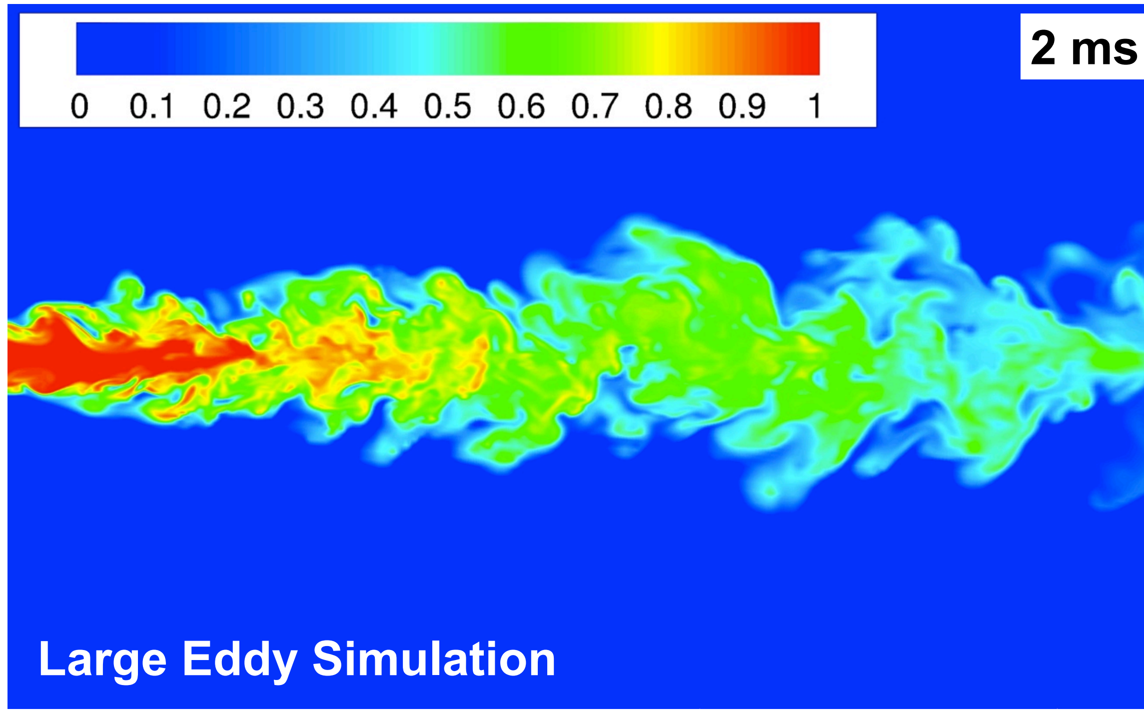
- **Supercritical Cylinder Pressures**
  - Interfacial diffusion layers develop as a consequence of vanishing surface tension forces and broadening gas-liquid interfaces
  - Lack of inter-molecular forces promotes diffusion dominated mixing processes prior to atomization
  - As a consequence, injected jets can potentially evolve in the presence of exceedingly large (but continuous) thermo-physical gradients in a manner that is markedly different from the classical assumptions



To investigate, we apply a real-fluid model with detailed thermo, transport

Rayleigh Images



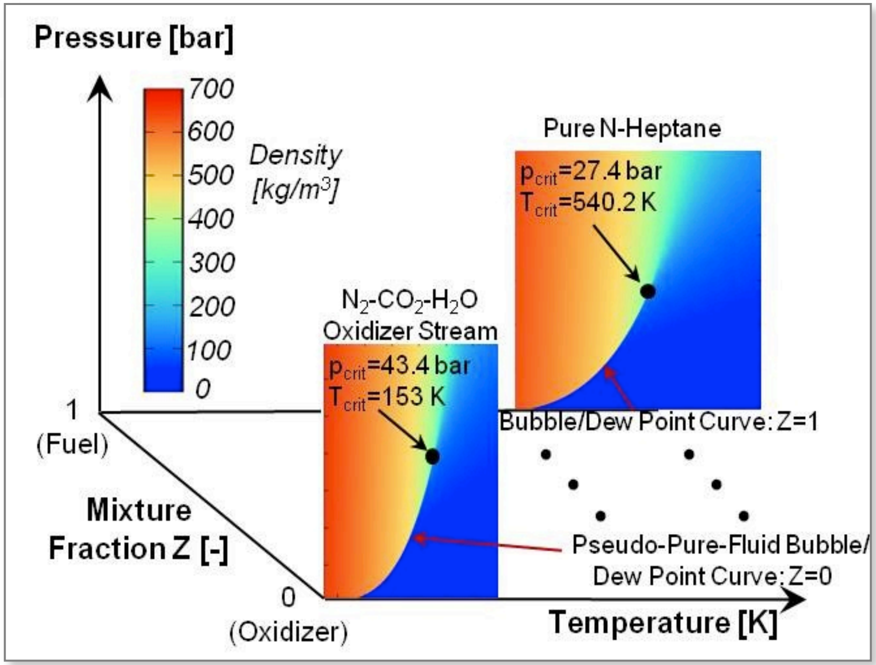


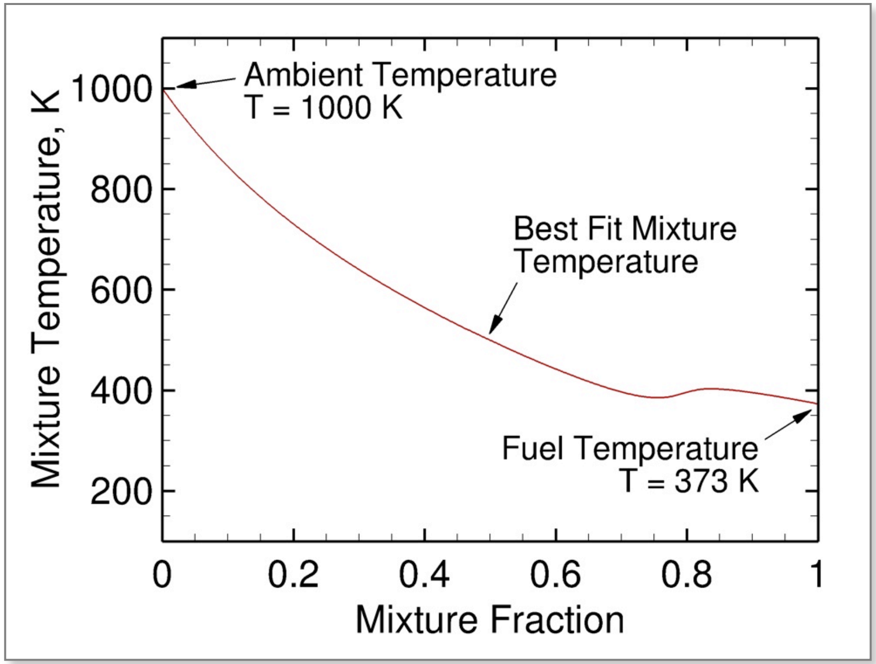
Available Data

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

Results have raised many questions that are now being jointly investigated through an optimal combination of LES, theory, and experimental observations

