Project ID: ACE007

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

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(with contributions from Rainer N. Dahms and Anthony Ruiz)

Combustion Research Facility
Sandia National Laboratories, Livermore, CA 94551

Support Provided by the DOE
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 simulations and models 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

Barriers

- Two sets of barriers addressed
  1 – Lack of fundamental knowledge of advanced engine combustion regimes
  – LTC technologies (i.e., understanding effects of fuel-injection, ignition-timing, heat-transfer, engine-geometry on fuel-air mixing, combustion, soot, emissions over broad operating ranges)
  2 – Lack of modeling capability for engine combustion and emission control
  – Efficient and routine use of High-Performance-Computing (HPC) to establish optimal balance between predictive and affordable models for advanced engine combustion research

Budget

- Total Project Funding
  - FY13 – $450K
  - FY14 – $450K

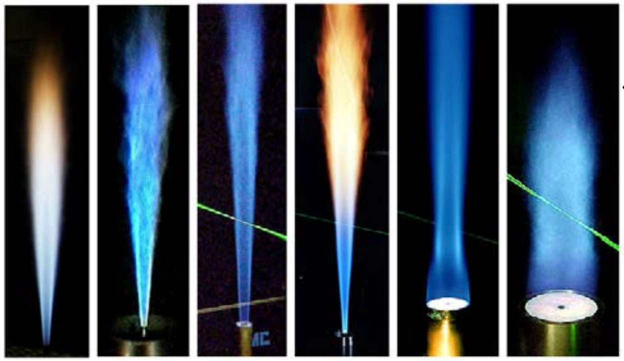
Partners

- PI's in the Engine Combustion Group (e.g., ECN, Pickett et al.)
- ≈ 50 collaborators and institutions
- Project lead: Joe Oefelein

Relevance … provide science-base for advanced model development

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

DOE Basic Energy Sciences Program



TNF Workshop
www.ca.sandia.gov/TNF

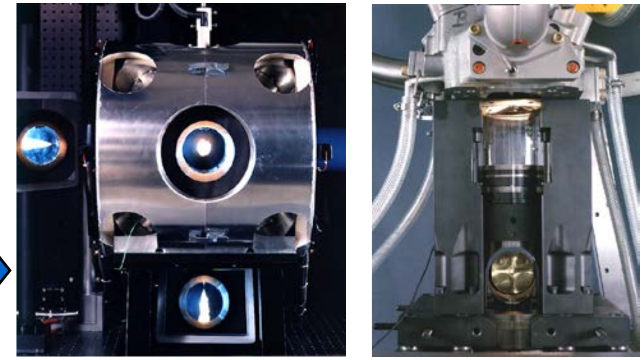
Detailed jet flame data for model development but low Reynolds number and simple fuels

Re ≈ *O(10,000)*

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

Re > *O(100,000)*

DOE Vehicle Technologies Program



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

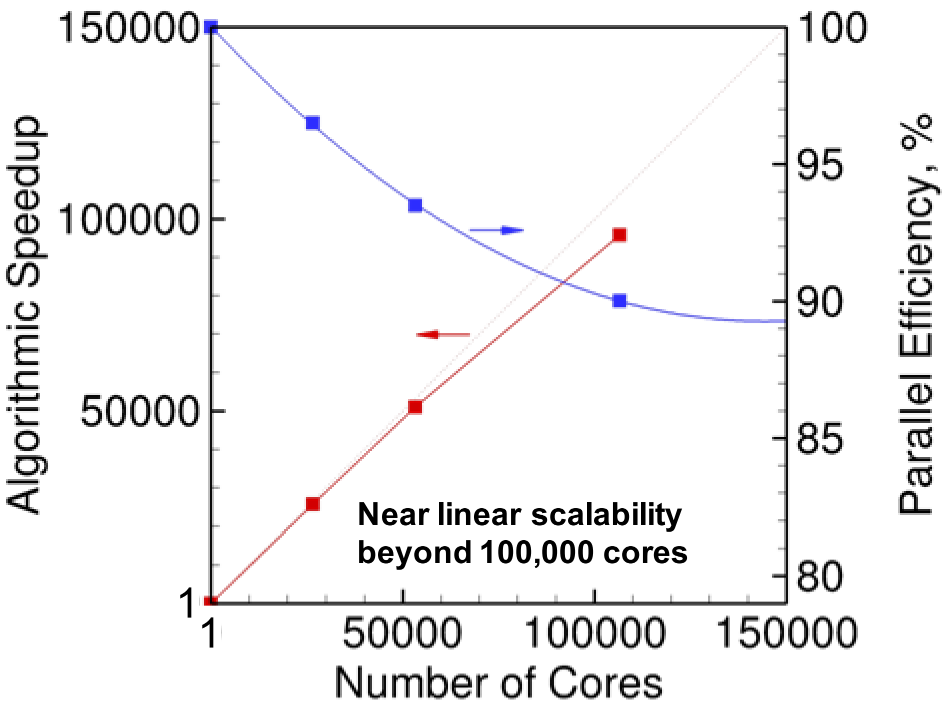
- **Goal … use "high-fidelity" LES and "first-principles" models to complement key experiments, bridge gap between basic/applied research**
  - **Detailed simulations that match geometry, operating conditions (i.e., high Re)**
  - **Retain full system coupling and incorporate detailed physics and geometry**
  - **Validation using available data, then joint analysis …**
    - **Fundamental insights not available from experiments alone**
    - **Data reduction aimed at affordable models for engineering**
- **Use high-performance computing as enabler (both local and DOE platforms)**

Milestones (FY14)

- ✓ Implement real-fluid model and perform detailed Large Eddy Simulation (LES) of the Engine Combustion Network (ECN) Spray-A case in collaboration with Pickett et al. (Q1, 12/31/13)
- ✓ Perform detailed comparisons between high-fidelity LES and available experimental data for Spray-A in preparation for 3rd Engine Combustion Network (ECN) workshop (Q2, 03/31/14)
- ✓ Complete fully-coupled first-principles LES of ECN Spray-A (including auto-ignition) and demonstrate pathway for development of reduced order models for engineering (Q3, 06/30/14)
- Complete first detailed LES of the optical Low Temperature Gasoline Combustion (LTGC) engine and initial comparisons with experimental data in coordination with VT LTGC project (Q4, 09/30/14)

Approach … 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)**
  - Staggered finite-volume differencing (non-dissipative, discretely conservative)
  - Dual-time stepping with generalized preconditioning (all-Mach-number formulation)
  - Detailed treatment of geometry, wall phenomena, BC's
  - Massively-parallel

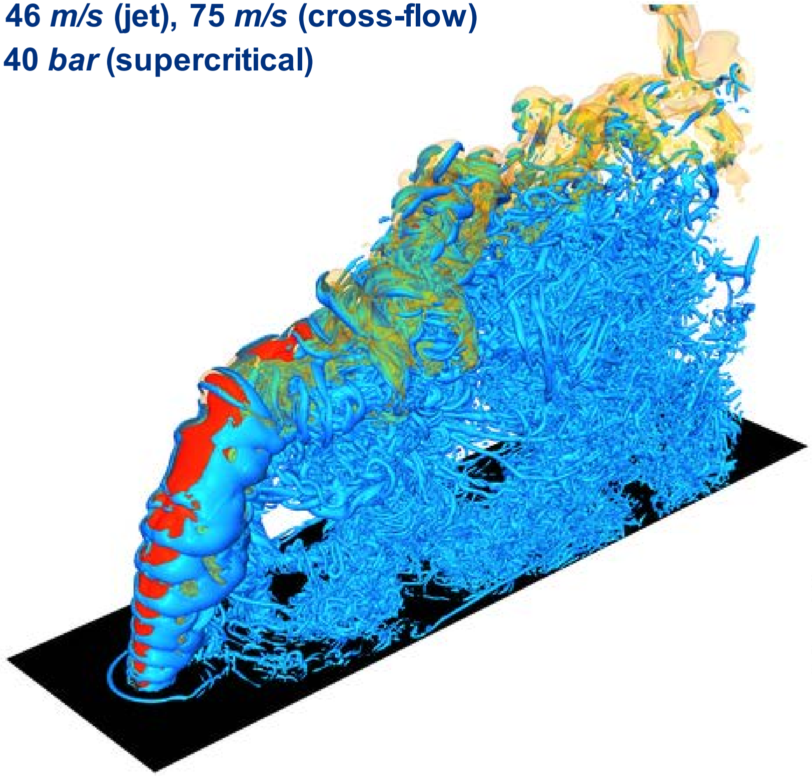


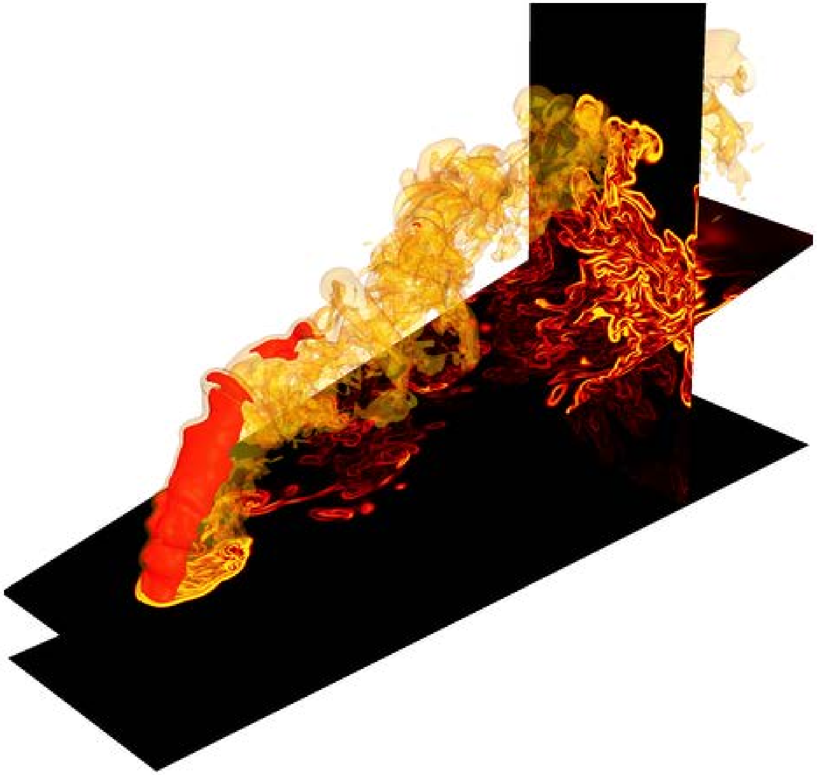
- Results from strong and weak scaling on Oak Ridge National Laboratory CRAY XK7 (Titan), June 2013
- Test case – jet-in-cross-flow, 500-million cells
  - Strong scaling: 24,000 to 120,000 cores, > 90% efficiency
  - Weak scaling: 500-million-cells/24,000-cores to 2-billion-cells/120,000-cores, < 4% increase in CPU time
- Currently being refactored for hybrid multi-core parallelism and GPU acceleration (MPI/OpenMP/OpenACC)

