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

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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**
  - **FY12 – $450K**
  - **FY13 – $450K**

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 (e.g., Pickett et al.)**
- **≈ 50 collaborators and institutions**
- **Project lead: Joe Oefelein (Lacaze, Dahms hired as FTE's)**

Project Objectives – Relevance

- **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 science, 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 first principles models and high-fidelity LES in concert with experiments**
  - **High-pressure high-Reynolds-number mixed-mode combustion, complex fuels, multiphase flow, sprays at relevant conditions**

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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: Spray-H (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.**
    - **Development of optimal grid generation capabilities in progress (RAPTOR code framework now directly interfaced with GridPro)**
  - **LES best practices, treatment of complex geometries, detailed model development (Drs. G. Lacaze, R. Dahms hired as Tech. Staff)**
    - **Development of Quality Assessment Techniques for Large Eddy Simulation of Propulsion and Power Systems in Complex Geometries**
    - **Development of High-Fidelity Models for Liquid Fuel Spray Atomization and Mixing Processes in Transportation and Energy Systems**
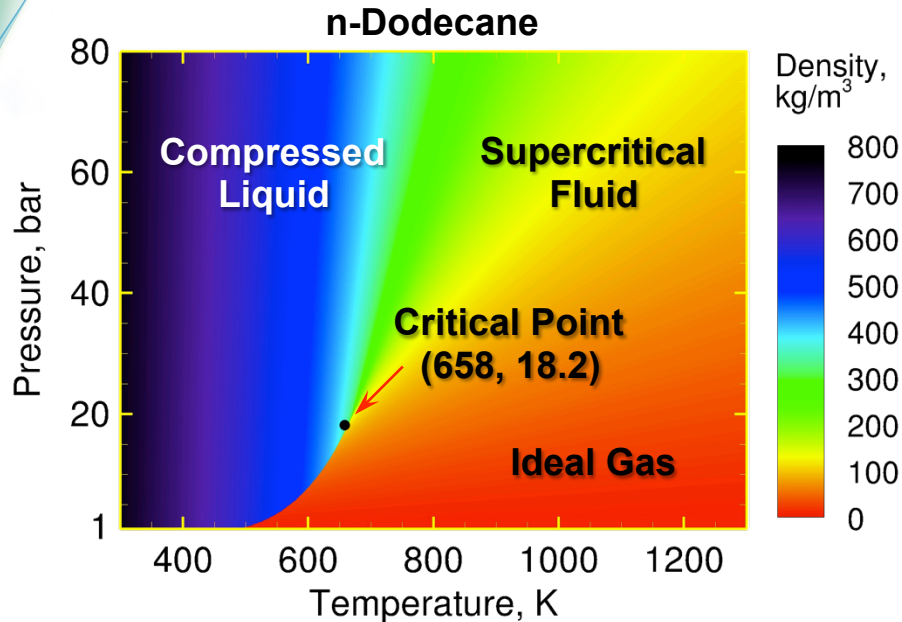
Approach/Strategy … application of first principles LES framework (RAPTOR)

- **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 numerics)**
  - **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**

Near linear scalability beyond 100,000 cores
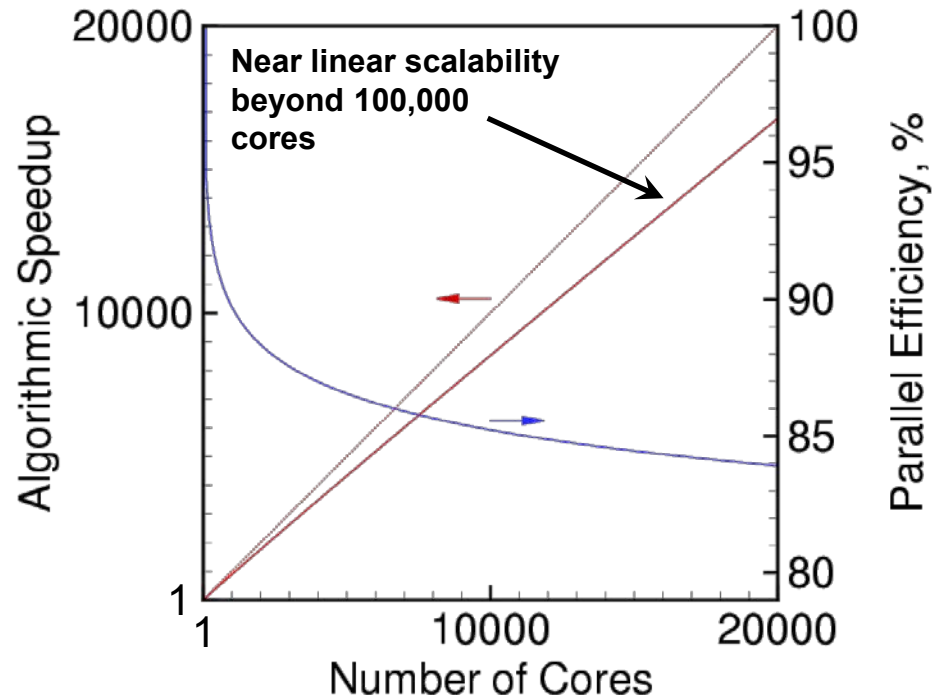
- **Strong (fine-grain) scaling attributes exhibited on the ORNL OLCF CRAY XK7 system (Titan … 18,688 nodes, AMD processors – 16 cores/node, NVIDIA® Tesla® GPU accelerators – 1 GPU/node … now 27 PF)**
  - **Single block, 1.28-million cells**
  - **20,000 blocks with 4^3 cells**
- **Weak (coarse-grain) scaling on 150,000 cores benchmarked as part of DOE 2009 Joule Code Metric**
- **Currently being refactored for multi-core parallelism, GPU acceleration**

Approach/Strategy … current focus on detailed treatment of complex fuels

n-Dodecane

Density, kg/m³

- Compressed Liquid
- Supercritical Fluid
- Critical Point (658, 18.2)
- Ideal Gas

Example Compounds

Compound	Formula	P_c, bar	T_c, K
Acetone	CH3COCH3	47.0	508
Ethanol	C2H5OH	61.5	514
Ethane	C2H6	48.7	305
Propane	C3H8	42.5	370
Benzene	C6H6	48.9	562
Heptane	C7H16	27.4	540
Octane	C8H18	25.7	544
Nonane	C9H20	22.9	595
Decane	C10H22	21.2	618
Undecane	C11H24	19.9	637
Dodecane	C12H26	18.2	658
Tridecane	C13H28	16.8	676
Tetradecane	C14H30	15.7	693

- **Provides detailed representation of gas/liquid EOS, thermodynamics, and transport**

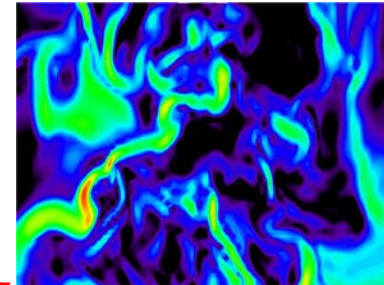- **Generalized to treat wide range of hydrocarbon mixtures (Fuel/Oxidizer/Products)**

J. C. Oefelein (2013). General package for evaluation of multicomponent real-gas and liquid mixture states at all pressures. *SAND Report*.
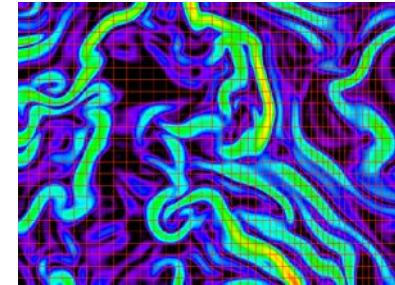
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Approach/Strategy … a word on the definition of "high-fidelity" LES

LES Grid Designed Using Layer Width Measurements

Location of maximum mean shear

Interrogation windows at x/d = 5, 10, 20

Jet exit d = 8.0 mm

LES of Scalar Dissipation

$\log(mm^{-2})$
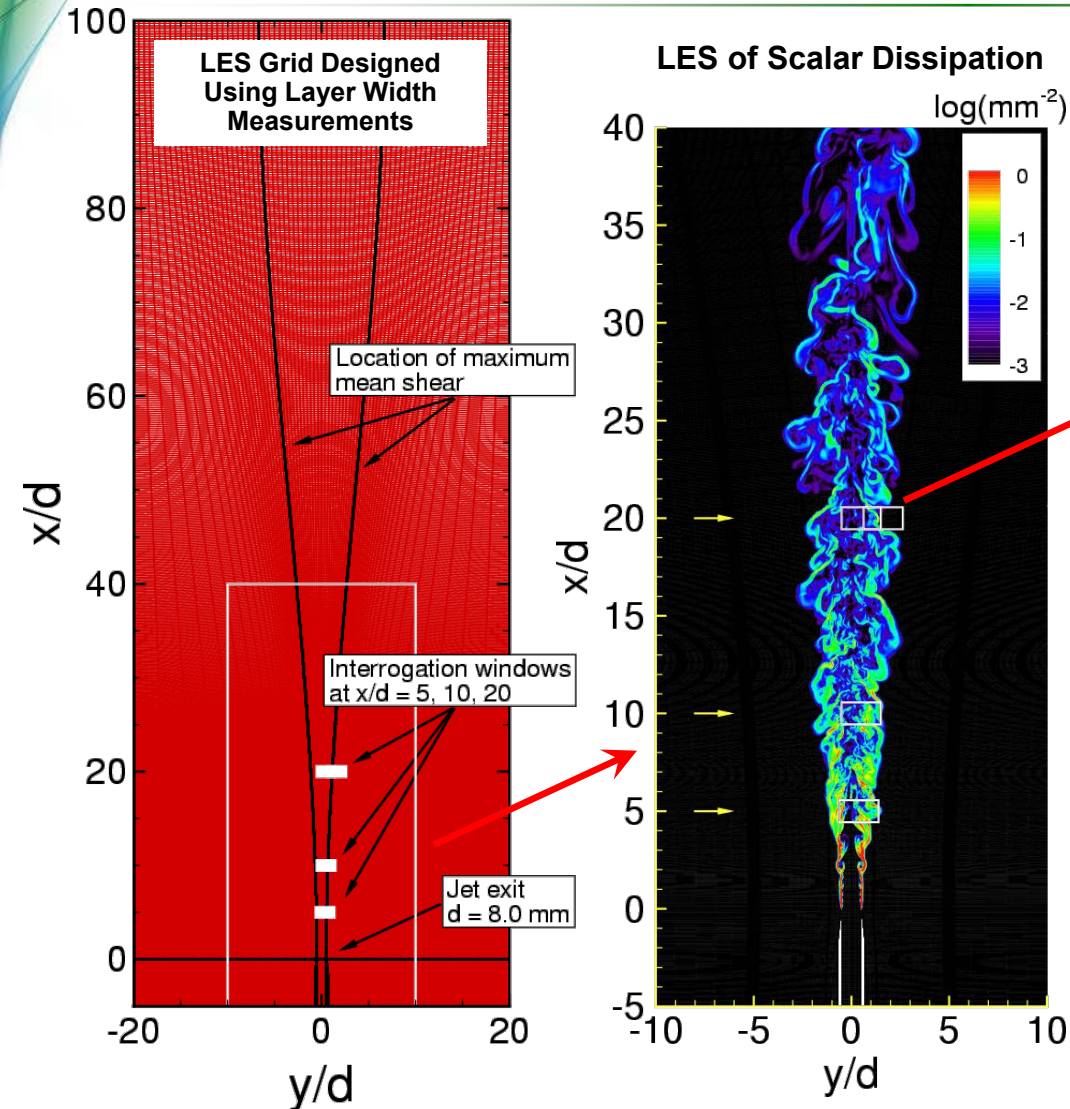
Close-up at x/d = 20 (10-million cell grid)