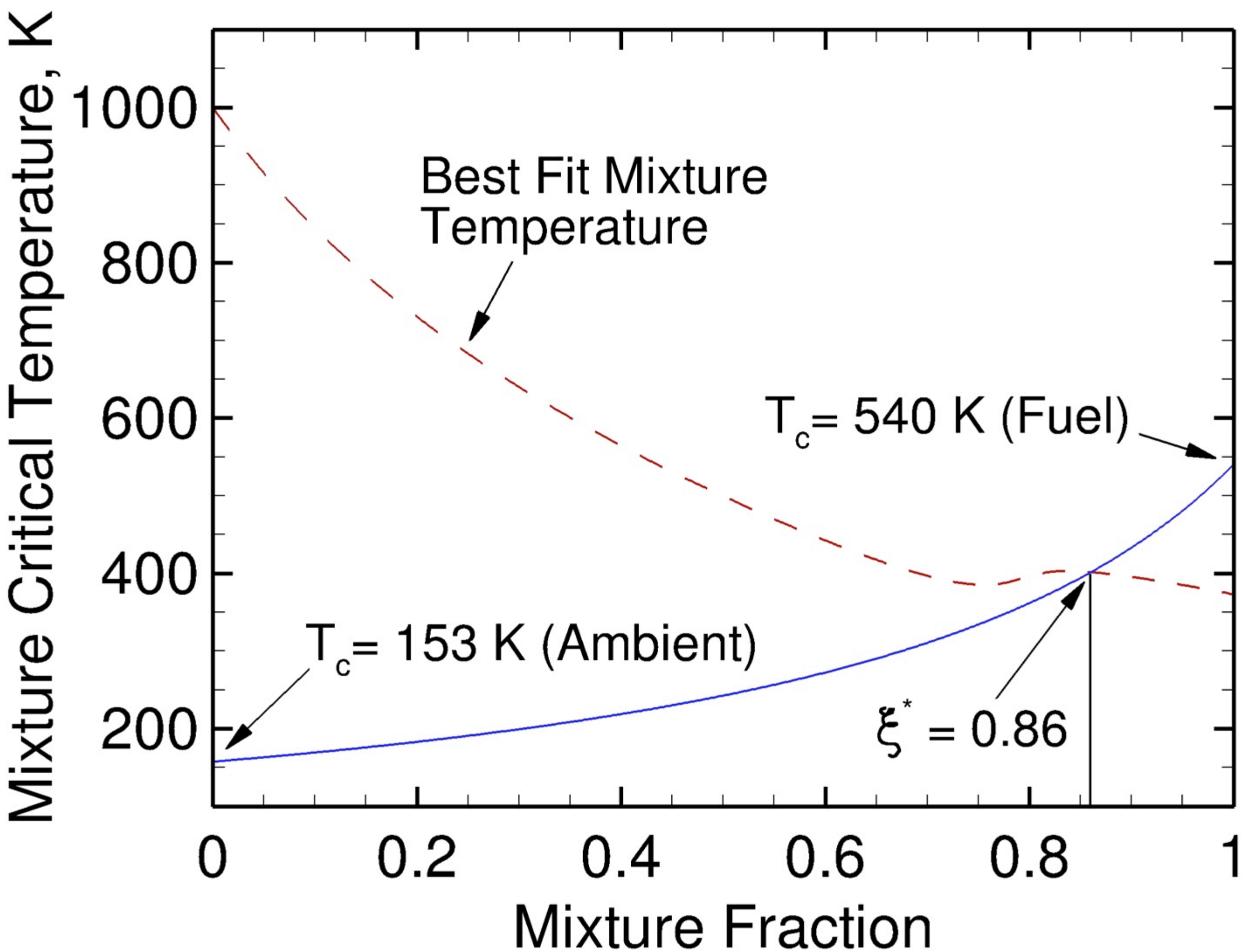
High-fidelity LES facilitates detailed analysis of mixture states