"High-fidelity" LES & "first-principles" models have specific definitions

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

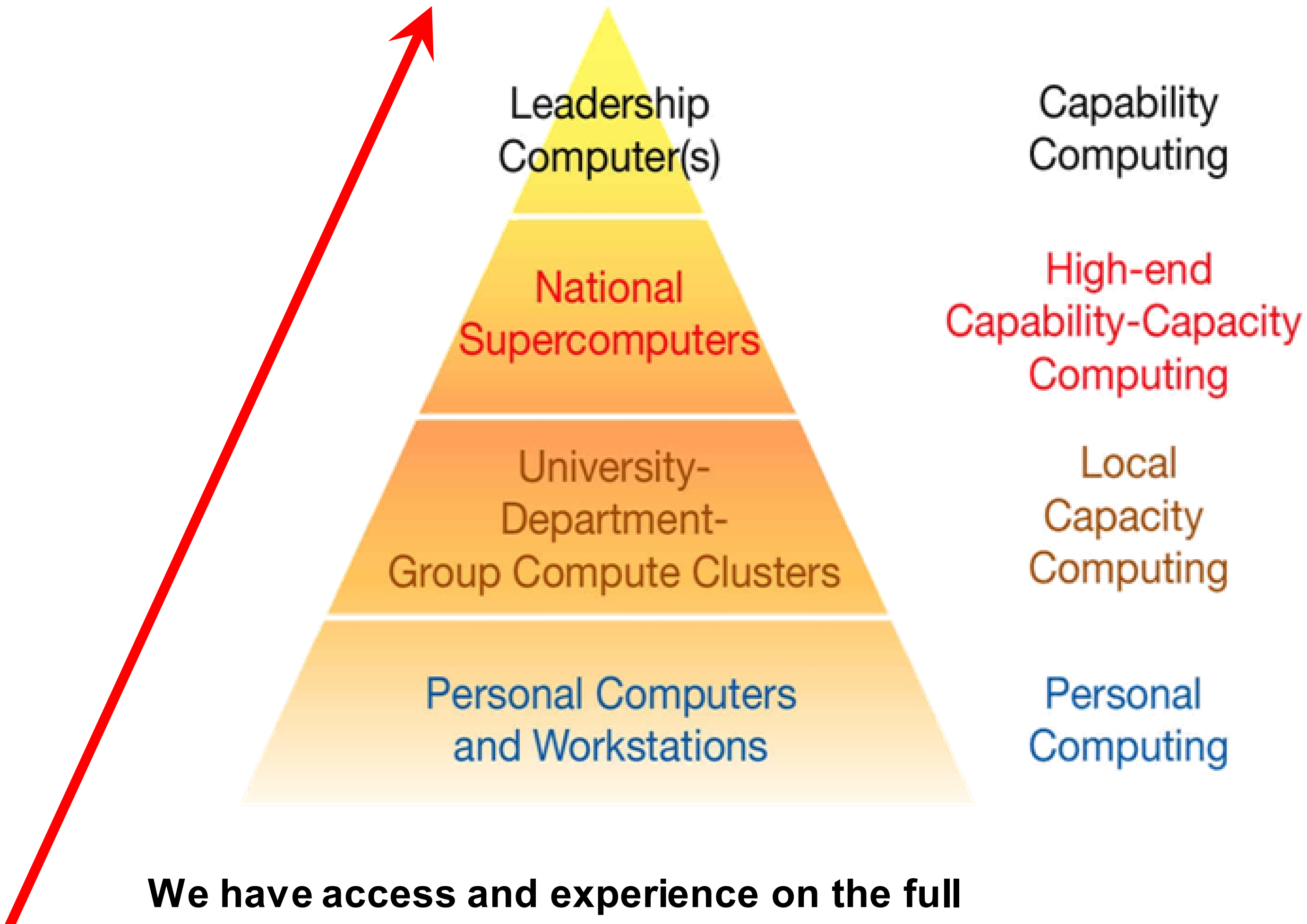
- Re = 100,000 (jet), 620,000 (cross-flow)
- U = 46 *m/s* (jet), 75 *m/s* (cross-flow)
- P = 40 *bar* (supercritical)





- High-fidelity LES implies we are resolving scalar dissipation with structurally/physically correct dynamics
- First-principles models implies the use of next generation models with no tuned constants (lim Δ➔0 = DNS)

Supporting Resources



We have access and experience on the full hierarchy of computer platforms for science

Supporting Resources

- OLCF (27 PF / Hybrid)
  - EERE-VT (INCITE/ALCC)
  - O(50-million CPU-HRS)

- ALCF (10 PF)
  - EERE-VT and SC-BES
  - 2014 ALCC, Proposed INCITE


In-house BES/VT midscale clusters (50 TF)

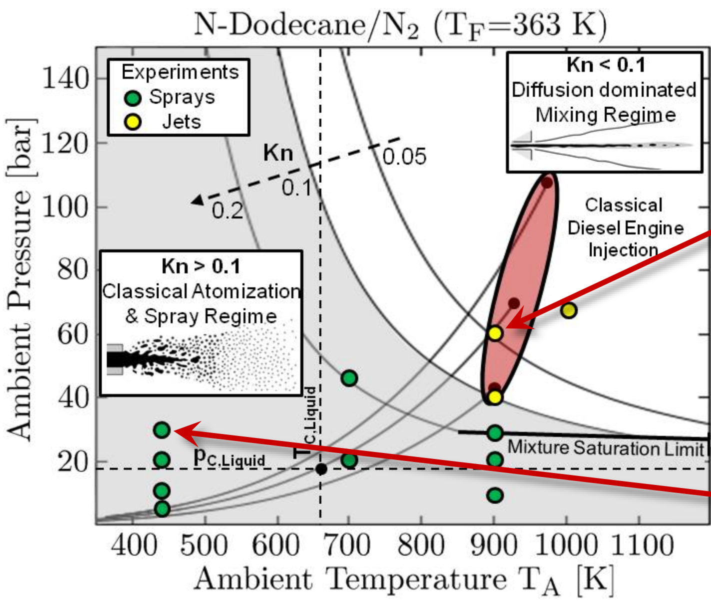
- NERSC (2.4 PF)
  - Office of Science (SC) – BES
  - O(5 – 10-million) CPU-HRS

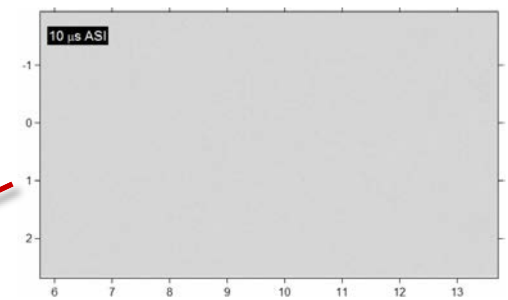
We have access and experience on the full hierarchy of computer platforms for science

Technical Accomplishments and Progress

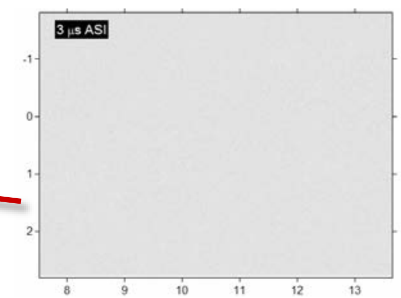
Fundamental differences between gasoline & diesel fuel sprays revealed

Regime diagram for n-dodecane injected into nitrogen





Diffusion dominated mixing (supercritical fluid)



Classical atomization and spray dynamics

R. N. Dahms and J. C. Oefelein. On the transition between two-phase and single-phase interface dynamics in multicomponent fluids at supercritical pressures. *Physics of Fluids*, **25**: 092103, 2013.