Rayleigh image with LES grid overlaid

Identical color map, number of contours, spatial location

Rayleigh imaging has provided quantitative insights ($CH_4/H_2/N_2$ flame in air co-flow, Frank et al.)

- **Successive refinements illustrate structural versus statistical simulations**
  - **1.3-million cells (engineering)**
  - **10-million cells (intermediate)**
  - **82-million cells ("high-fidelity")**

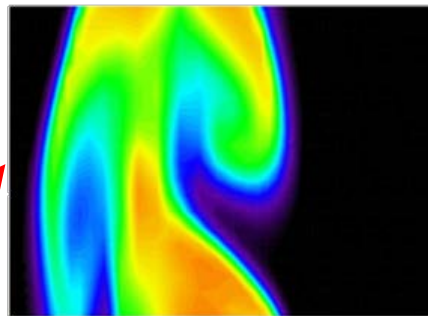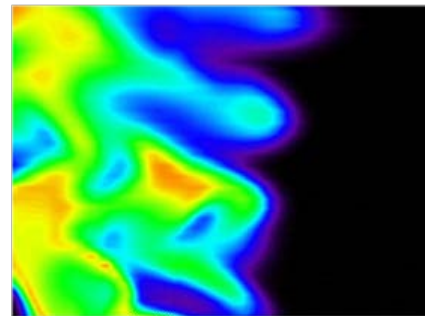# Approach/Strategy … structural versus statistical simulations

Mixture Fraction
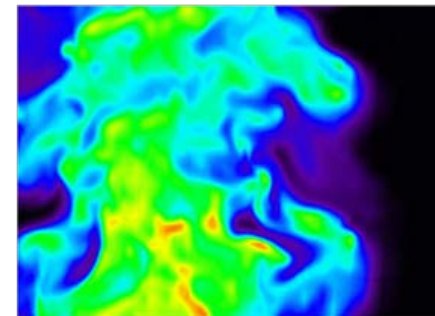
Experiment
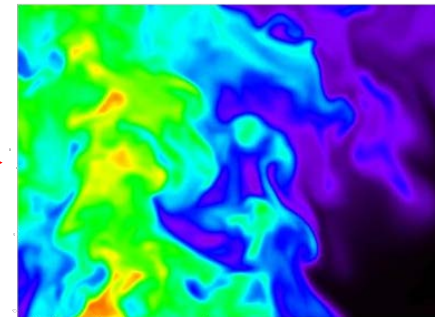
LES

1.3-million cells
$\Delta t = 1.00\ \mu s$

10-million cells
$\Delta t = 0.50\ \mu s$

82-million cells
$\Delta t = 0.25\ \mu s$

0.9

0.0

Statistically Correct?

Structurally Correct

Frank, J. H., Kaiser, S. A. and Oefelein, J. C. (2011). Analysis of scalar mixing dynamics in LES using high-resolution imaging of laser Rayleigh scattering in turbulent non-reacting jets and non-premixed jet flames. *Proceedings of the Combustion Institute*, **33**:1373–1381.
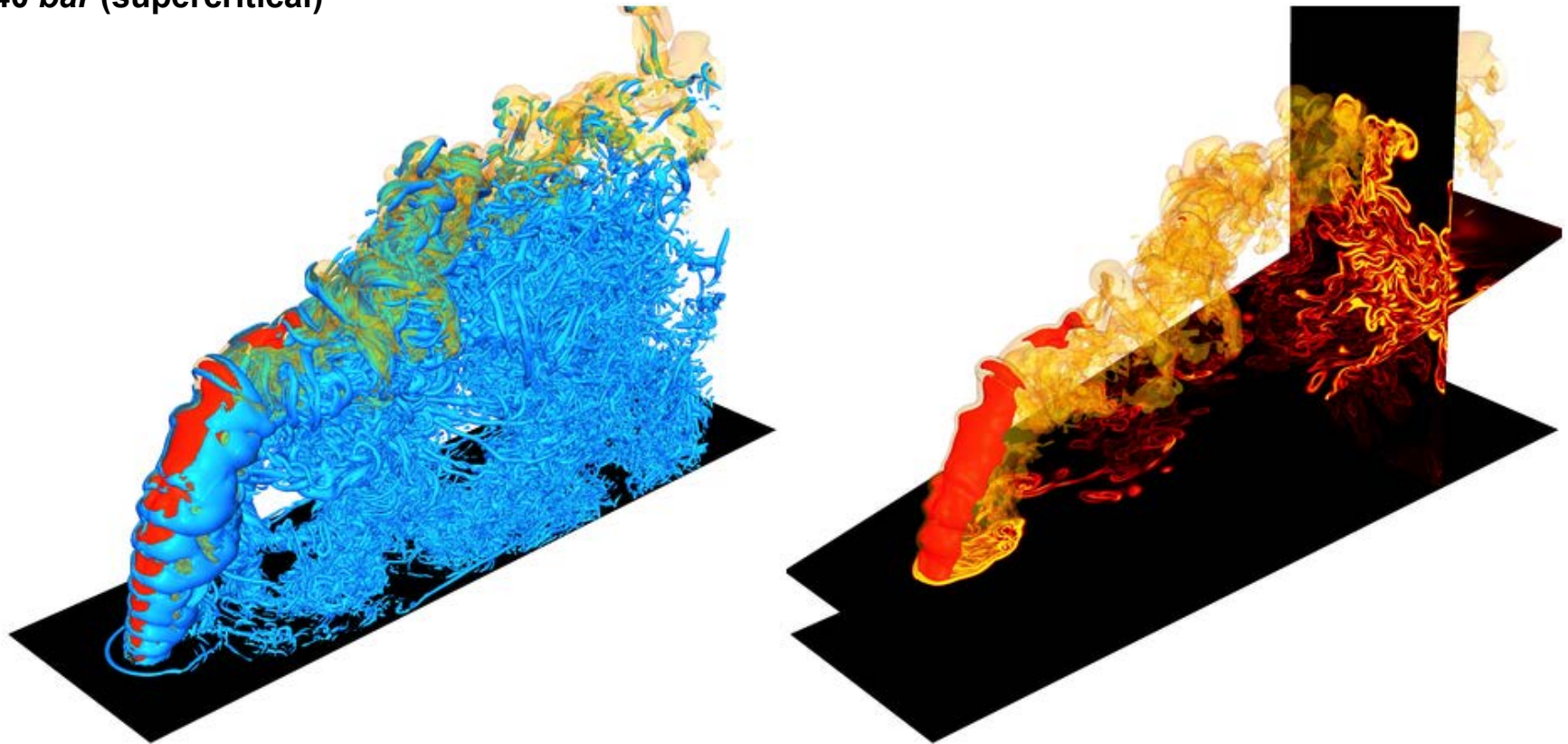
Approach/Strategy … structural versus statistical simulations

Liquid n-Decane-air jet-in-cross-flow

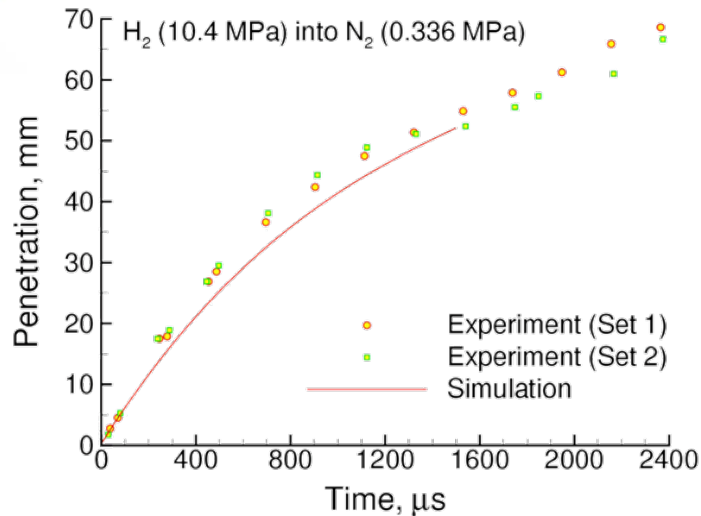**Re = 100,000 (jet), 620,000 (cross-flow)**
U = 46 *m/s* (jet), 75 *m/s* (cross-flow)
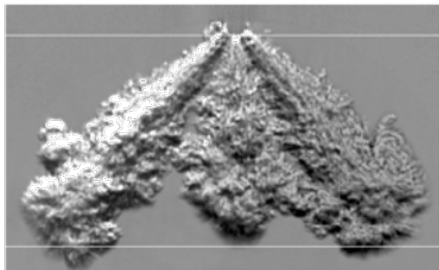**P = 40 *bar* (supercritical)**

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Technical Accomplishments and Progress ... ...