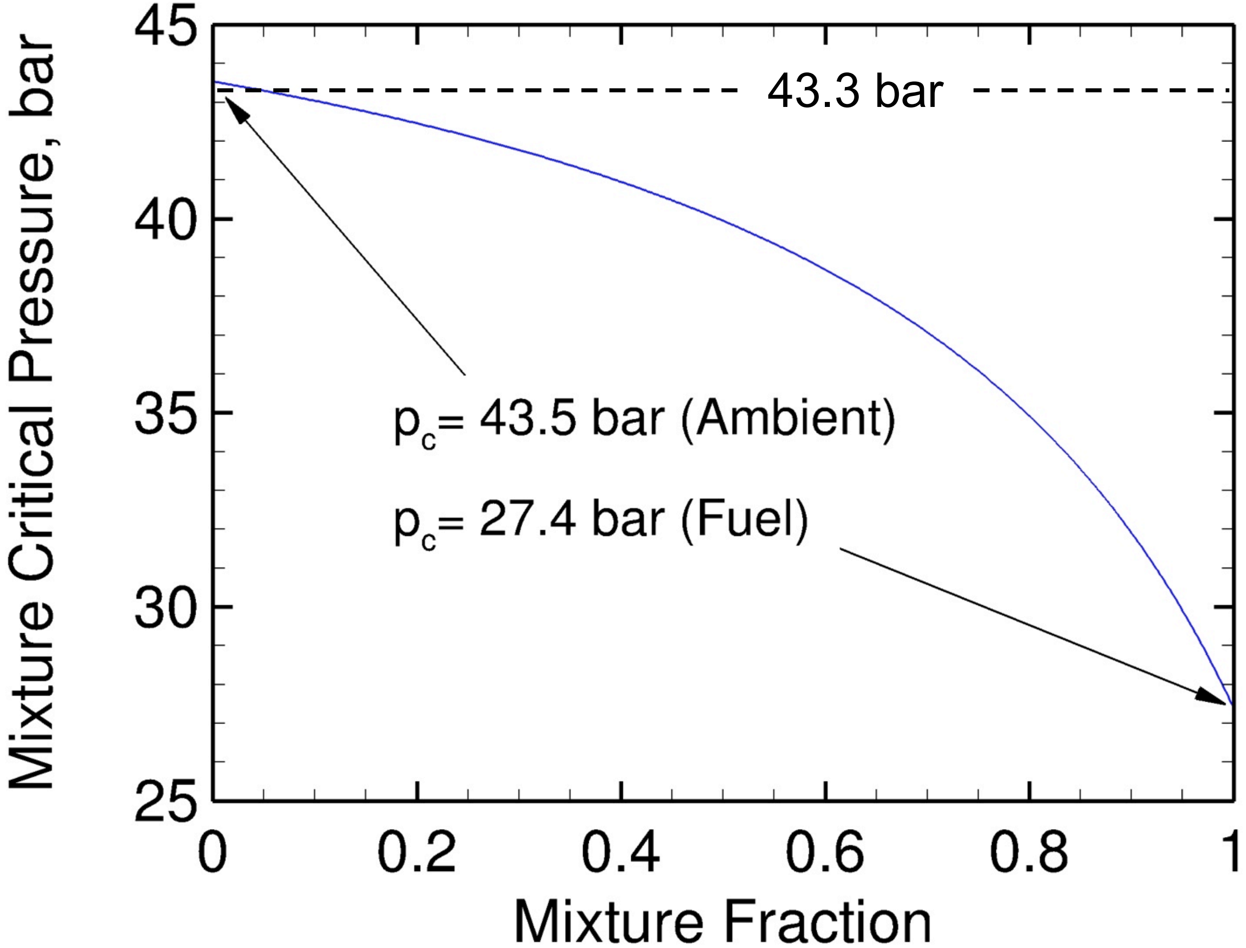


- Introduce mixture fraction variable to analyze local instantaneous mixture states
  - ξ= 0 refers to "oxidizer" (N2-CO2-H2O)
  - ξ= 1 refers to fuel (C7H16)
- Scatter data of temperature conditioned on mixture fraction processed from LES
  - Maps temperature of local multicomponent mixture to mixture fraction
  - Facilitates development of thermodynamic regime diagram

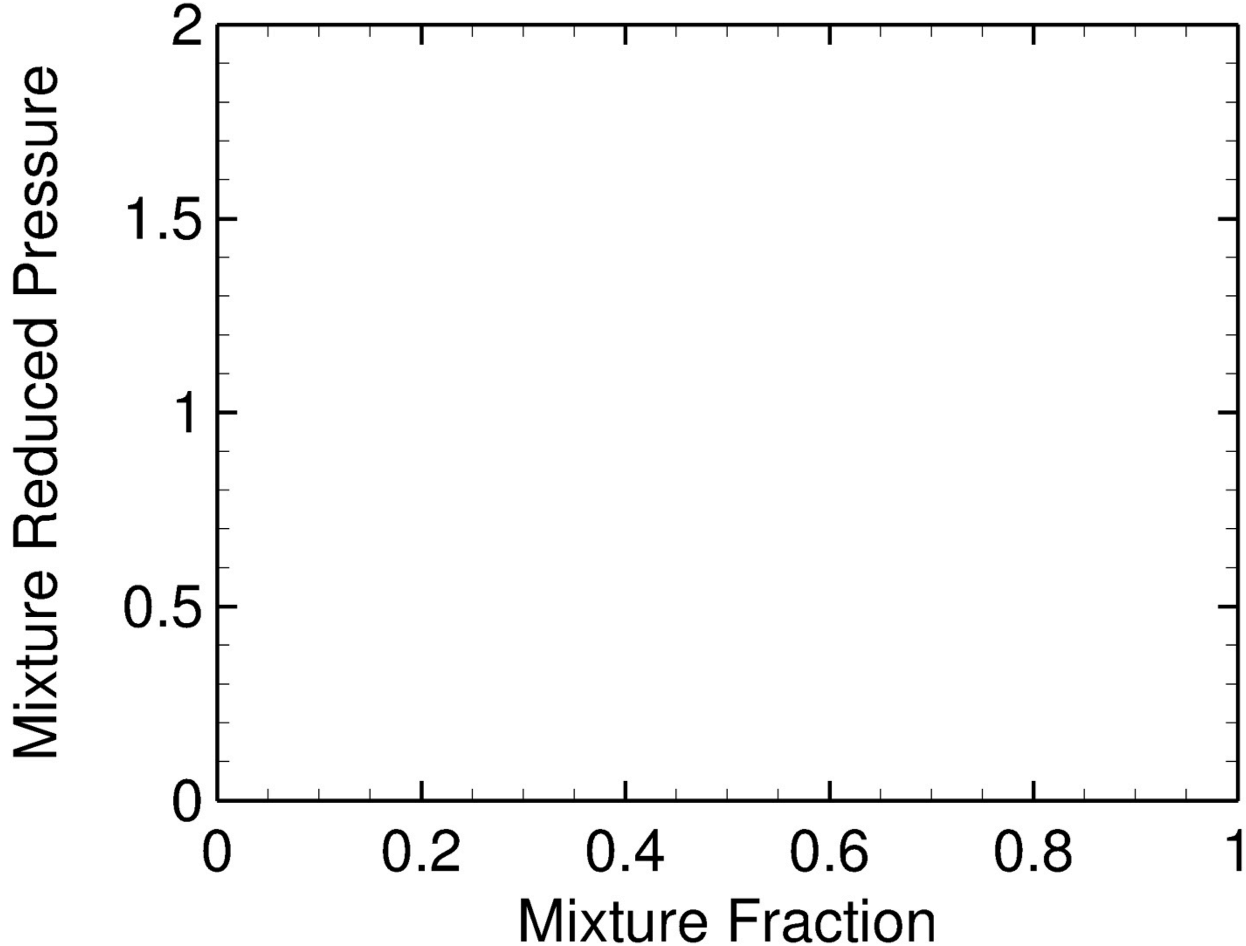
Mixture critical temperature as function of mixture state ($T > T_c$ for $\xi < 0.86$)



Mixture critical pressure as function of mixture state ($p > p_c$ for $\xi > 0.05$)