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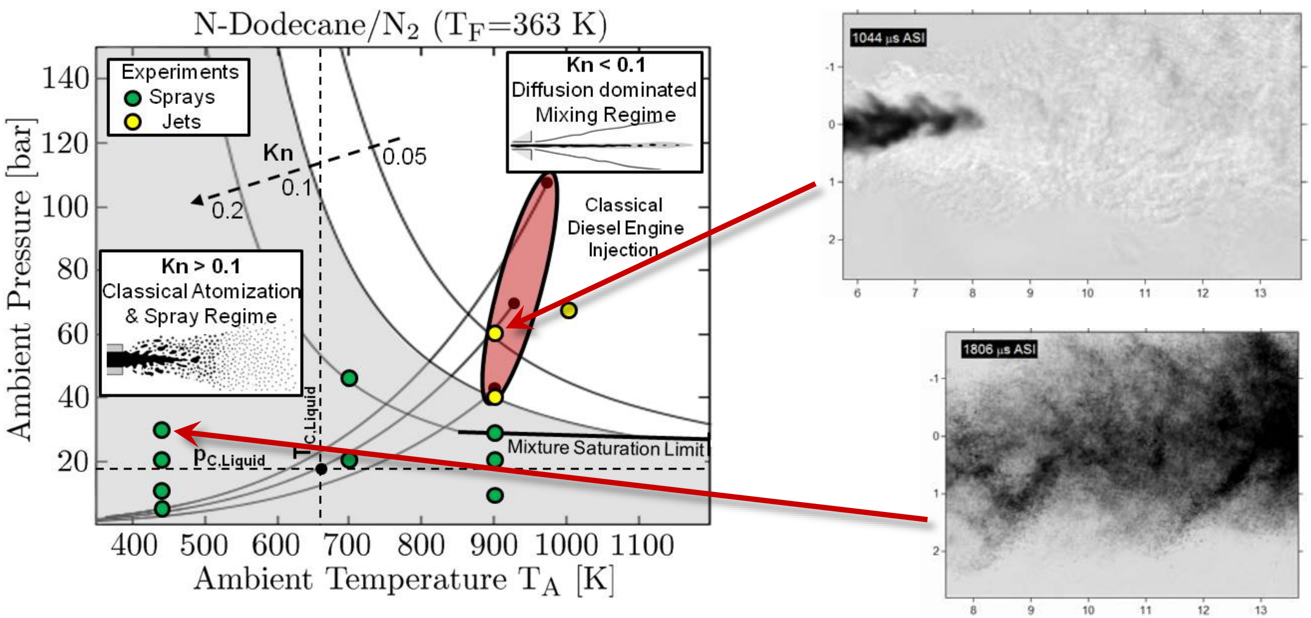


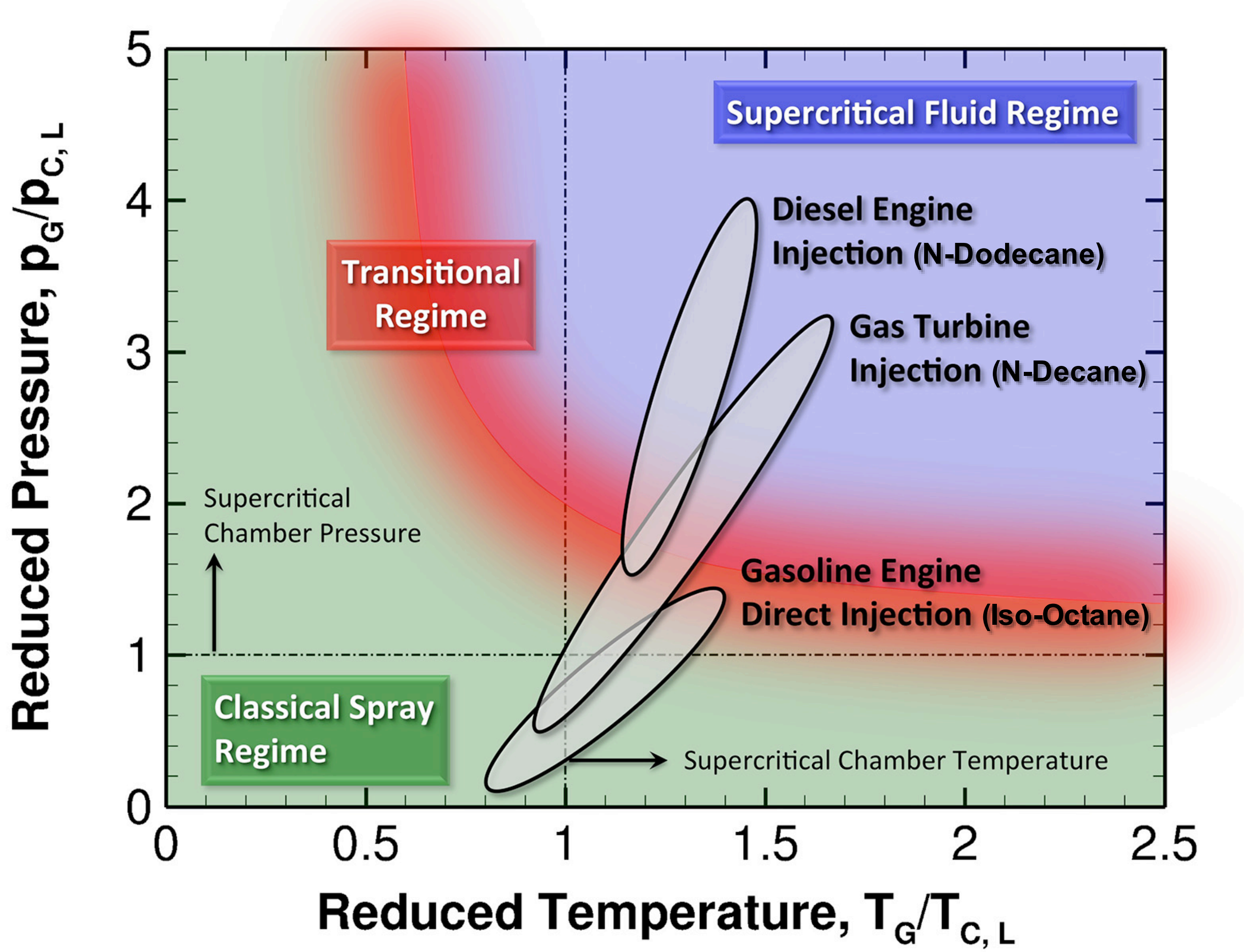
Diffusion dominated mixing (supercritical fluid)

Classical atomization and spray dynamics

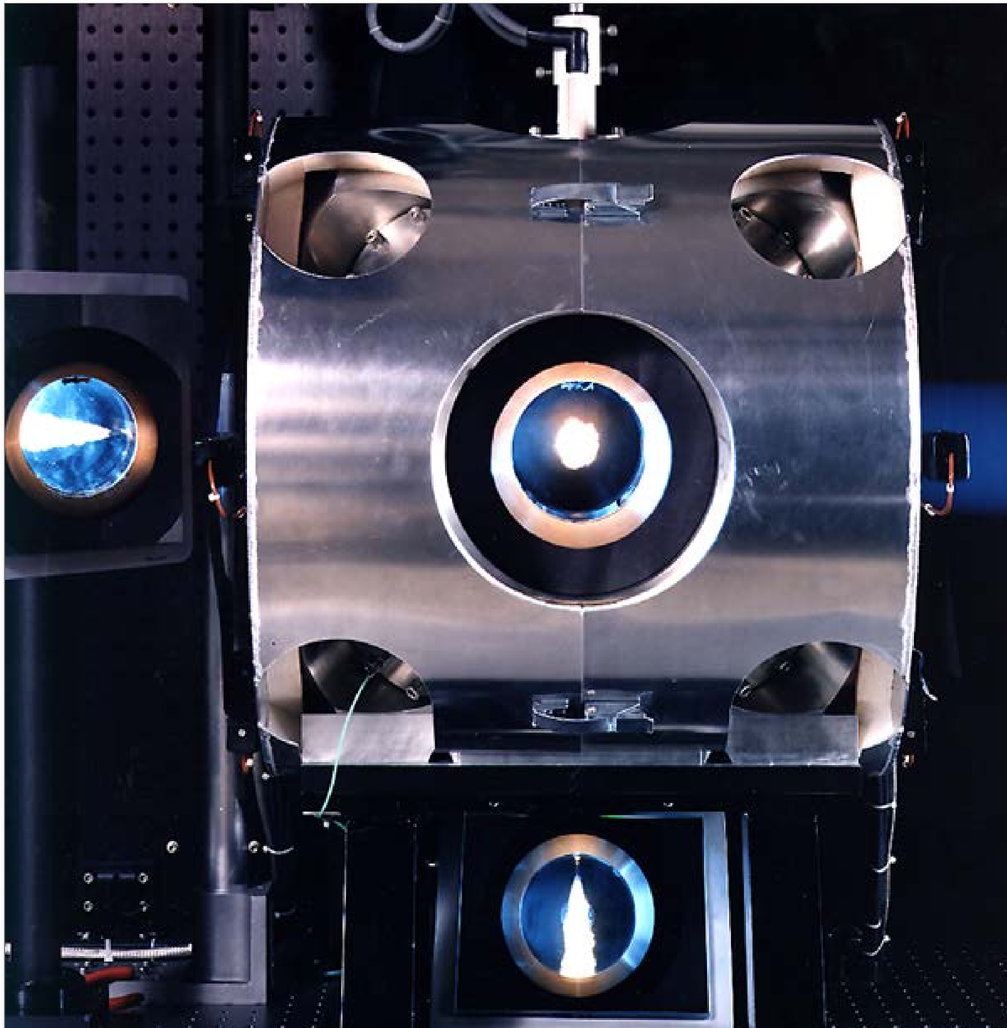
- **Classical Lagrangian drop models do not correctly account for diffusion dominated mixing in the supercritical fluid regime (drops not present)**
- **Advanced spray models must account for both extremes**

R. N. Dahms and J. C. Oefelein. On the transition between two-phase and single-phase interface dynamics in multicomponent fluids at supercritical pressures. *Physics of Fluids*, **25**: 092103, 2013.