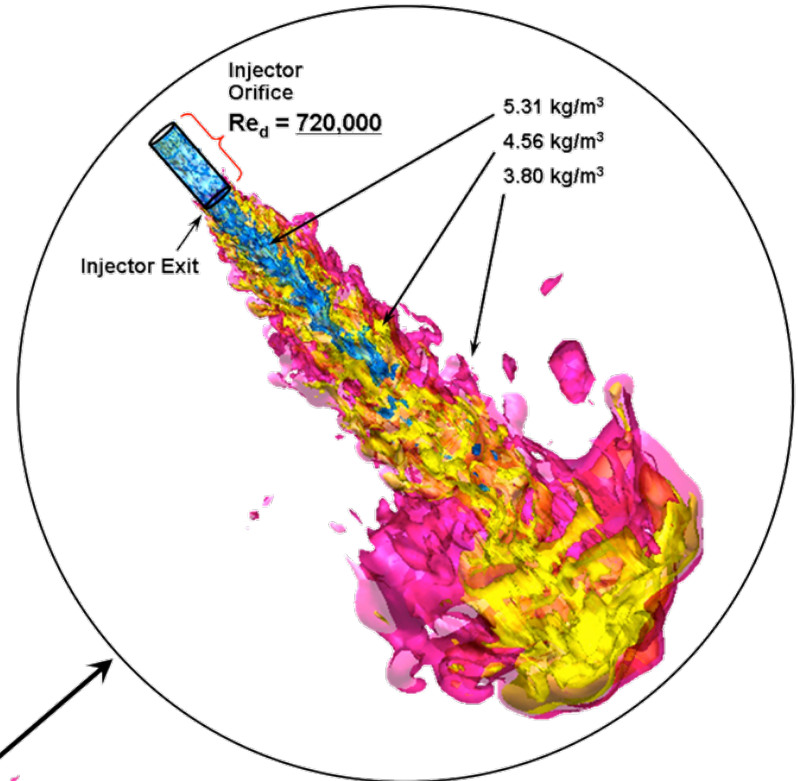**We have developed a new quantitative understanding of high-pressure fuel injection processes**

H_2 (10.4 MPa) into N_2 (0.336 MPa)

- Experiment (Set 1)
- Experiment (Set 2)
- Simulation

Comparison of LES with experimental measurements of jet penetration rate

Injector Orifice

$Re_d = \underline{720,000}$

5.31 kg/m³
4.56 kg/m³
3.80 kg/m³

Injector Exit

Shadowgraph (U. Wisconsin)
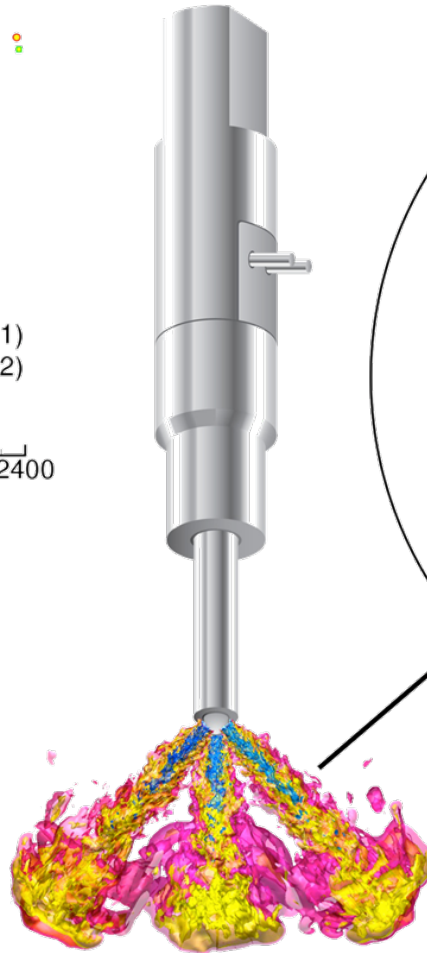
Large Eddy Simulation

Orifice Diameter	0.8 *mm*
Injection Pressure	10.4 *MPa*
Injection Temperature	298 *K*
Chamber Pressure	0.336 *MPa*
Chamber Temperature	298 *K*

# Effects of pressure on liquid injection processes are not well understood

10 bar

➜ **"Low" (subcritical) pressure**

- Molecular interface separates injected liquid from ambient gases
- Interactions between dynamic shear forces and surface tension promote primary atomization and breakup
- Spray evolves from dense to dilute state in classically assumed manner

60 bar
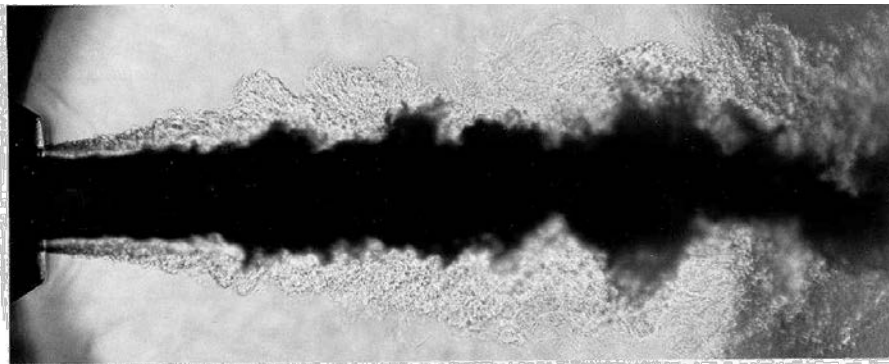

➜ **"High" (supercritical) pressure**

- Interfacial diffusion layers develop presumably due to lower surface tension
- Lack of inter-molecular forces promotes diffusion dominated turbulent mixing prior to atomization
- Interfacial region between jets interact in presence of exceedingly large gradients

Shear-coaxial injection of N2 and He
(N2: p_c = 34 bar, T_c = 126 K)

W. Mayer, *et al*. (1998). Atomization and breakup of cryogenic propellants under high-pressure subcritical and supercritical conditions. *Journal of Propulsion and Power*, **14**(5): 835-842.

Sandia high-pressure combustion vessel (Pickett et al.)
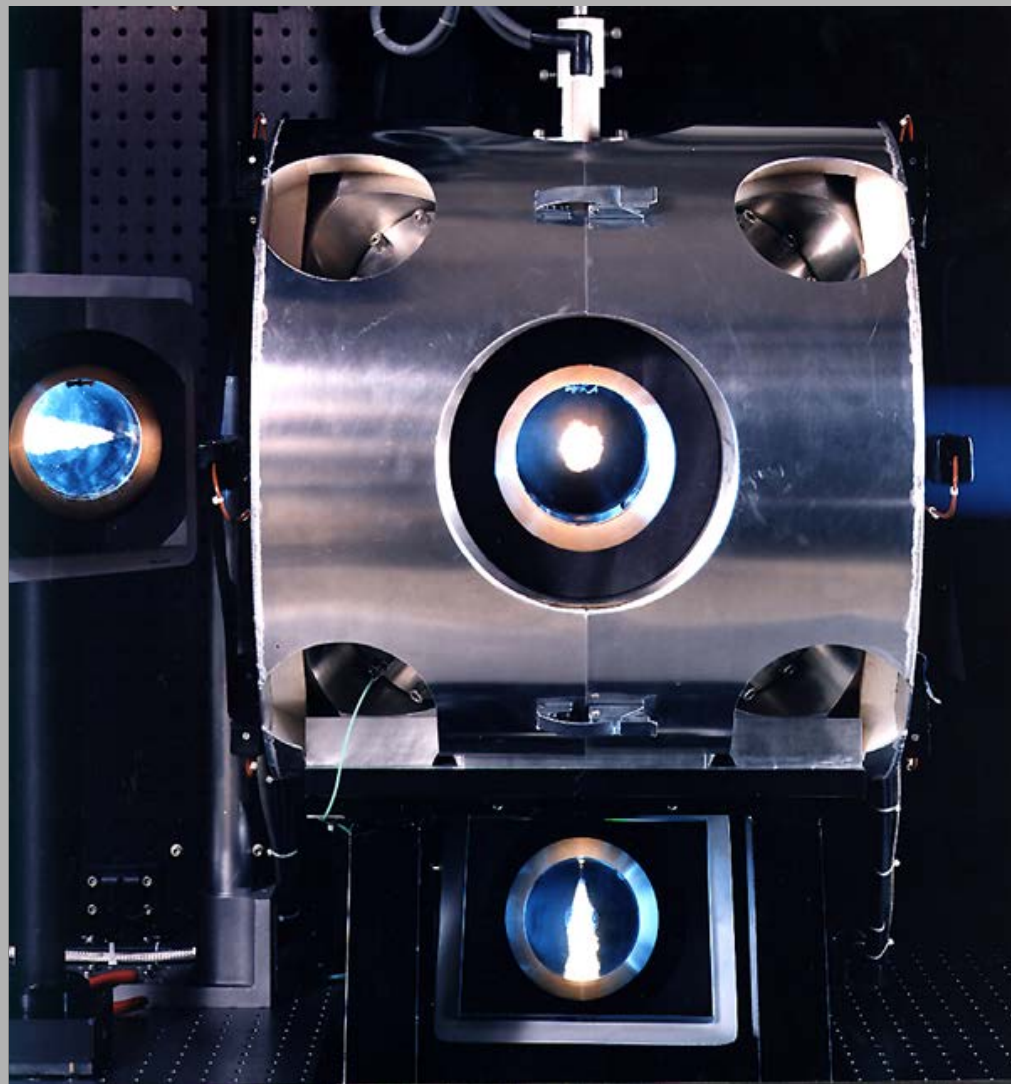
Peak Injection Conditions
Fuel pressure: 2000 *bar*
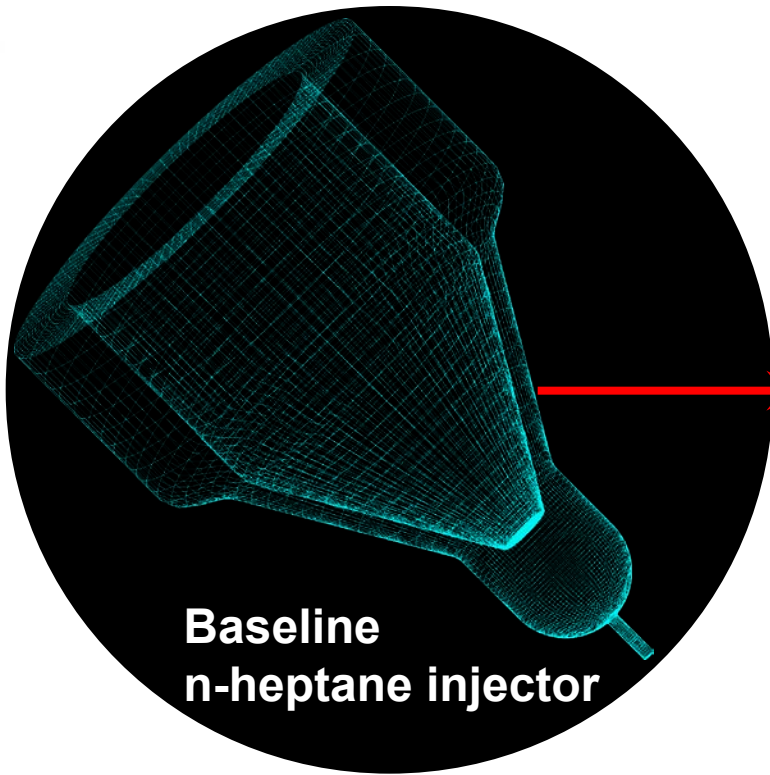(diesel, gasoline, biofuels)