Envelope of mixture states mapped to thermodynamic regime diagram



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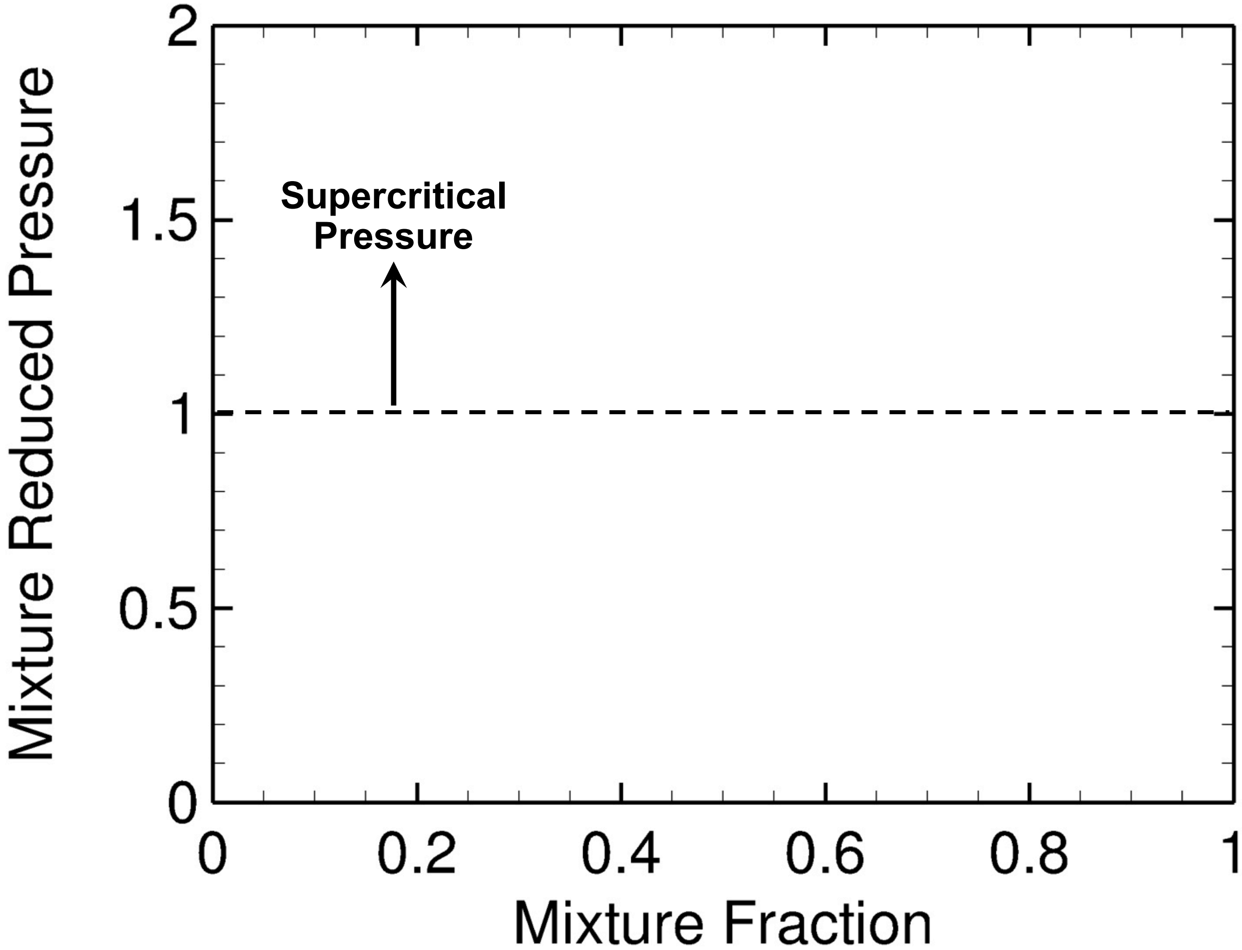

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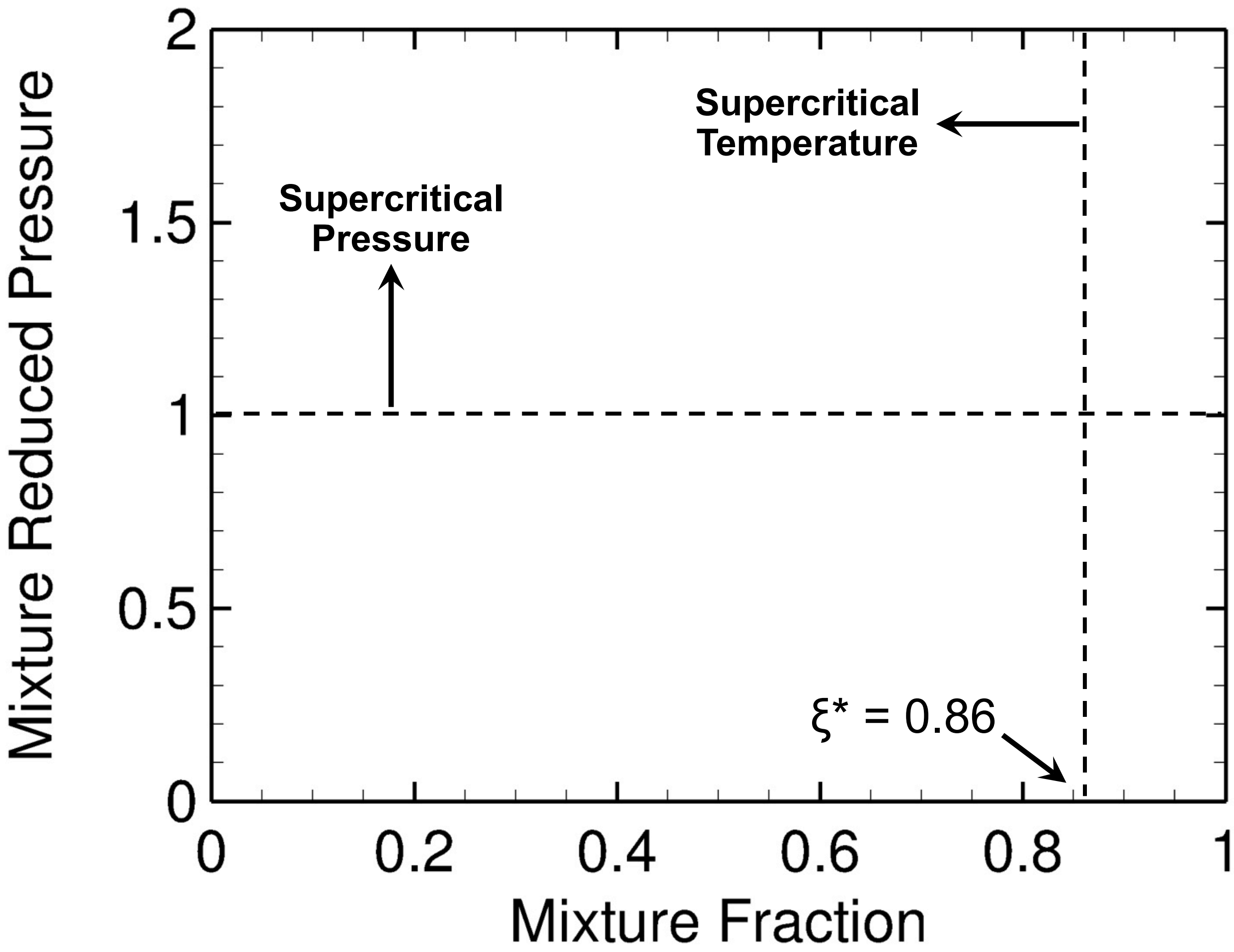