Analysis has now been generalized and extended to a variety of systems



Based on this we performed LES of Spray-A case using real-fluid model



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

Peak Injection Conditions

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

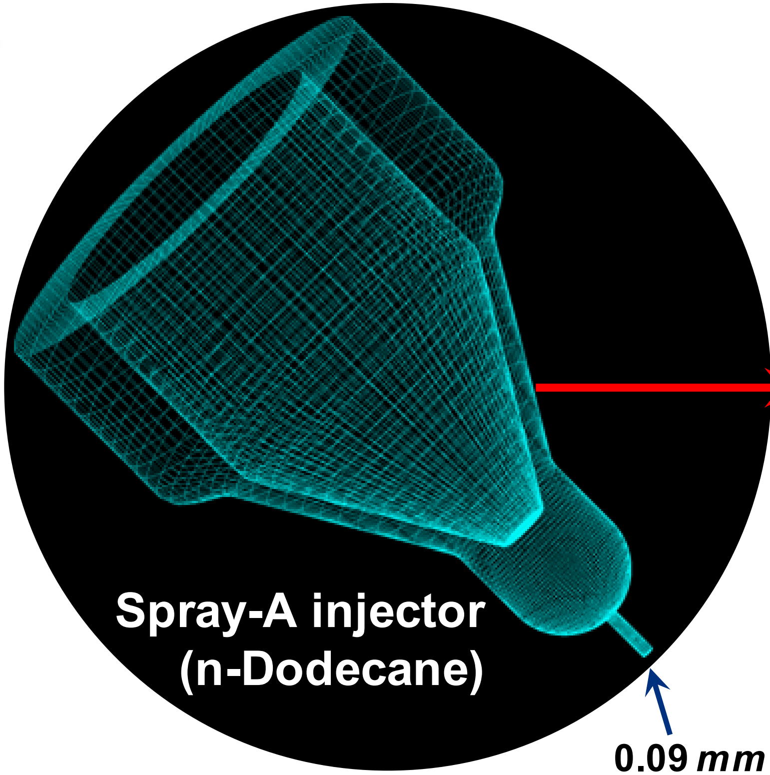
Peak Chamber Conditions

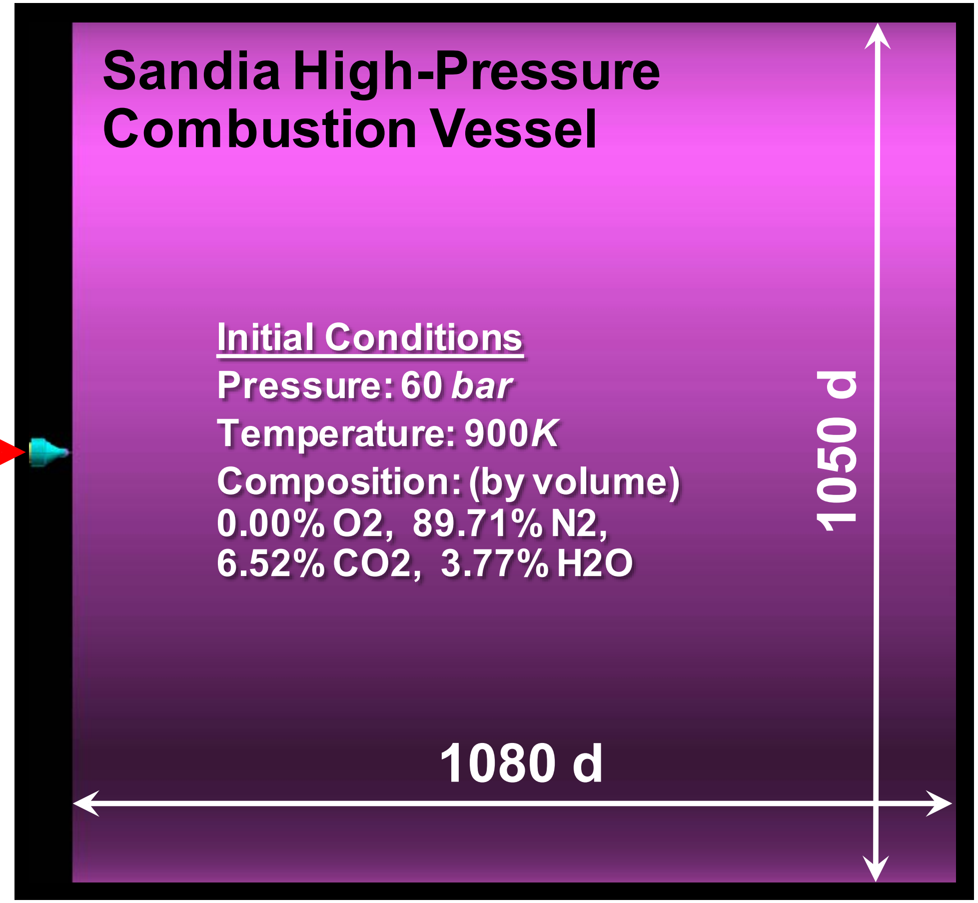
Pressure: 350 *bar*
Temperature: 1300 *K*
Composition: 0 – 21% O_2