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

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

LES at identical conditions …

Combustion Vessel

Initial Conditions
Pressure: 43.3 *bar*
Temperature: 1000 *K*
Composition: (by volume)
0.00% O2, 89.71% N2,
6.52% CO2, 3.77% H2O

1050 d

1080 d

Computational Domain

**Baseline
n-heptane injector**

Injection Conditions

Peak Re_d:	150,000
Temperature:	373 *K*
Density:	620 *kg/m³*
Peak Velocity:	554 *m/s*
Nozzle Diameter:	0.1 *mm*

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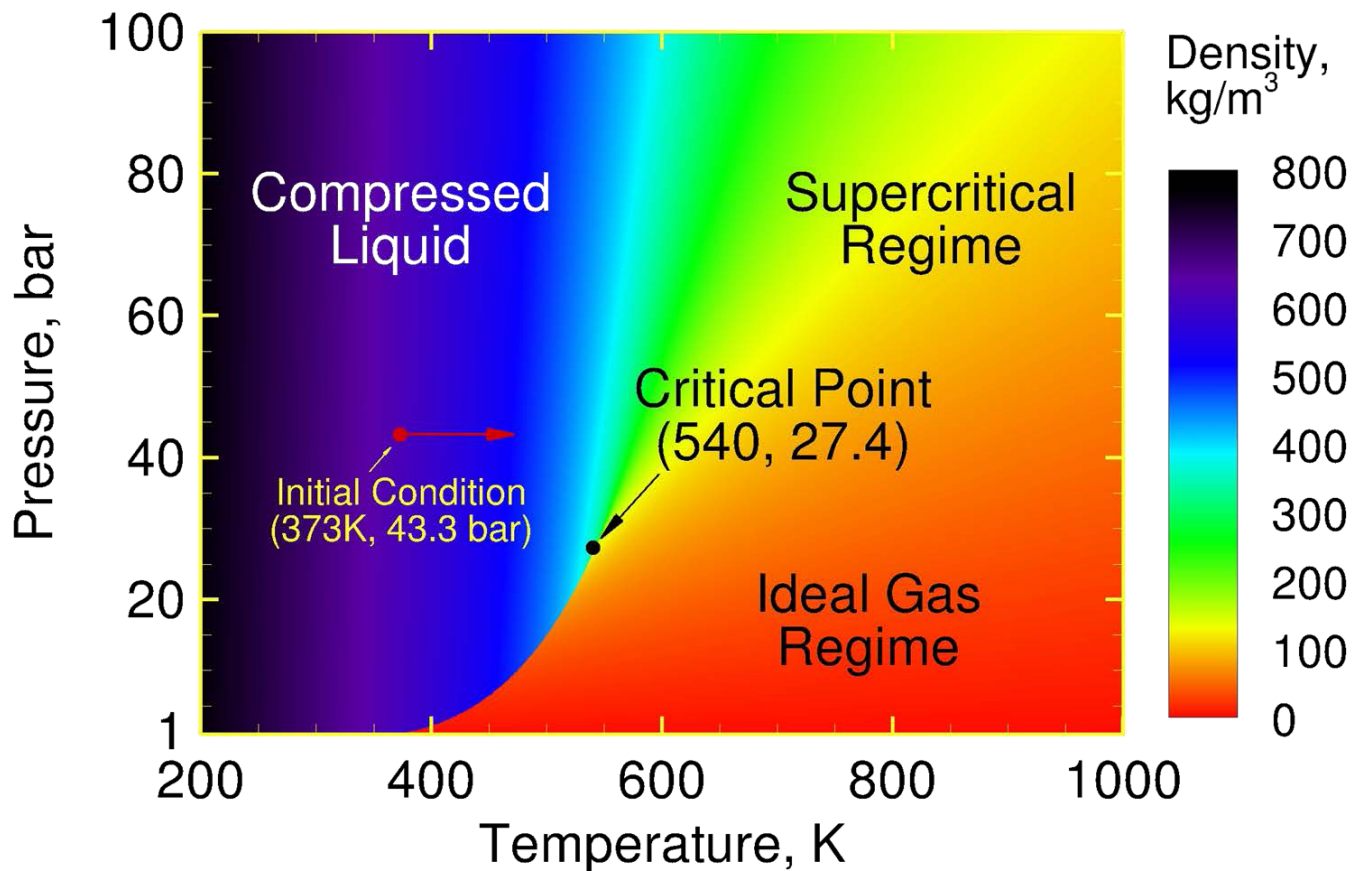
n-Heptane is being injected as a compressed liquid at supercritical pressure
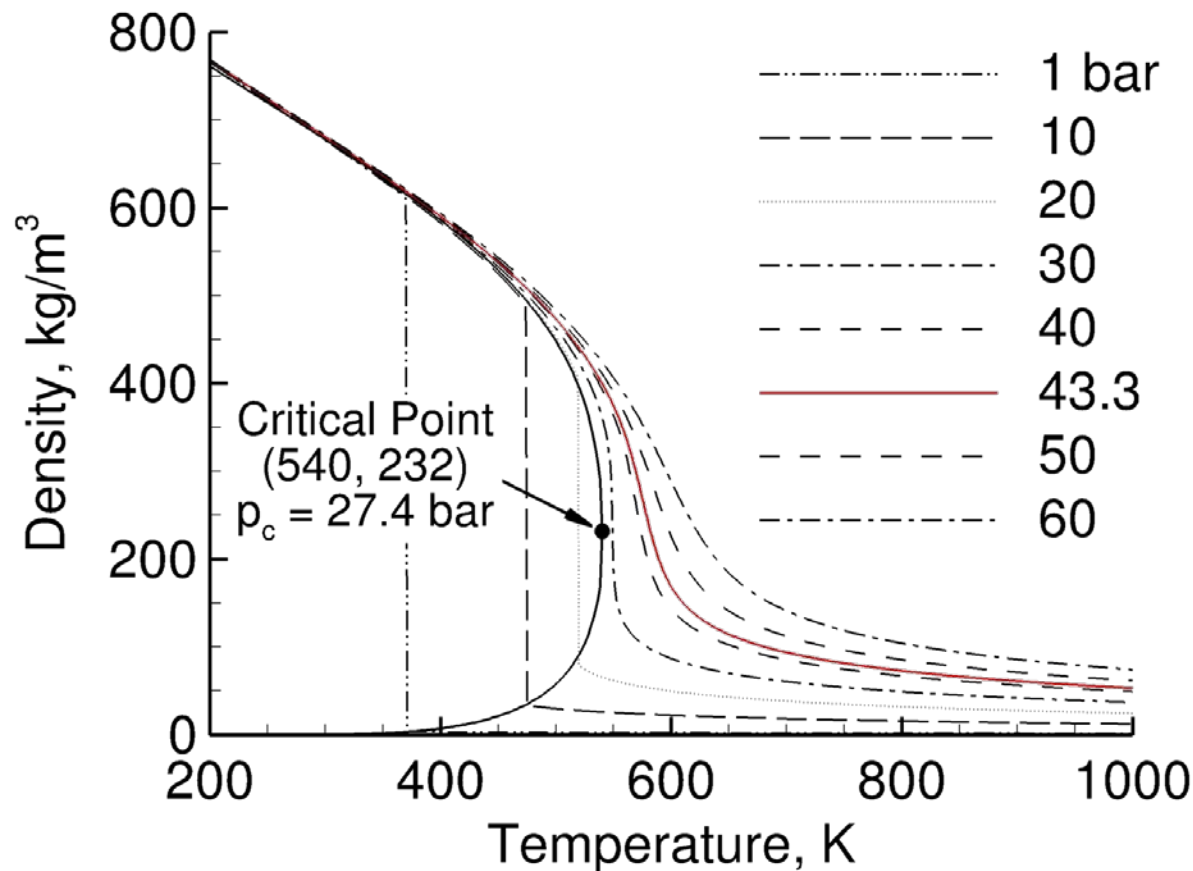
Thermodynamic considerations