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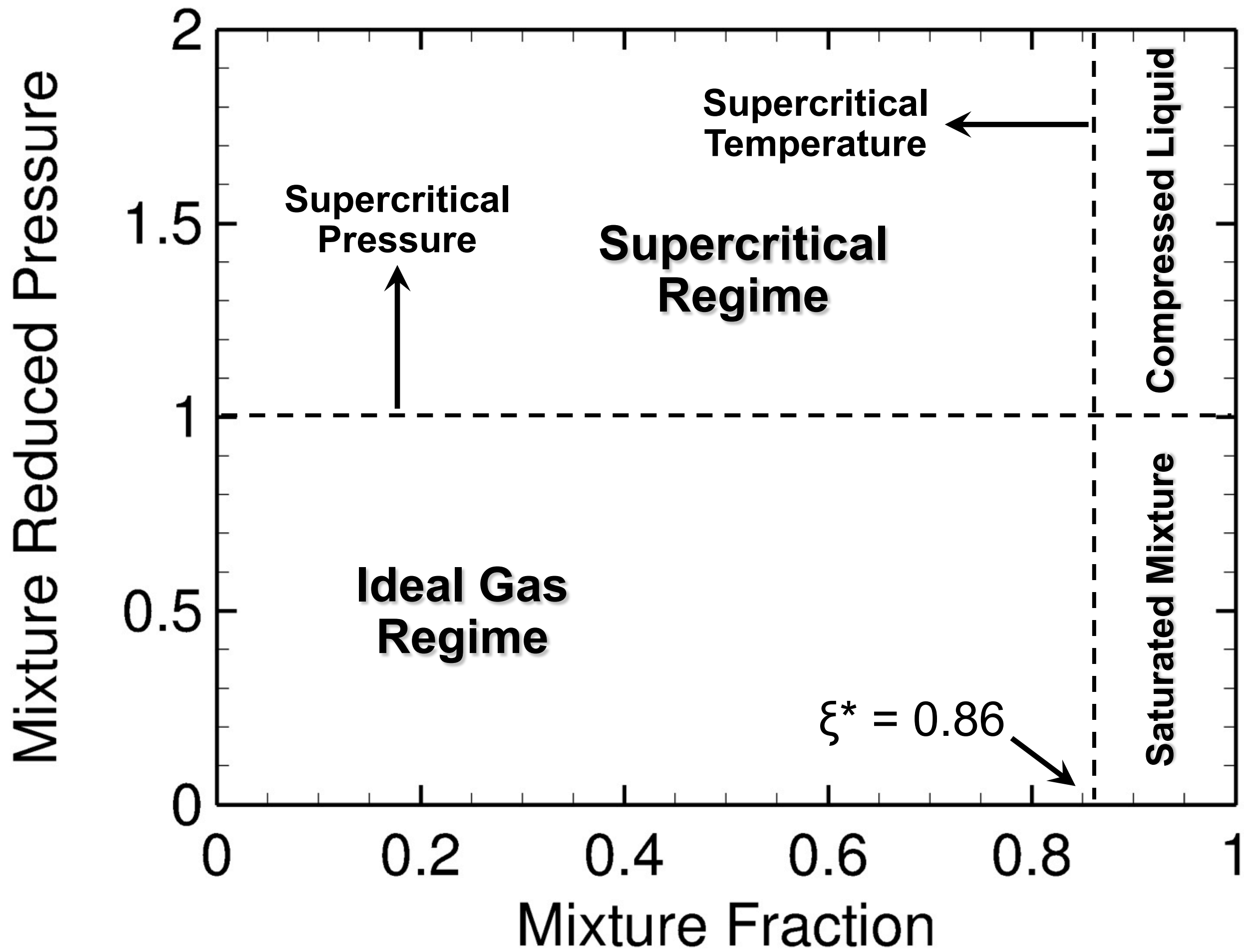

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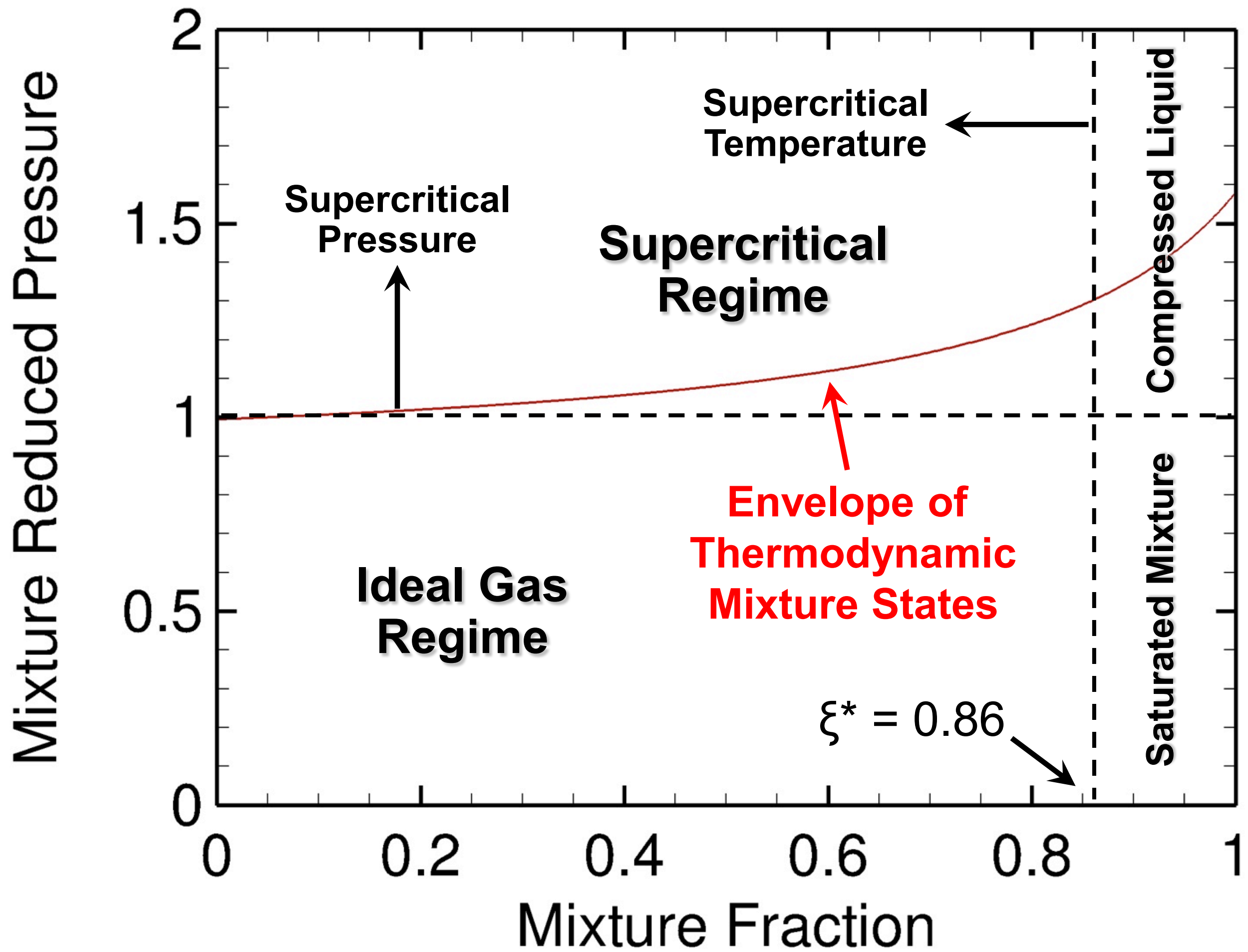
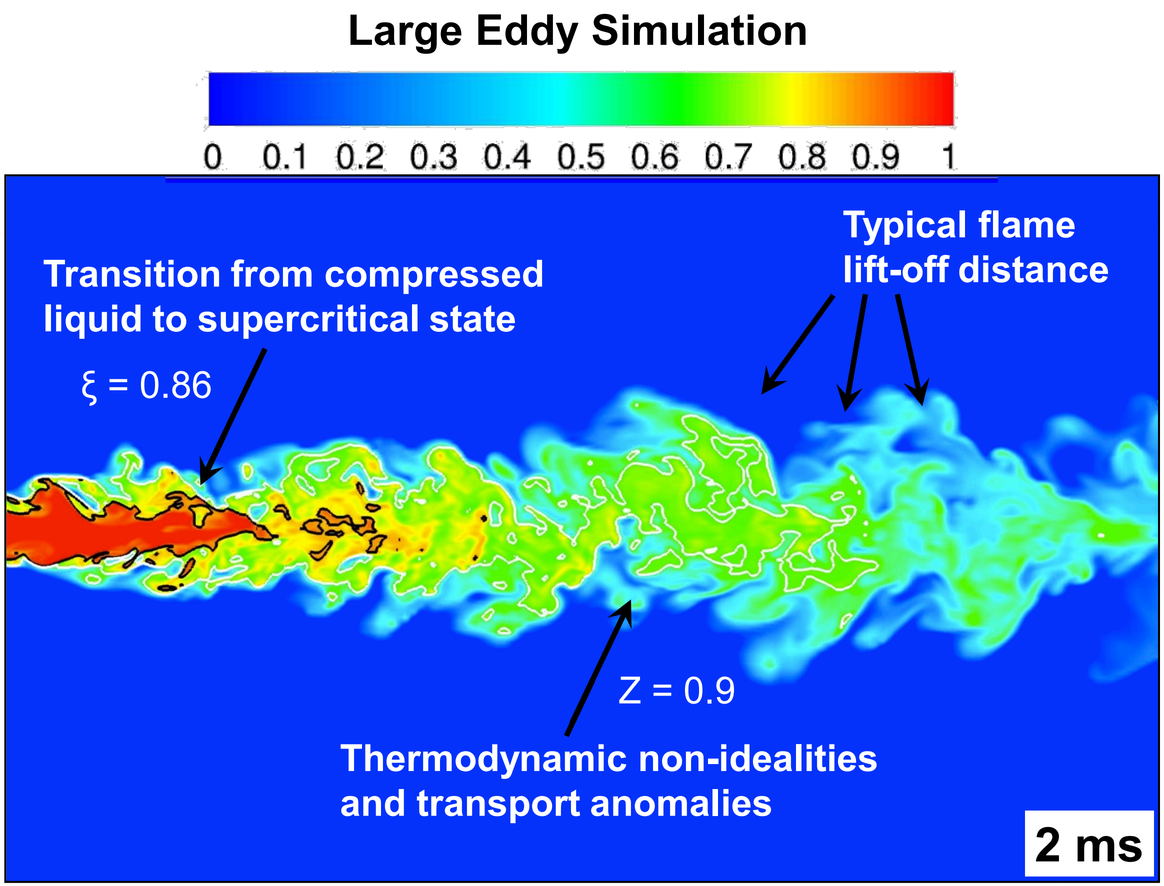