Available Data

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

Computational domain includes injector tip and vessel



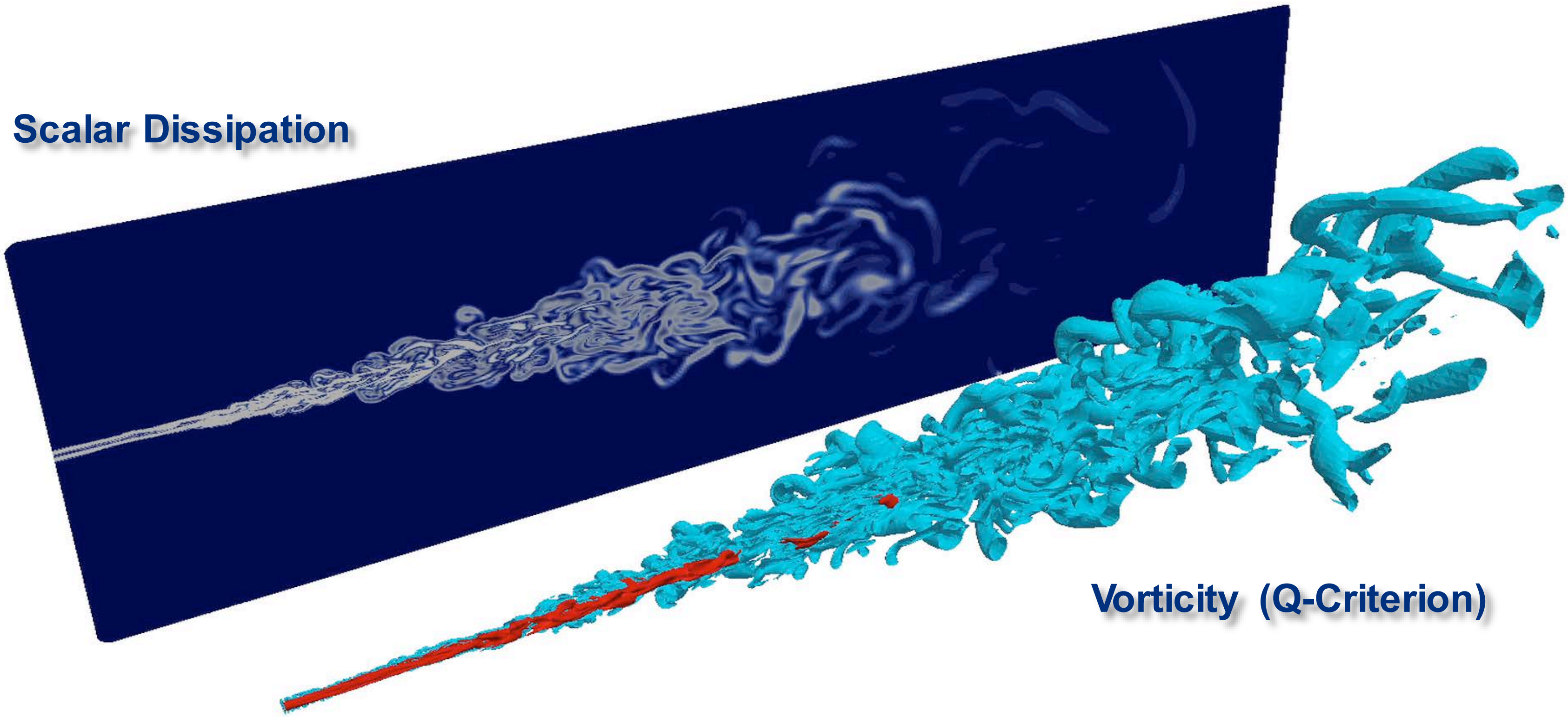


Computational Domain

Injection Conditions

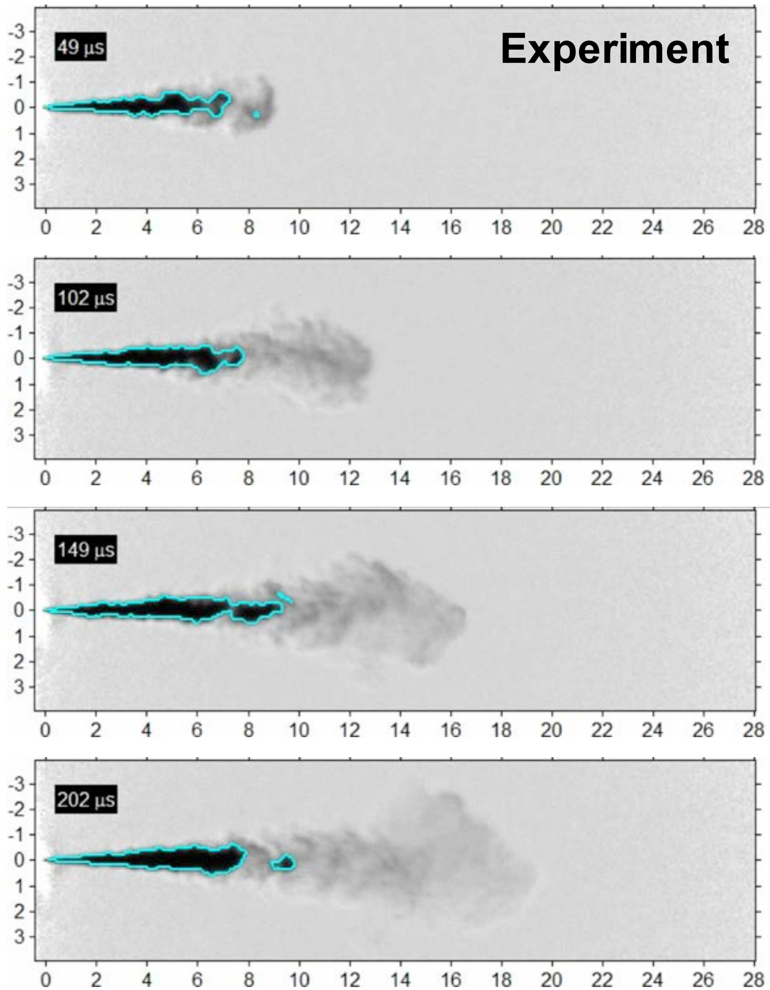
Peak Velocity:	600 *m/s*
Peak Re_d:	117,000
Density:	650 kg/m^3
Temperature:	363 *K*

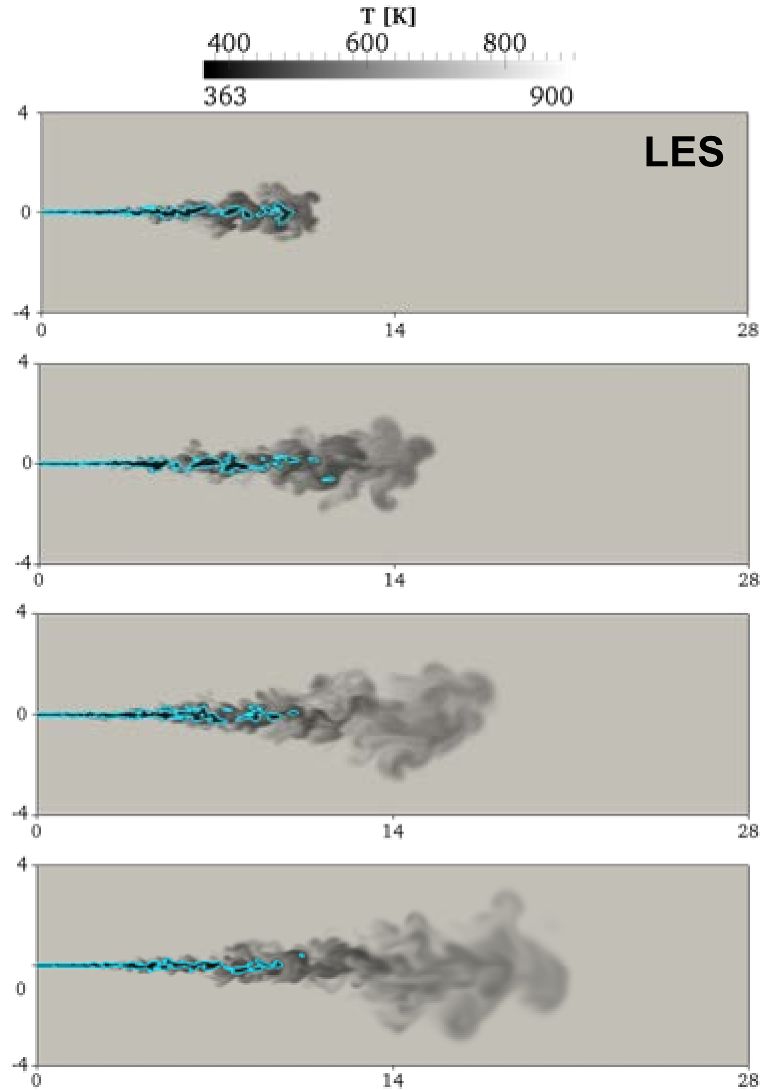
Transient evolution of jet shows detailed structural flow interactions



We performed detailed comparisons with experimental data for ECN3

What are the optimal liquid-vapor penetration thresholds to compare?





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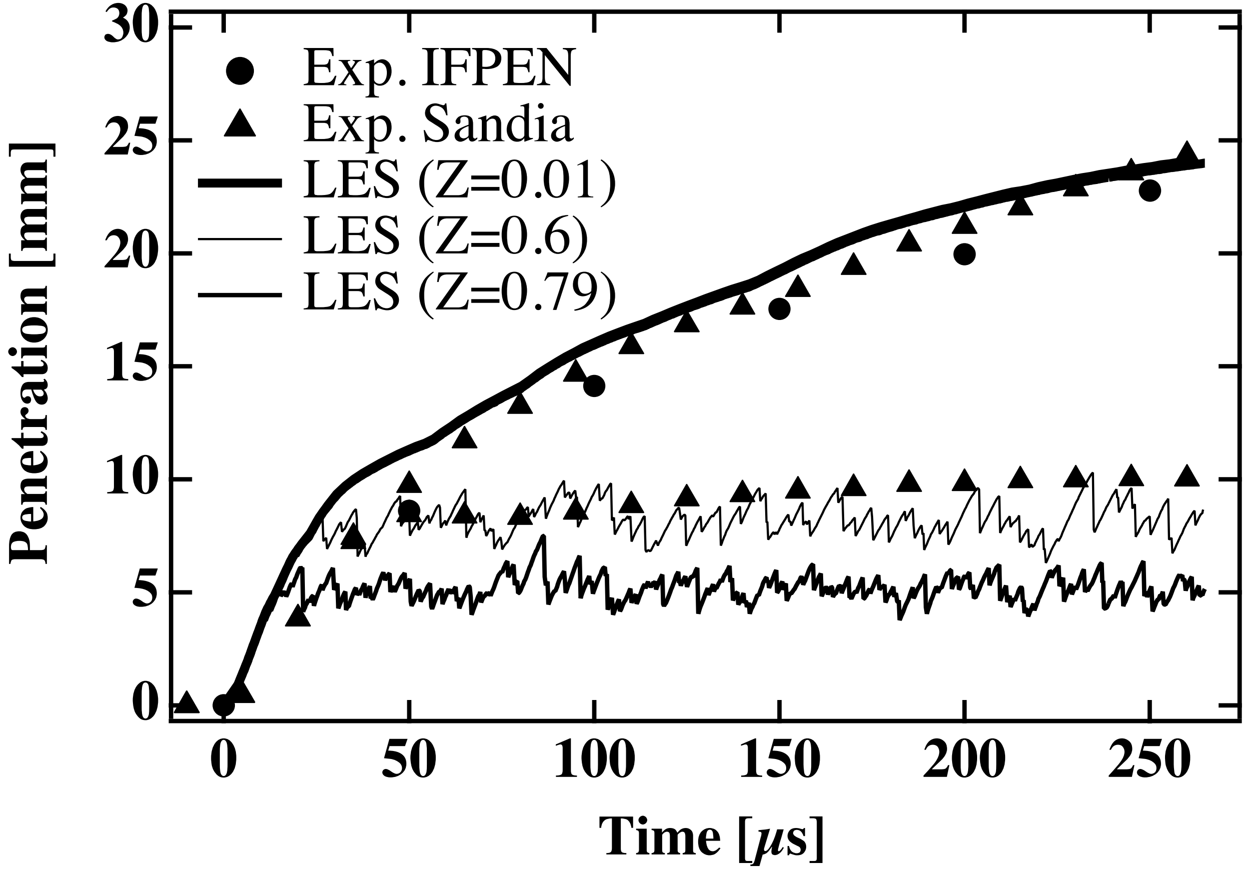
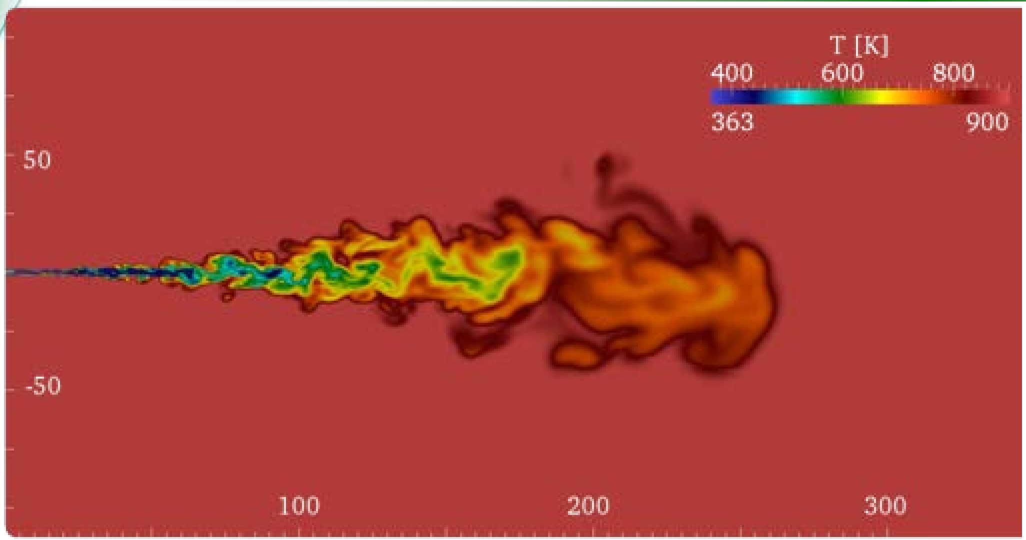
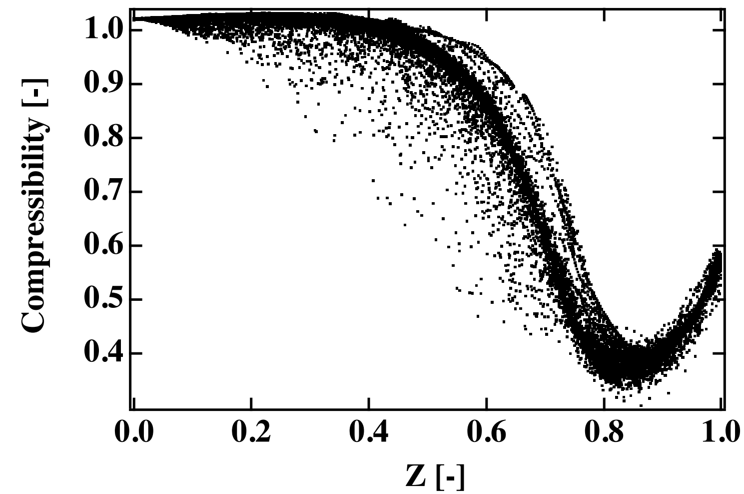
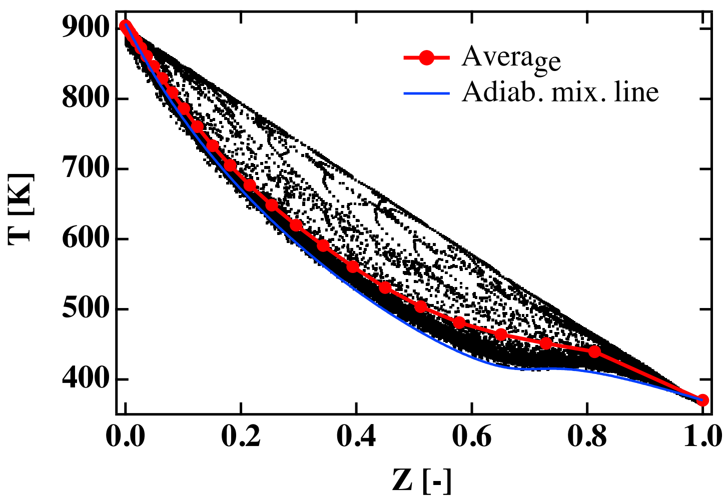
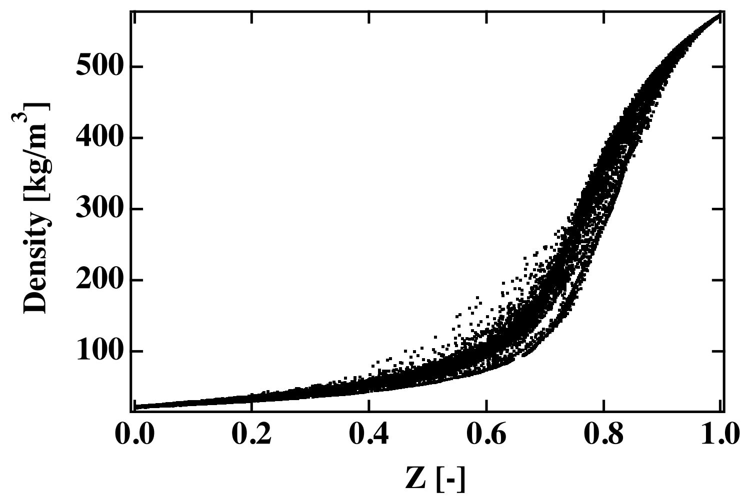