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

Real fluid model ... comparisons with data provide reasonable agreement

Rayleigh Images
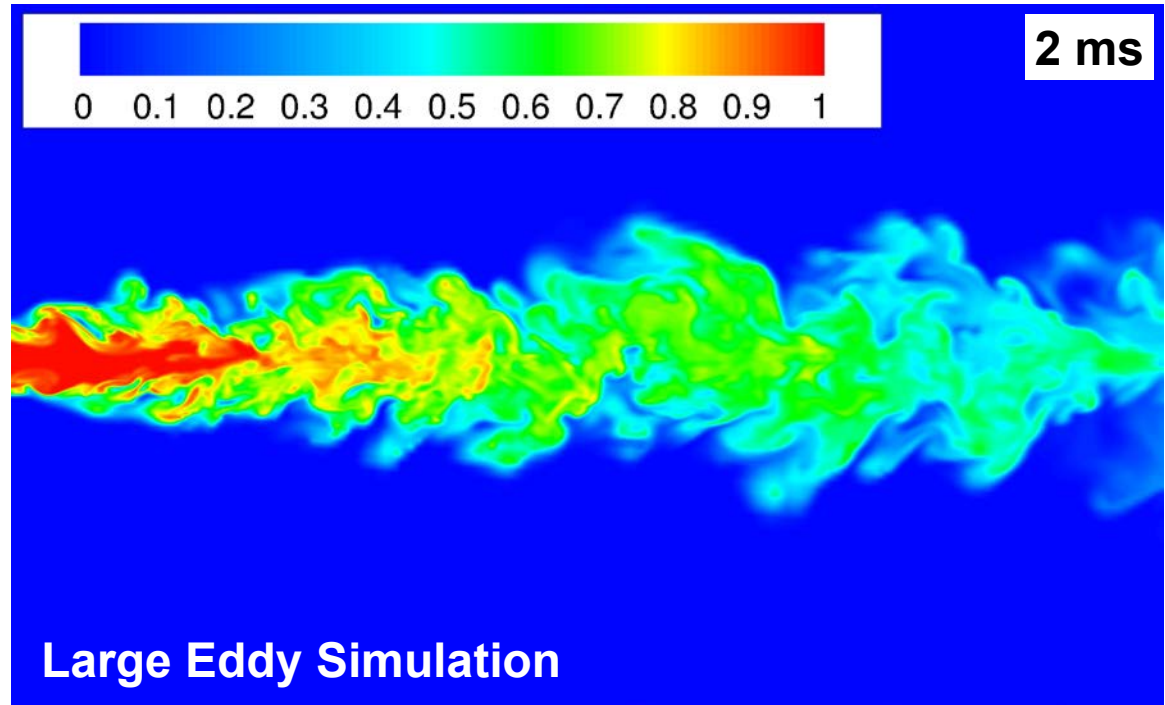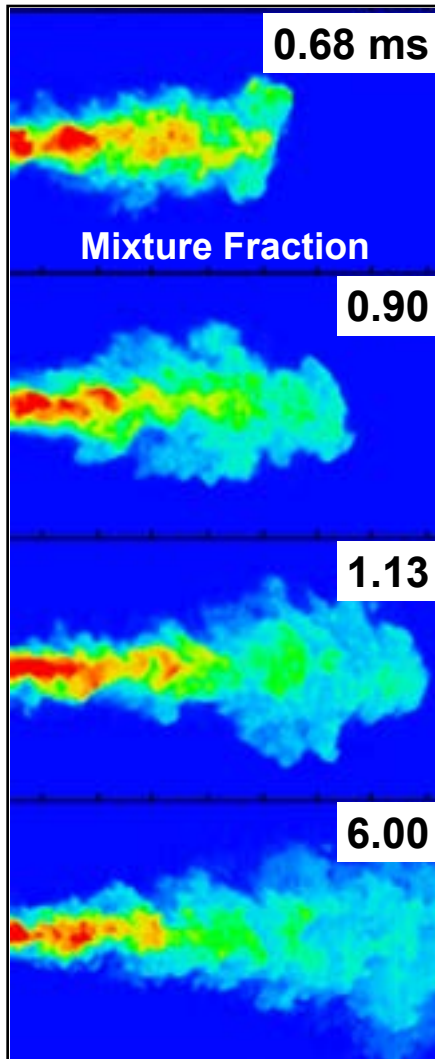
0.68 ms

Mixture Fraction

0.90

1.13

6.00

2 ms

0   0.1   0.2   0.3   0.4   0.5   0.6   0.7   0.8   0.9   1

Large Eddy Simulation

Available Data

⇒ **Internal injector geometry**

⇒ **Rate of injection**

✓ **Rayleigh scattering images**

✓ **Schlieren movies**

✓ **Liquid length versus time**

✓ **Vapor length versus time**

Results facilitate detailed analysis of "gas-liquid" interface dynamics

Large Eddy Simulation

Typical flame lift-off distance

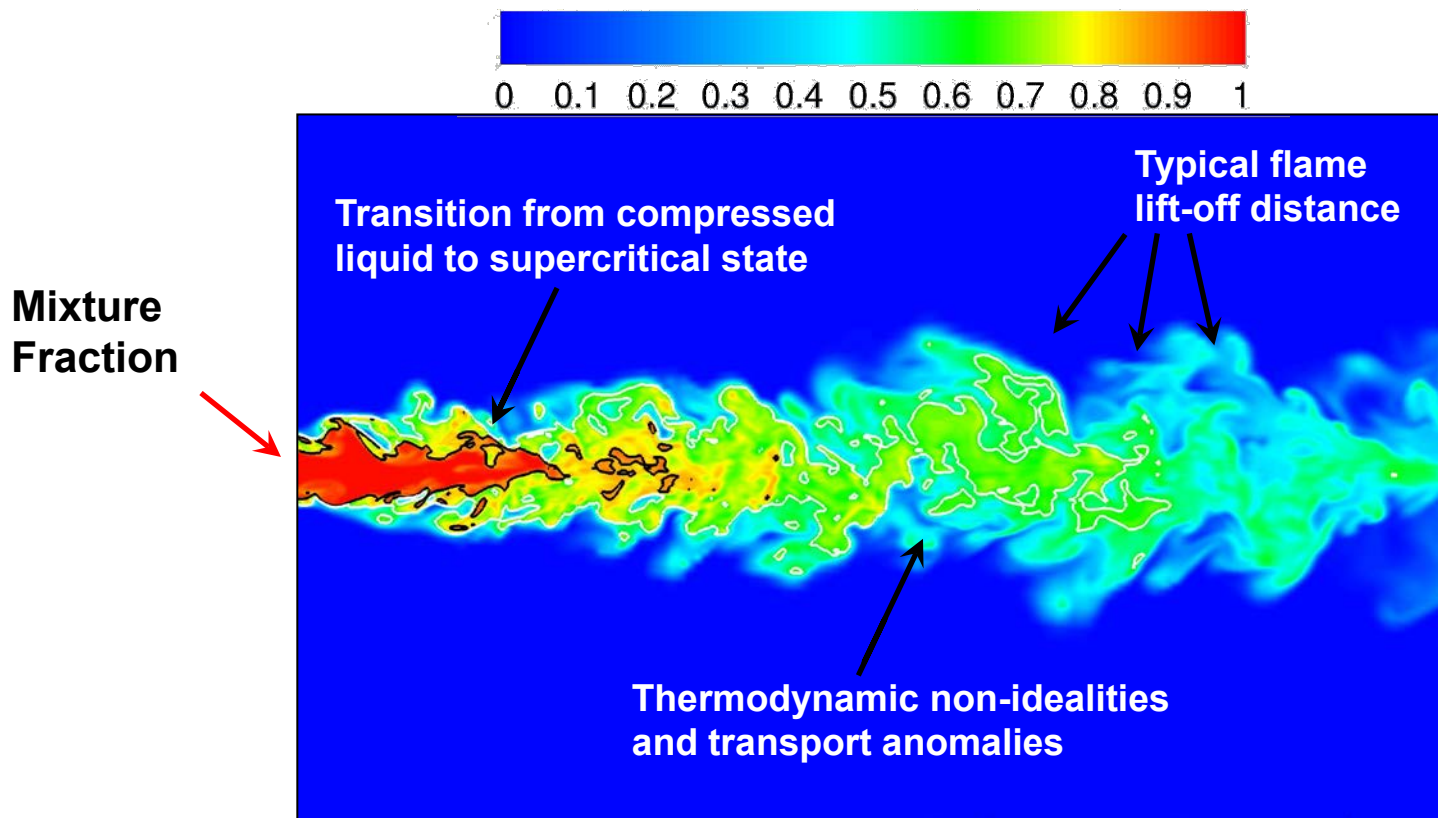Transition from compressed liquid to supercritical state