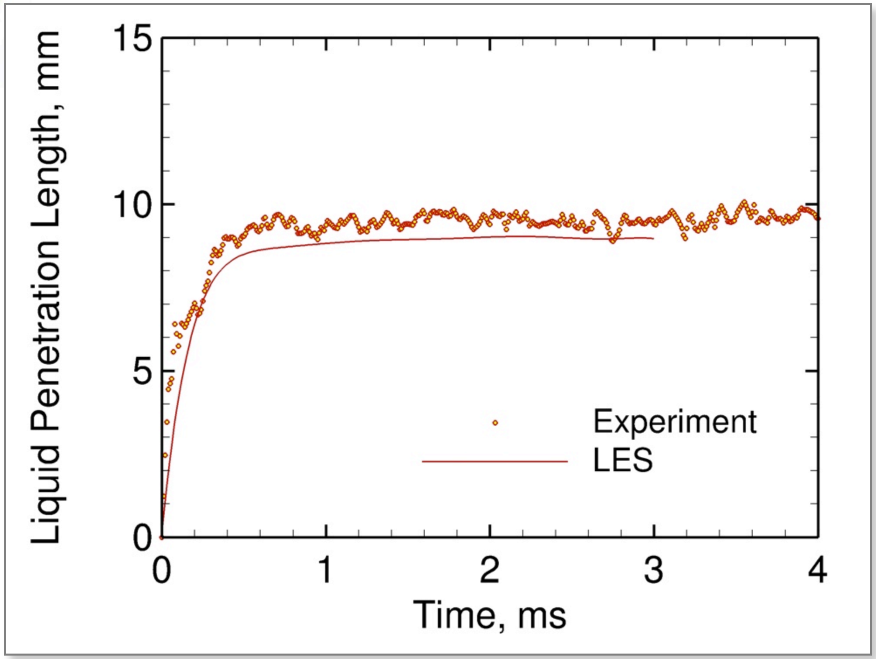
Mixing path never crosses liquid/vapor regime

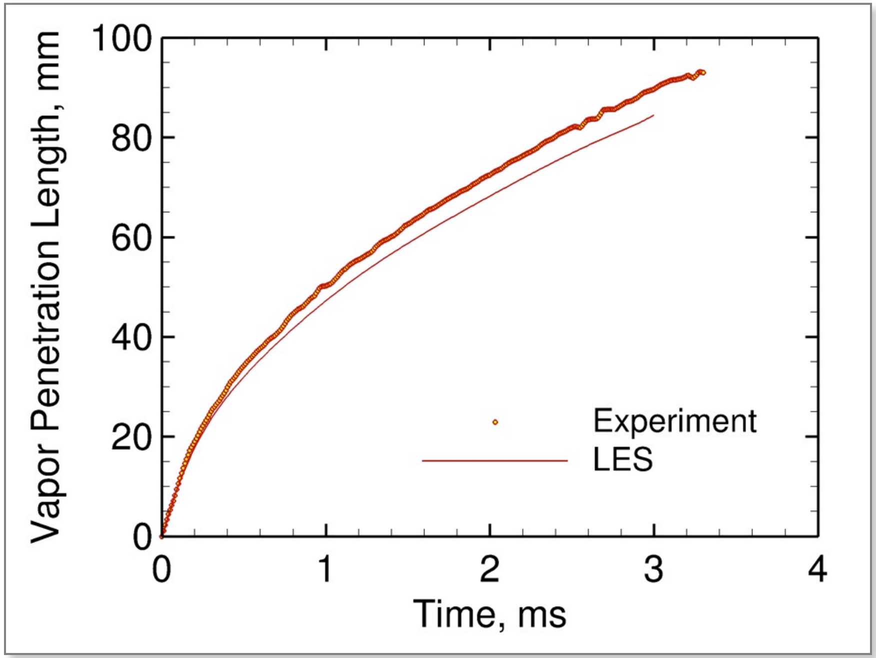
Full-field thermodynamic analysis provides revealing insights



- Mixture conditions vary from compressed liquid to supercritical state
- Significant thermodynamic non-idealities and transport anomalies
- Classical two-phase flow models do not necessarily account for this