We have also extracted complementary data not available from experiments



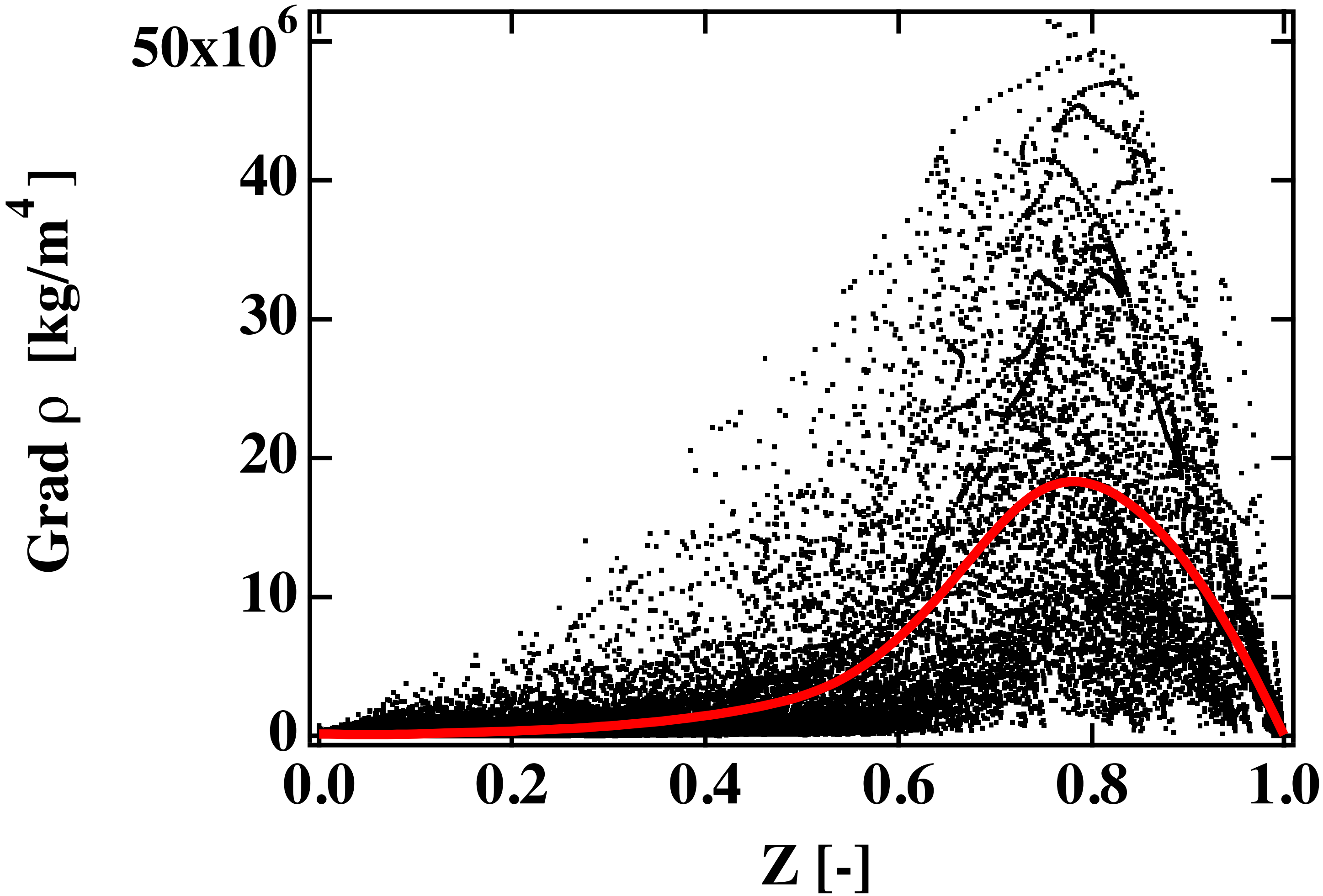




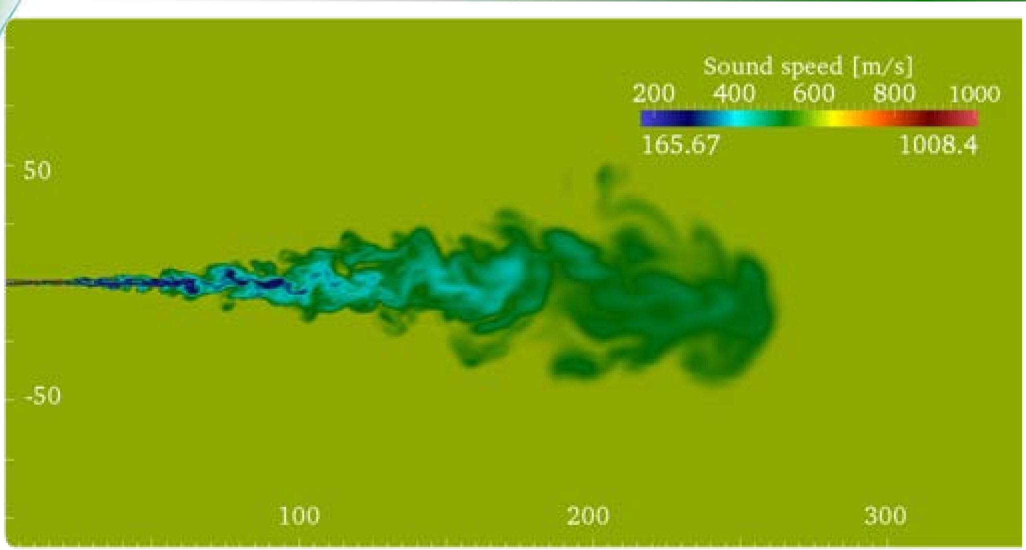


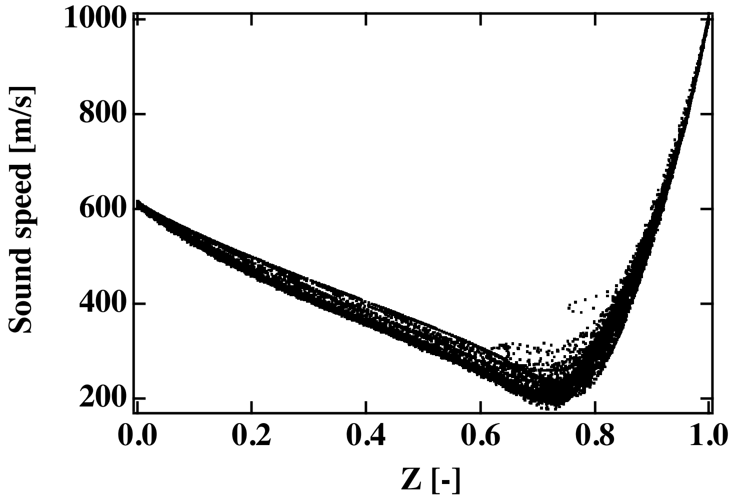
Non-ideal thermodynamics and transport govern mixture state prior to ignition