Mixture Fraction

Thermodynamic non-idealities and transport anomalies

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

Real-fluid model, equilibrium theory, and gradient theory facilitate analysis
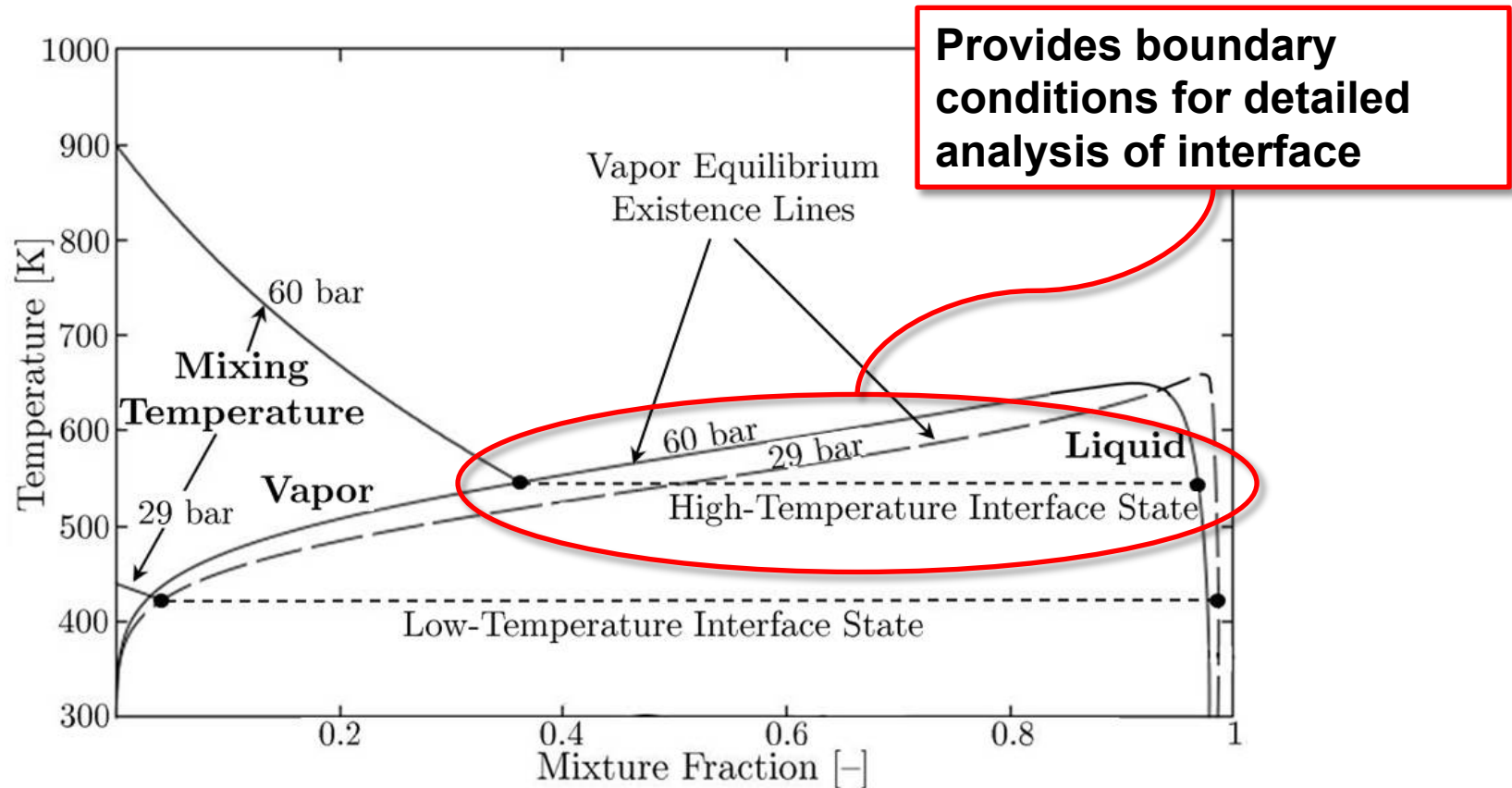
Provides first quantitative description of high-pressure interface dynamics
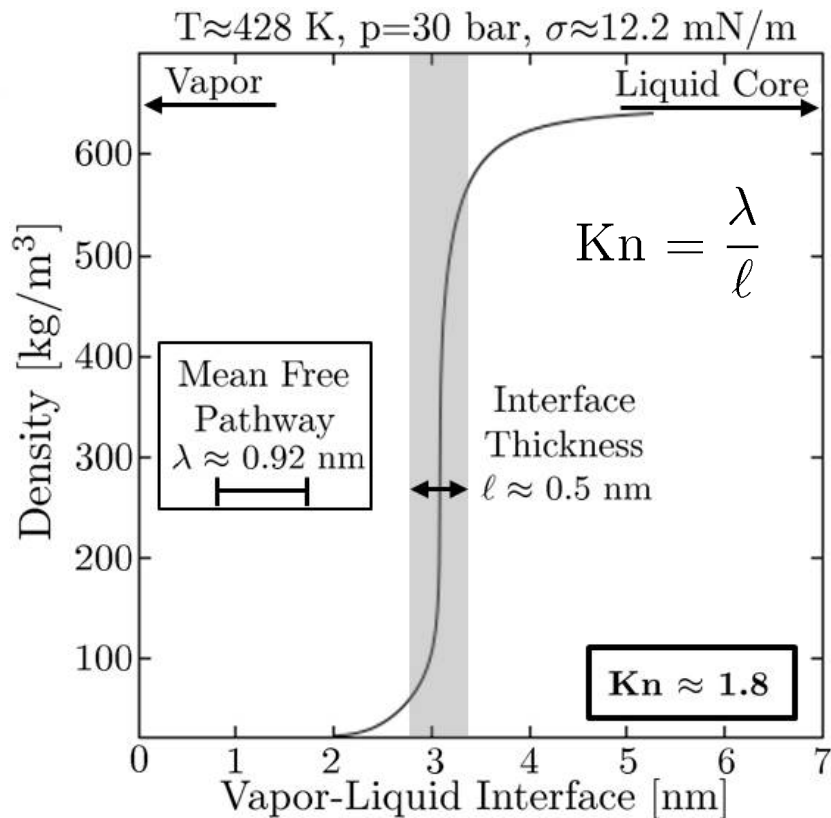
Kn > 0.1: Molecular Interface
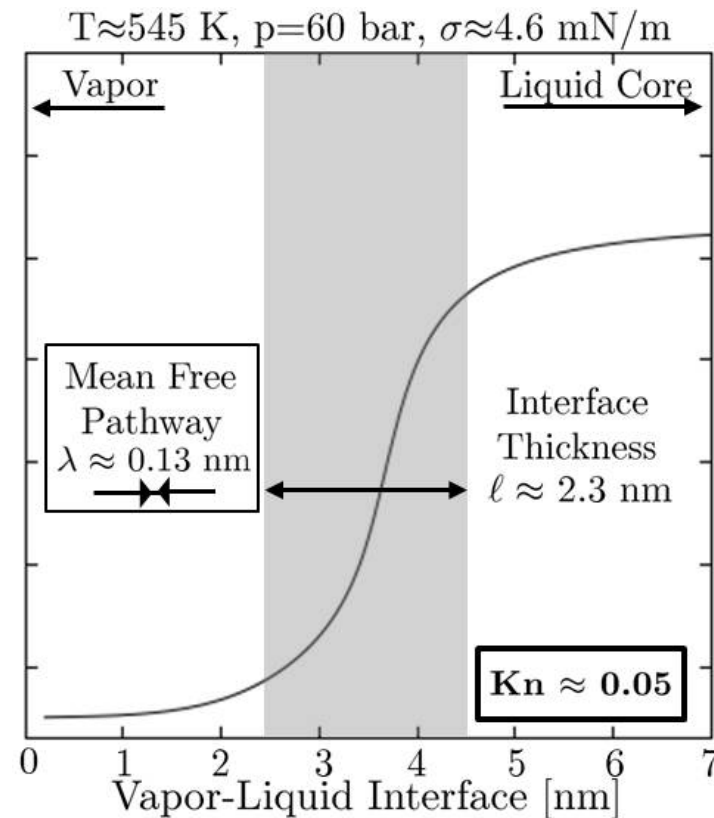
Kn < 0.1: Continuum Regime

Transition from spray to diffusive mixing occurs through combination of vanishing surface tension, broadening interfaces, reduced mean free path

Facilitates construction of predictive regime diagrams for specific systems

N-Dodecane/N_2 (T_F=363 K)

Predicted trends have been used to guide experiments (Pickett et al.)
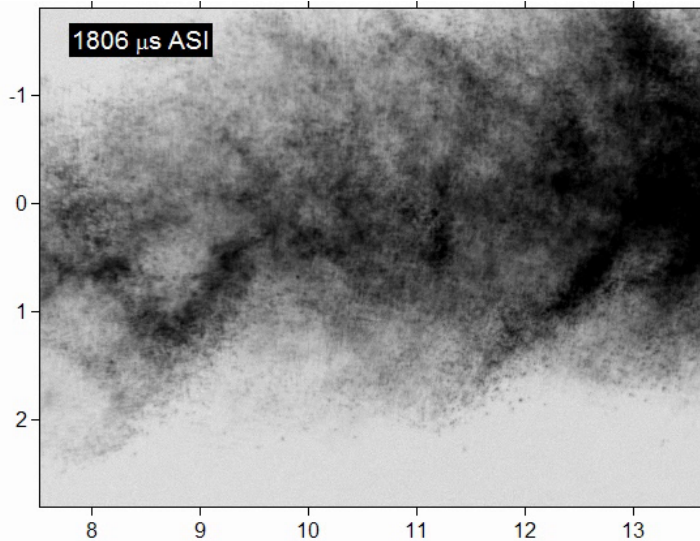
Results provide new insights directly relevant to model development, design

- **Theory provides first quantitative explanation applicable at device level**

  – **Knudsen-number criterion reveals that interfacial diffusion layers develop due to vanishing surface tension and broadening vapor-liquid interfaces**