Liquid and vapor penetration rate versus time





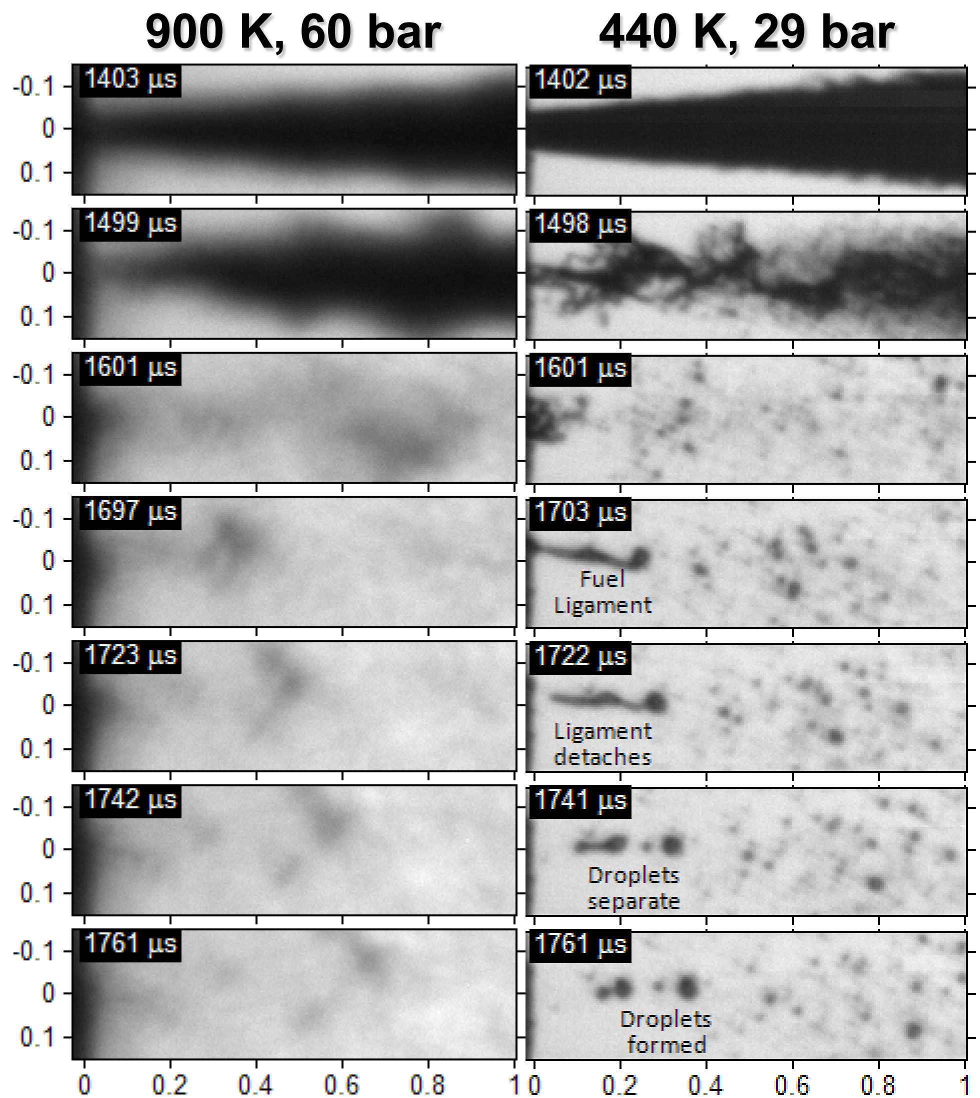
Mixture fraction thresholds of 0.86 and 0.05, respectively, produce reasonable agreement without the use of tuning constants

Observations …

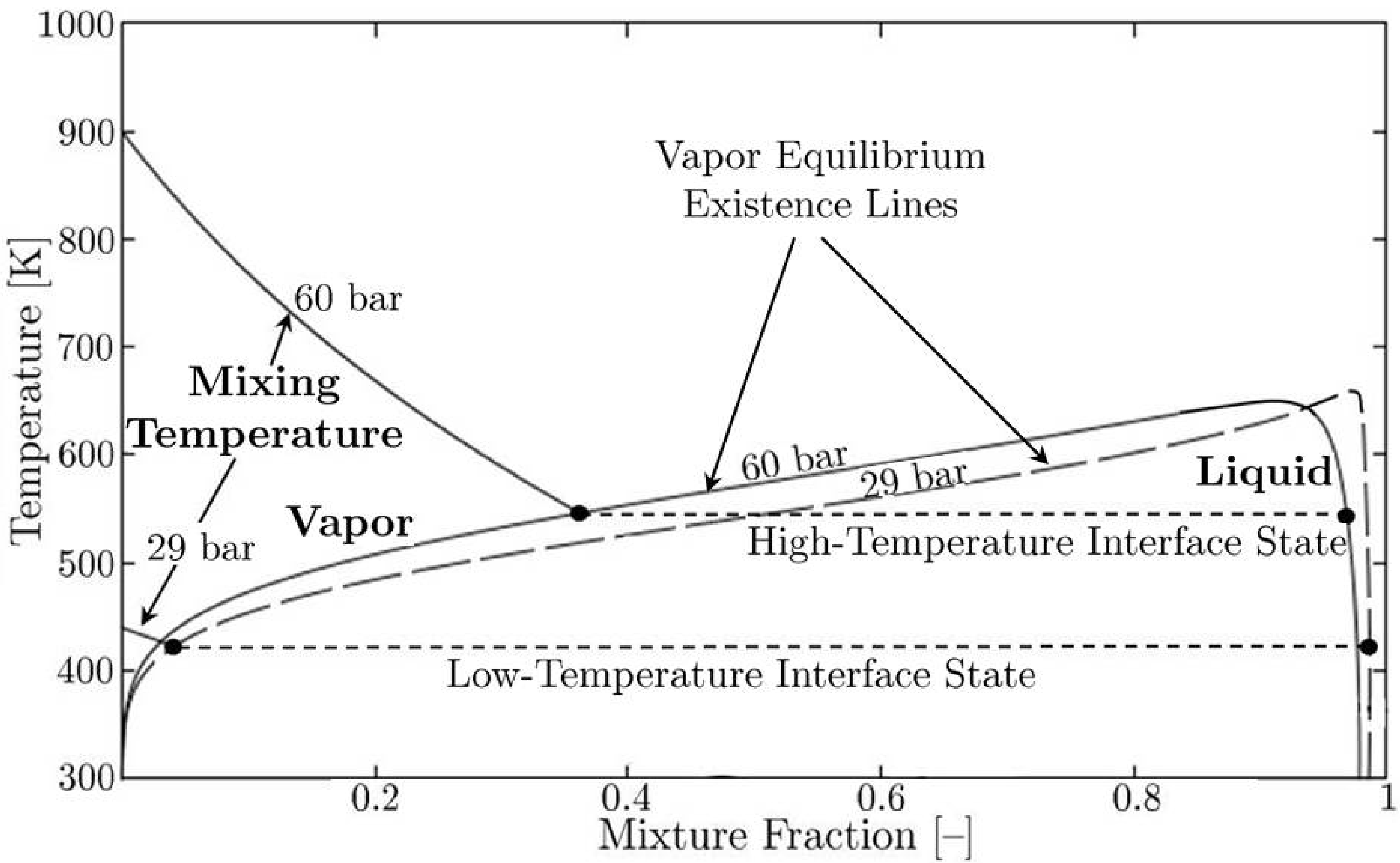
- Real-fluid model appears to capture behavior of arbitrary multiphase mixtures at certain high-pressure supercritical conditions
  – Analysis of baseline n-heptane case reveals that the envelope of mixture conditions varies from a compressed liquid to supercritical state
  – 1st order vapor-liquid phase transitions do not occur, which implies a distinct gas-liquid interface does not exist
  – Suggests that 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
  – Instead, non-ideal real-fluid behavior must be taken into account using detailed equation of state, thermodynamics and transport models