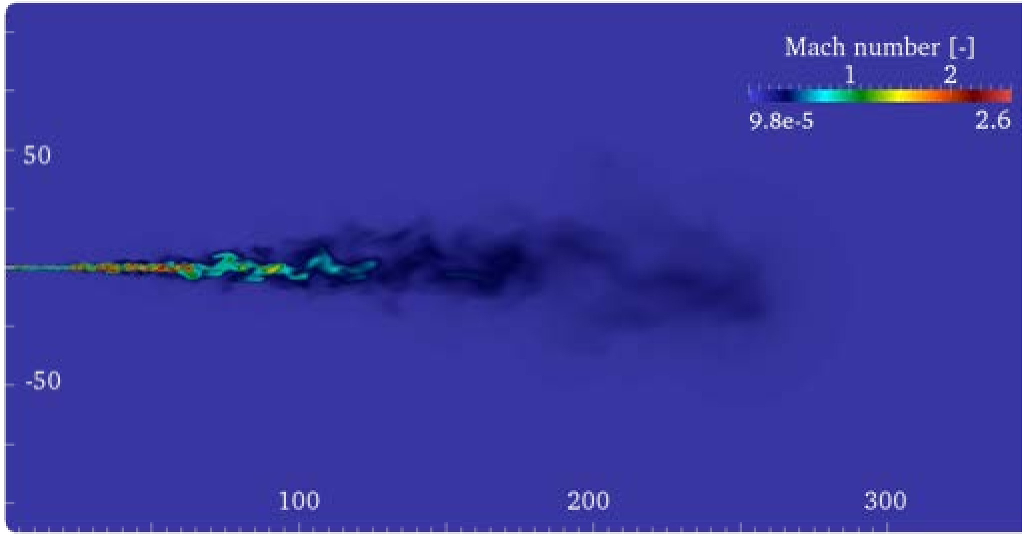
Large property gradients in shear-layer dominate transient mixing

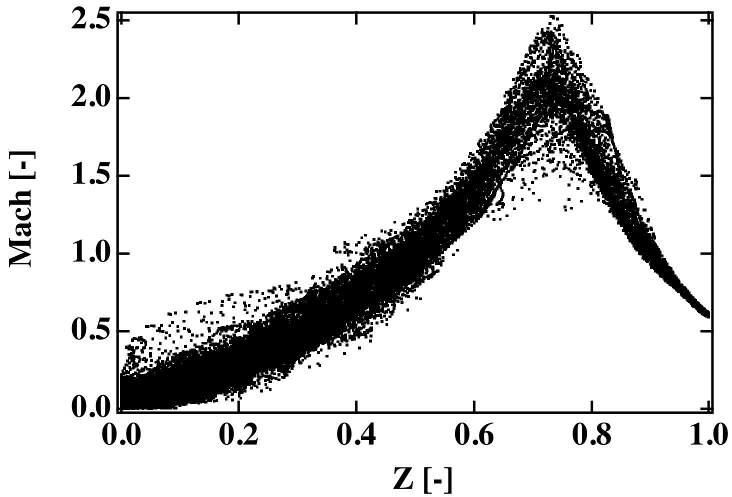


Localized supersonic regions caused by wide variation in sound speed









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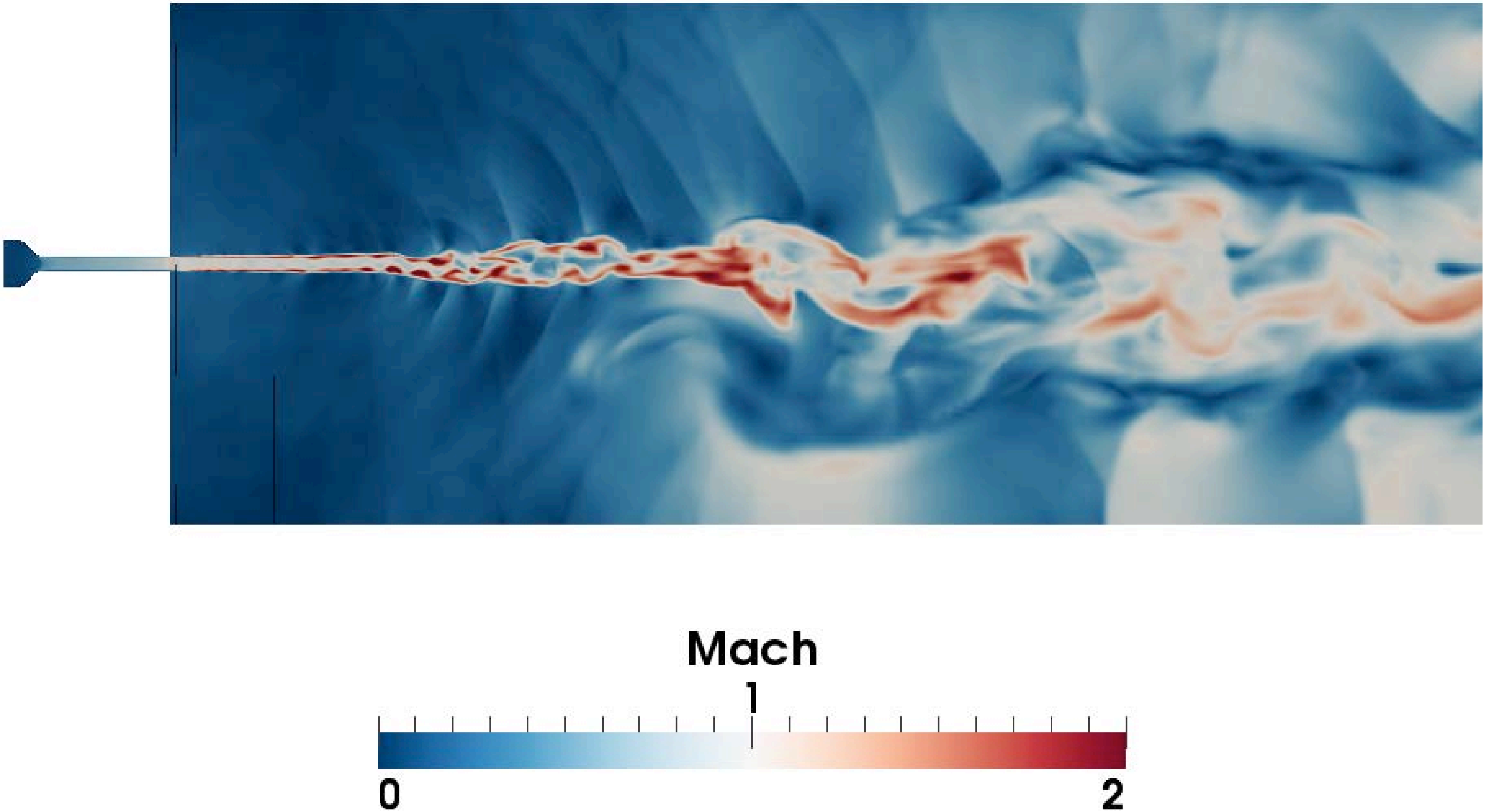
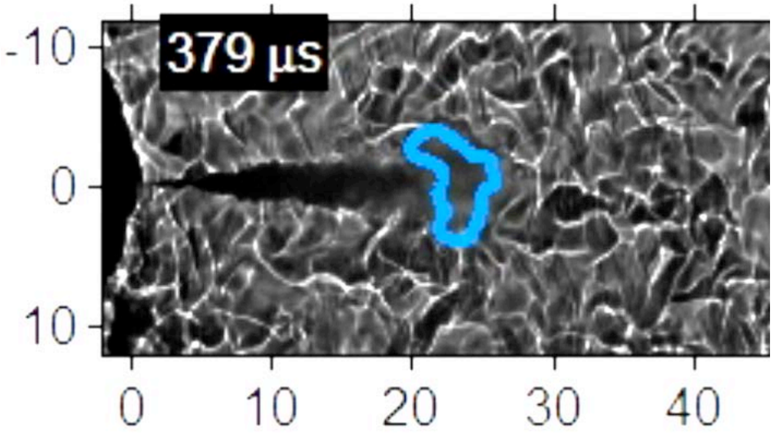
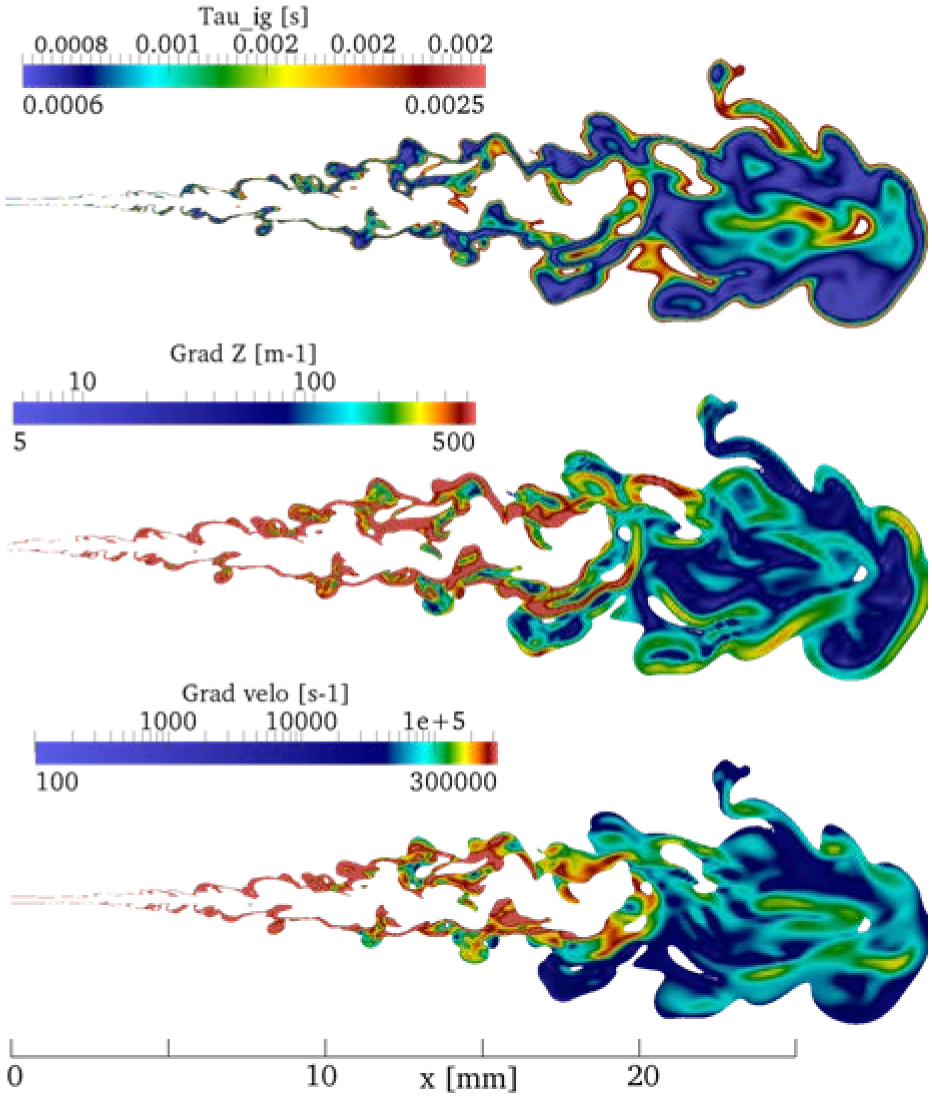