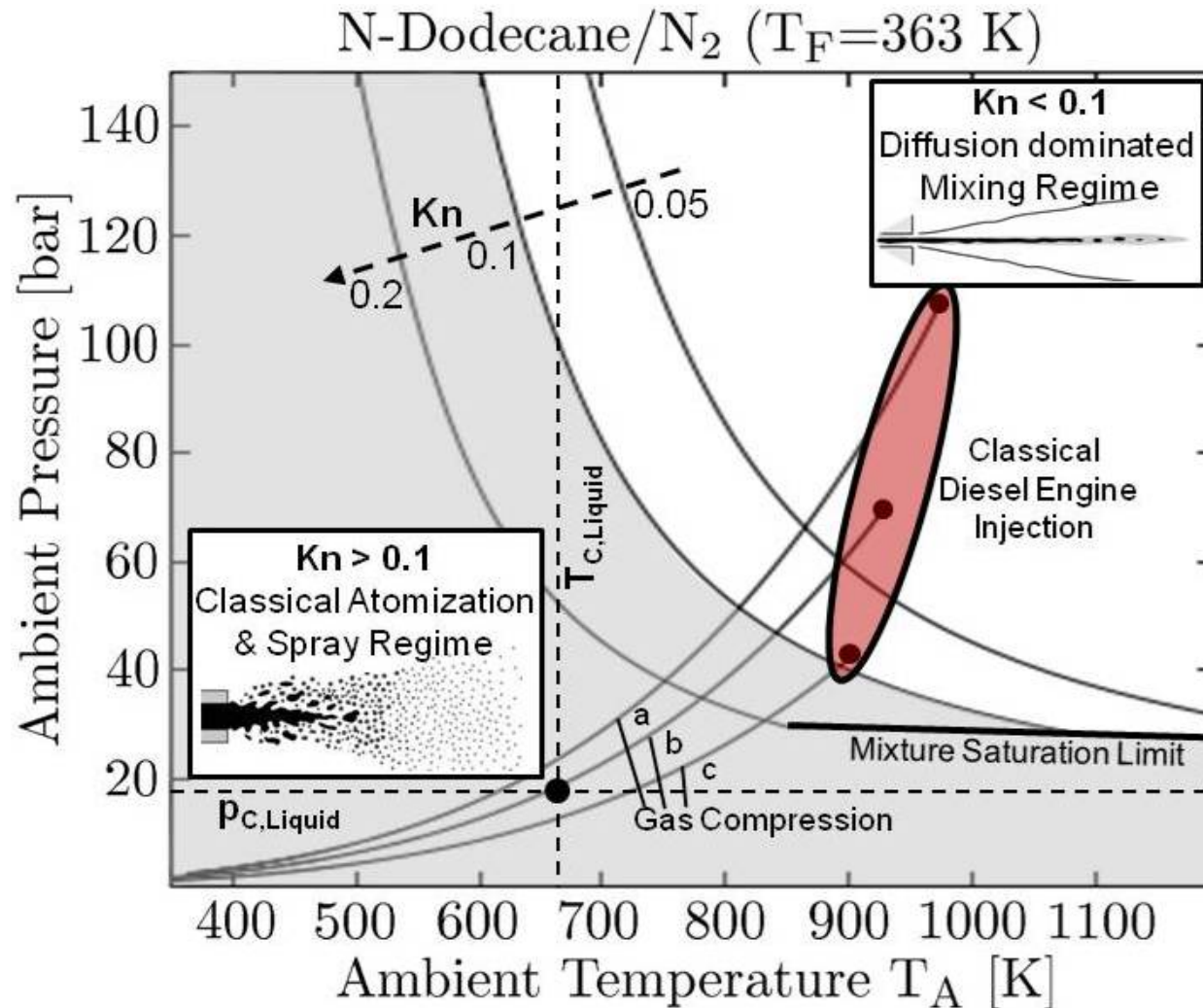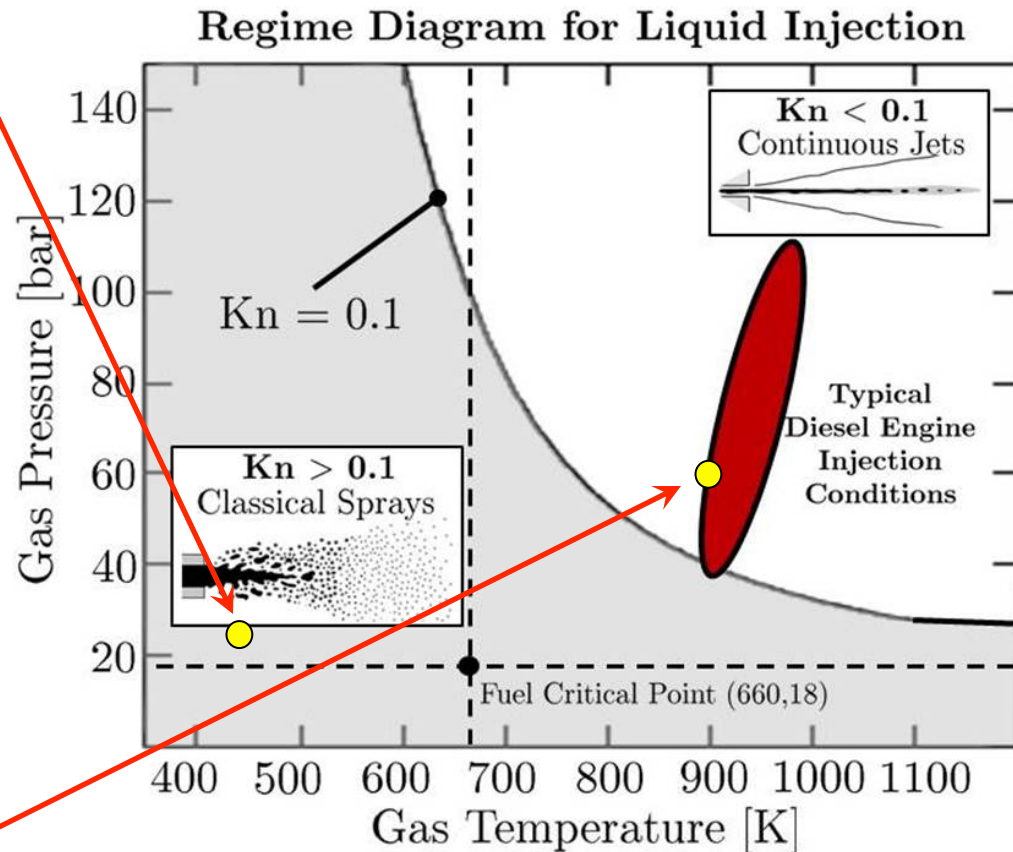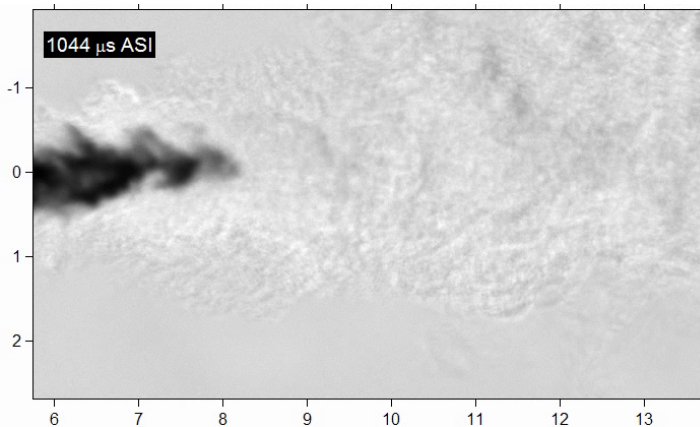 – **As pressure increases, interface enters the continuum regime due to increasing thickness and significant decrease in mean molecular path**

- **Results demonstrate classical view of jet atomization (which is currently widely assumed) is not applicable**

  – **Distinct gas-liquid interface does not exist, conventional spray model theory is not valid**

  – **Lack of inter-molecular forces promote diffusion over atomization**

  – **Real fluid thermodynamics and transport for supercritical mixtures must be considered instead**

Regime Diagram for Liquid Injection
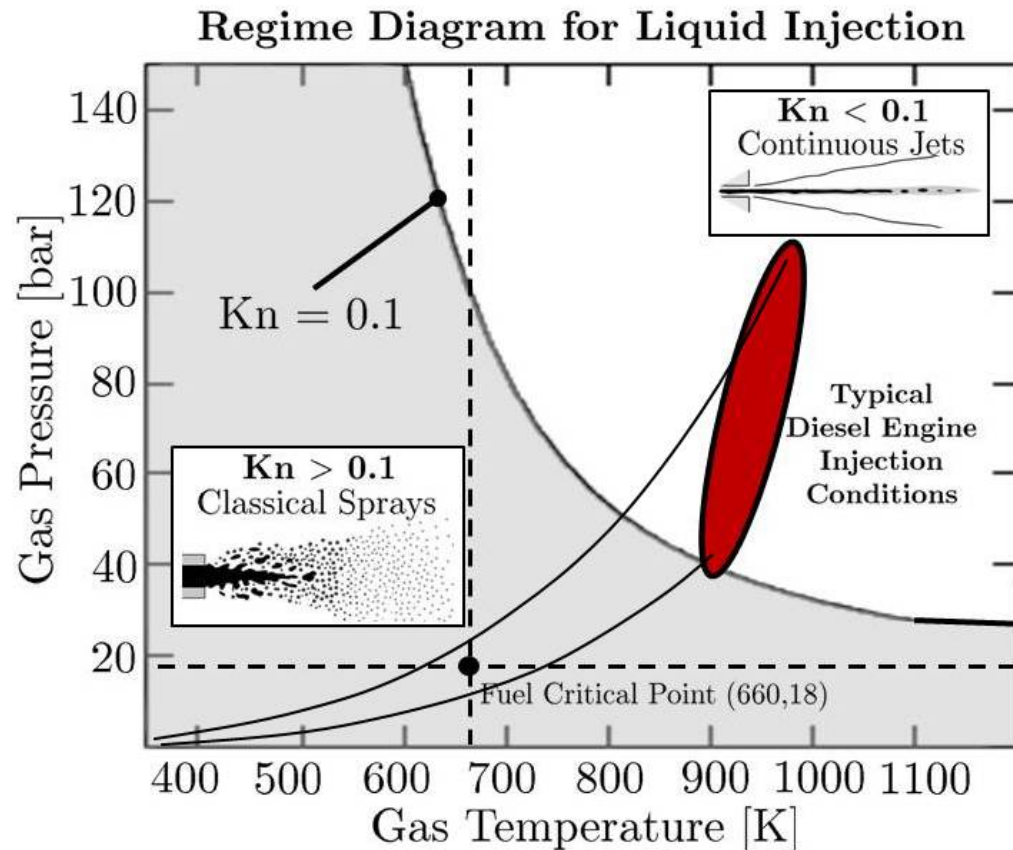
Collaborations and Institutions …
Special thanks to Dr. Rainer Dahms