These observations have helped guide experimental investigations

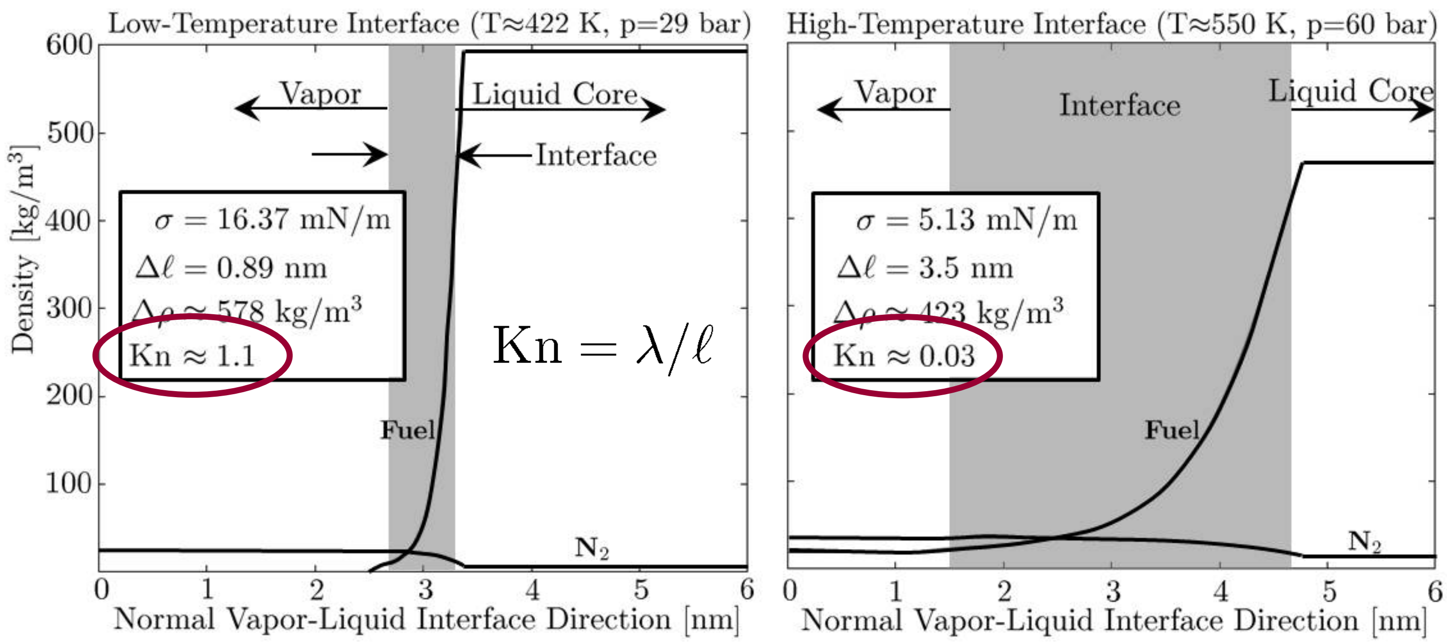
- Shift emphasis to Spray-A case
  - Collaboration with Pickett, Manin
  - More realistic n-dodecane, nitrogen mixtures
  - T_c = 658 K, P_c = 18.2 bar
- End-of-injection visualization
  - Best chance to observe surface tension effects
  - Two conditions considered (right)
- Experiments show
  - Evidence of surface tension at low-temperature condition
  - More diffusive injection process at high-temperature condition and no apparent formation of drops
- Why?



Combination of real-fluid model and equilibrium theory provides insights



Addition of gradient-theory provides complete quantitative picture



- **Gradient theory facilitates reconstruction of multicomponent gas-liquid interfaces**
  - **Enables simultaneous estimates of surface tension and interfacial thickness**
  - **Real-fluid model combined with equilibrium theory provides boundary conditions**
- **Knudsen-Number Criterion**
  - **Low temperature state: Kn > 0.1, which implies a non-continuum interface processes**
  - **High temperature state: Kn < 0.1, which implies continuum regime**
- **Results have provided new and revealing quantitative insights**
  - **Transition from classical spray to diffusion dominated mixing occurs through a combination of vanishing surface tension and broadening of the interface**

Proposed future work

- Continue detailed analysis of Spray-A (and n-heptane) case in collaboration with Pickett, ECN participants, related focal points
  - Use real-fluid/equilibrium/gradient-theory model to provide detailed mapping of multiphase regimes as a function of pressure, fuels, engine conditions
  - Begin parallel effort aimed at treatment of classical dense spray phenomena following approach demonstrated here (Lagrangian-Eulerian drop tracking)
  - Incorporate combustion closure for n-dodecane system into overall model framework with emphasis on auto-ignition (also n-heptane, iso-octane)
  - Continue to establish collaborative interactions aimed at reducing high-fidelity benchmark simulations to economical engineering models
- Work toward LES of combustion processes in HCCI engines at operating conditions identical to the experiment of Dec et al.
  - Need to improve proficiency and workflow for high-quality grid generation
- Expand collaborative activities related to priority research defined as part of the DOE BES/VTP PreSICE workshop
  - Focus on two central issues: 1) the dynamics of fuel injection and sprays, and 2) cycle-to-cycle variation and stochastic nature of in-cylinder flows

Collaborations and Institutions … Special thanks to Dr. Rainer Dahms

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  - 8351 Reacting Flow Research
  - 8353 Combustion Chemistry
  - 8362 Engine Combustion
  - 8365 Thermal/Fluid Science and Engineering
  - 8367 Hydrogen & Combustion Technology
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- Professor J. Doom, Minnesota State University
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- Professor B. Geurts, University of Twente, The Netherlands
- Professor D. Haworth, The Pennsylvania State University
- Professor J. Janika, Technical University of Darmstadt, Germany
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Summary

- Project provides significant link between DOE Office of Science and EERE Vehicle Technologies program (basic → applied)
  - Addresses barriers related to both AEC research and development of advanced simulation capabilities
  - Dedicated resources, facilities (CRCV, INCITE, etc.)
- Primary focus … complement development of engineering models for RANS, LES at device relevant conditions
  - Direct coupling with key target experiments (anchor)
  - Application of science-based models at identical conditions
  - Joint analysis to understand model performance, limitations
    - Critical trade-offs between cost and accuracy
    - Uncertainties as a function of fidelity and method
    - Implementation requirements as function of model