- CRF Departments 8351, 8353, 8362, 8365, 8367 (Arienti, Barlow, Chen, Dahms, Debusschere, Frank, Lacaze, Michelsen, Miles, Musculus, Najm, Pickett, Settersten, Shaddix, Siebers, Templeton)
  - 8351 Reacting Flow Research
  - 8353 Combustion Chemistry
  - 8362 Engine Combustion
  - 8365 Thermal/Fluid Science and Engineering
  - 8367 Hydrogen & Combustion Technology
- Professor W. Anderson, Purdue University
- Professor J.-Y. Chen, University of California, Berkeley
- Professor B. Cuenot, CERFACS, France
- Professor A. Dreizler, Technical University of Darmstadt, Germany
- Professor B. Geurts, University of Twente, The Netherlands
- Professor D. Haworth, The Pennsylvania State University
- Professor J. Janika, Technical University of Darmstadt, Germany
- Professor A. Kempf, Duisburg-Essen University, Germany
- Professor T. Lieuwen, Georgia Institute of Technology
- Professor K. Mahesh, University of Minnesota
- Professor S. Menon, Georgia Institute of Technology
- Professor M. Modest, University of California, Merced
- Professor C. Pantano, University of Illinois at Urbana-Champaign
- Professor T. Poinsot, CERFACS, France
- Professor S. Pope, Cornell University
- Professor C. Rutland, University of Wisconsin, Madison
- Professor R. Santoro, The Pennsylvania State University
- Professor V. Sick, University of Michigan
- Professor J. Sutton, Ohio State University
- Professor H. Wang, University of Southern California
- Professor V. Yang, Georgia Institute of Technology

- Dr. C. Carter, Air Force Research Laboratory, WPAFB, OH
- Dr. A. Dord, General Electric Global Research
- Dr. T. Drozda, NASA Langley Research Center
- Dr. S.-Y. Hsieh, General Electric Aviation
- Dr. B. Hu, Cummins, Inc.
- Dr. I. Leyva, Air Force Research Laboratory, EAFB, CA
- Dr. M. Oschwald, The German Aerospace Center (DLR)
- Dr. S. Rahman, NASA Johnson Space Center
- Dr. R. Sankaran, Oak Ridge National Laboratory
- Dr. V. Sankaran, United Technologies Research Center
- Dr. K. Tucker, NASA Marshall Space Flight Center
- Dr. D. Talley, Air Force Research Laboratory, EAFB, CA
- Dr. D. Walker, General Electric Global Research

- <u>Postdoc's and Students</u>
- Judith Segura, Stanford University, Dec 2000 – Sep 2004
- Tomasz Drozda, University of Pittsburgh, Oct 2005 – Oct 2008
- Victoria Lee, Cal. Polytechnic State University, Summer 2006, 2007
- Vaidyanathan Sankaran, Georgia Tech., Feb 2006 – Oct 2008
- Robert Knaus, UIUC, Summer 2007, 2008
- Joshua Smith, University of Adelaide, Australia, 2007
- Jeffrey Doom, University of Minnesota, Jan 2009 – Aug 2010
- Bing Hu, University of Wisconsin, Madison, Jan 2009 – Sep 2011
- Guilhem Lacaze, CERFACS, Toulouse France, Aug 2009 – Present
- Ville Vuorinen, Helsinki University of Technology, Finland, 2009
- Rainer Dahms, Aachen University, Germany, Jul 2010 – Present
- Matthieu Masquelet, Georgia Institute of Technology, 2011
- Raphael Mari, CERFACS, Toulouse France, Apr 2011 – Sep 2011
- Anthony DeFilippo, U. C. Berkeley, Sep 2011 – Dec 2012
- Anthony Ruiz, CERFACS, Toulouse France, June 2012 -- Present

Proposed future work

- **Continue detailed analysis of direct-injection processes for <u>both</u> Diesel and Gasoline in collaboration with Pickett et al. and ECN participants**
  - 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)

- **Work toward LES of combustion processes in HCCI engines at operating conditions identical to the experiment of Dec et al.**
  - Proficiency and workflow for high-quality grid generation and interface with RAPTOR code framework has been significantly improved (e.g. next slide)

- **Expand collaborative activities related to ECN and priority research defined as part of the DOE BES/VT PreSICE workshop (e.g. next slides)**
  - Development of Quality Assessment Techniques for Large Eddy Simulation of Propulsion and Power Systems in Complex Geometries (w/Lacaze)
  - Development of High-Fidelity Models for Liquid Fuel Spray Atomization and Mixing Processes in Transportation and Energy Systems (w/Dahms)

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RAPTOR code framework now directly interfaced with GridPro

Time-varying body-fitted multi-block grid
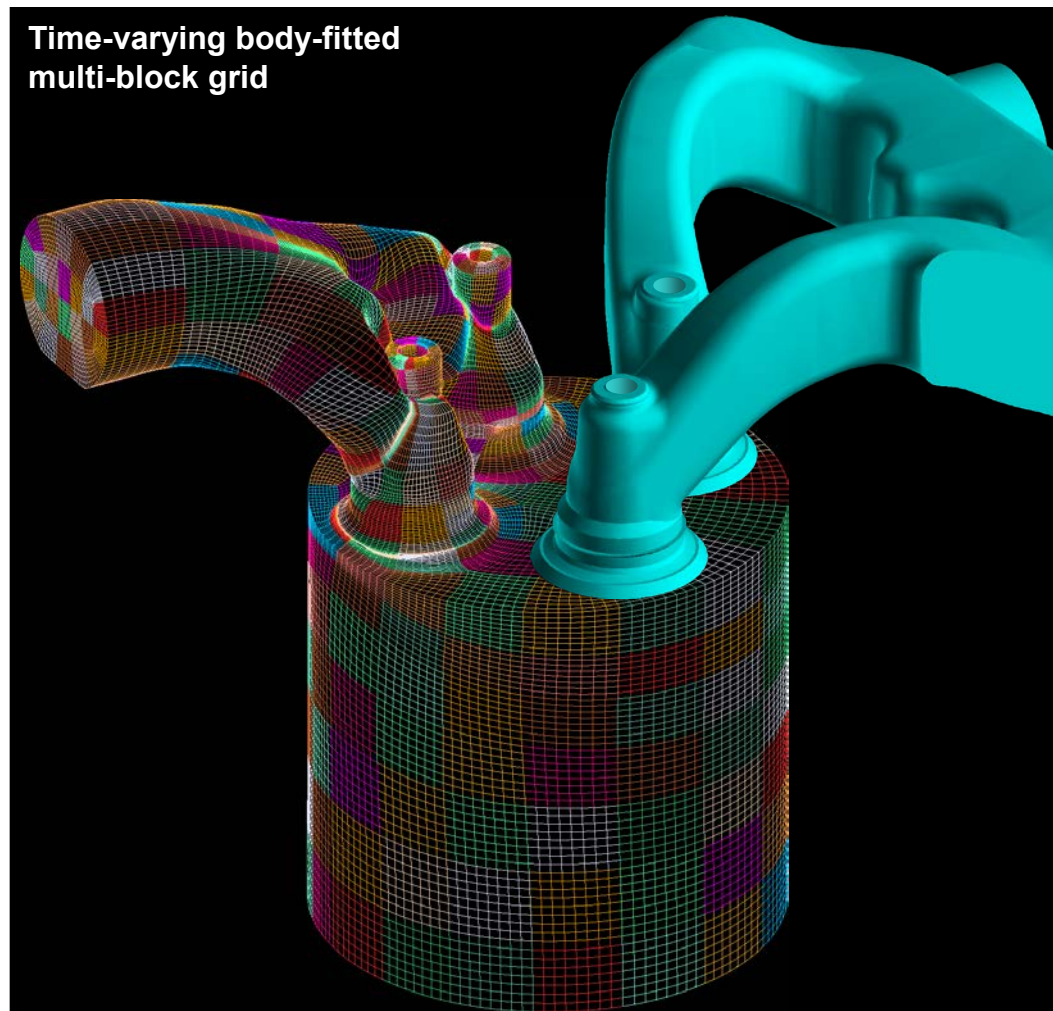
CRF optical HCCI engine, Dec et al.

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Development of quality assessment techniques for LES

- **Development of LES is complicated by the interdependence of different subgrid models, competition between modeling and numerical errors, model variability, and numerical implementation**
    - **Control of accuracy is critical for development of predictive LES**
    - **When accuracy not sufficient, results misleading and intractably erroneous**
        - **Poor numerics and/or grid quality**
        - **Lack of appropriate spatial or temporal resolution**
        - **Ill-posed boundary conditions**
        - **Inaccurate models**

- **Have begun to establish quantitative metrics to assess quality of LES**
    - **Goal to establish clear set of quantitative implementation requirements**
    - **Move beyond bulk error from multiple competing sources**
    - **Understand and control three distinct forms of error**
        - **<u>Discretization errors</u> associated with numerical techniques due to 1) temporal integration, 2) spatial differencing, and 3) related stabilization schemes**
        - **<u>Conceptual errors</u> associated with model itself due to 1) basic assumptions and 2) range of subgrid-scales it is specified to work over**
        - **<u>Total model residual errors</u> due to discretization of the sub-models themselves**

Model development for liquid fuel spray atomization, mixing, and combustion

1. **Primary atomization (sheet, filament and lattice formation)**

2. **Secondary breakup (particle deformation and coalescence processes)**

3. **Dilute spray dynamics**
   - *a.* Drop dispersion
   - *b.* Multicomponent drop vaporization
   - *c.* Two-way coupling between the gas and dispersed liquid phase
     - – Turbulence modulation (damping of turbulence due to particle drag effects)
     - – Turbulence generation (production of turbulence due to particle wakes)

4. **High-pressure supercritical phenomena**
   - *a.* Real-fluid equations of state, detailed thermodynamics and transport
   - *b.* Multicomponent mixtures, extreme property gradients, preferential transport

5. **Turbulent mixed-mode combustion**
   - *a.* Thermodynamic non-idealities, transport anomalies
   - *b.* Complex hydrocarbon chemistry, high-pressure chemical kinetics

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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 for engine design
  - Unique first principles solver for Large Eddy Simulation (LES)
  - Dedicated computational resources and facilities

- **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

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