Detailed analysis reveals transient mixture state just prior to autoignition



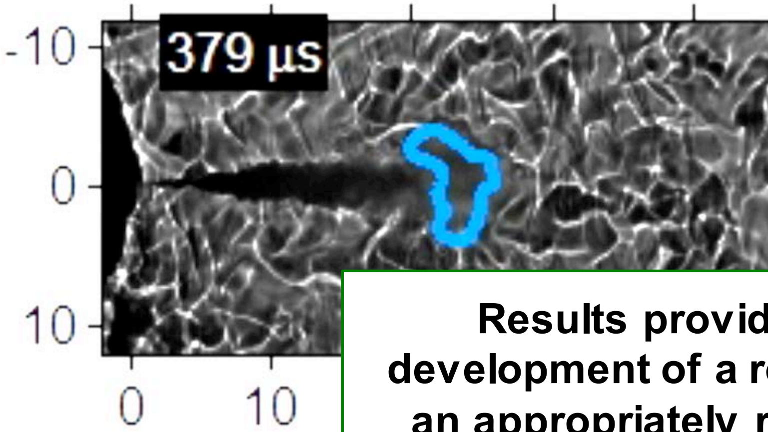


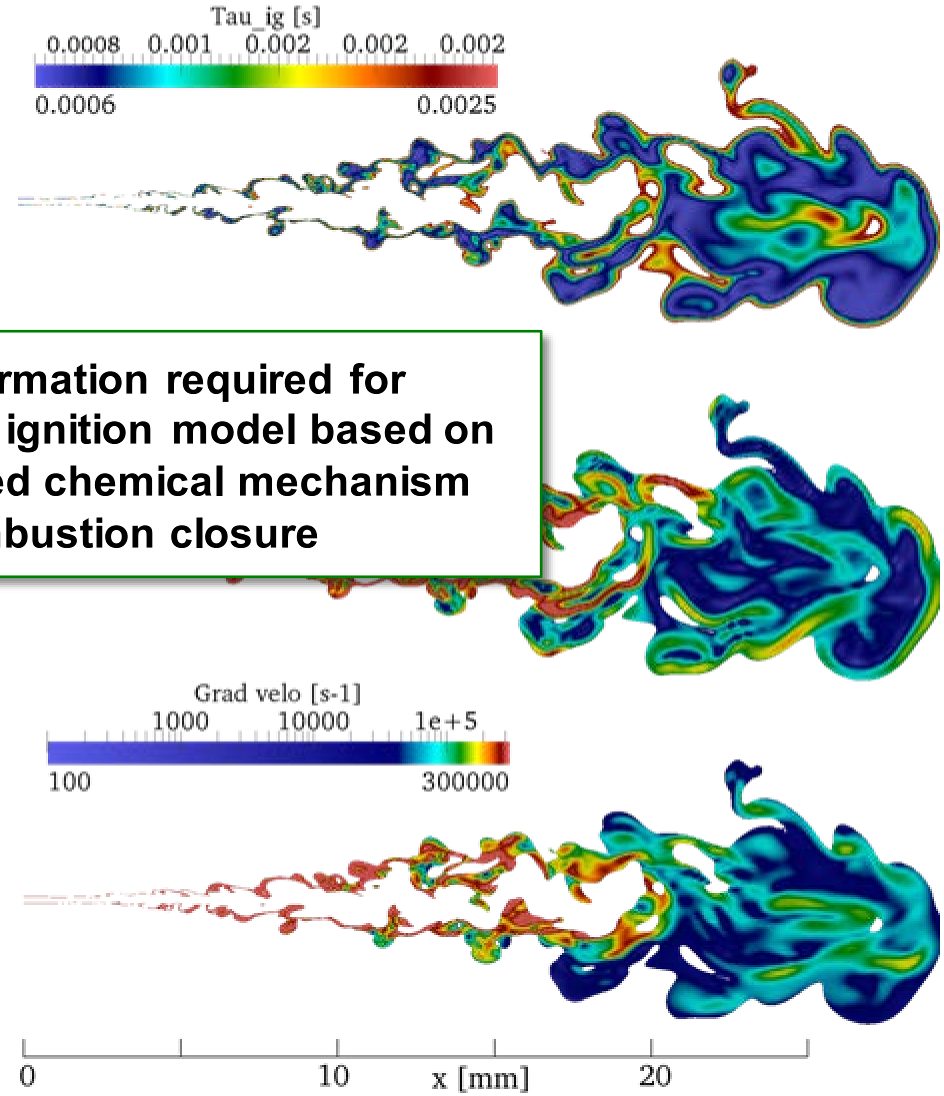
Autoignition most likely to occur where:

- **Ignition Delay Time,**
- **Scalar Dissipation Rate, and**
- **Strain Rate**

are simultaneously minimized

Detailed analysis reveals transient mixture state just prior to autoignition





Results provide information required for development of a robust ignition model based on an appropriately reduced chemical mechanism and related combustion closure

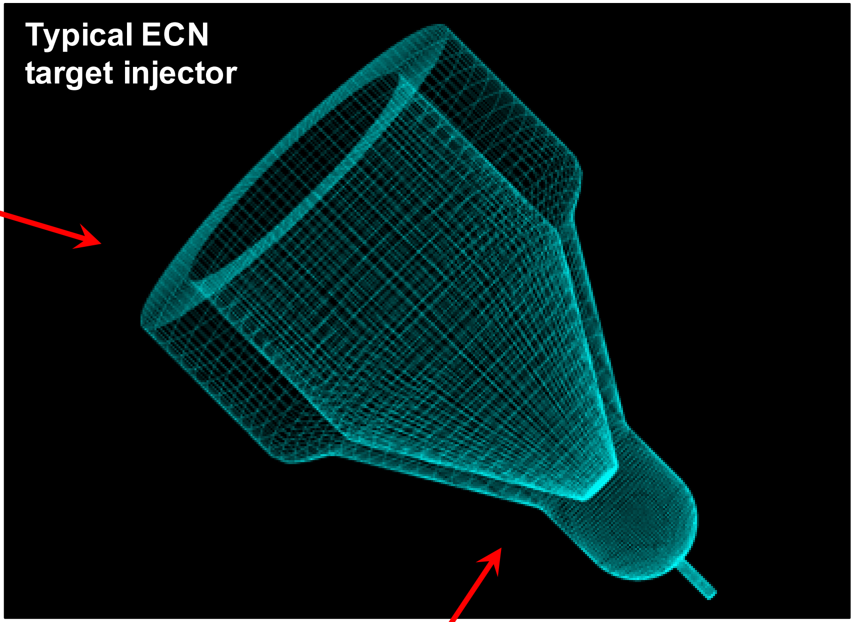
Autoignition most likely to occur where:

- Ignition Delay Time,
- Scalar Dissipation Rate, and
- Strain Rate

are simultaneously minimized

Proposed future work

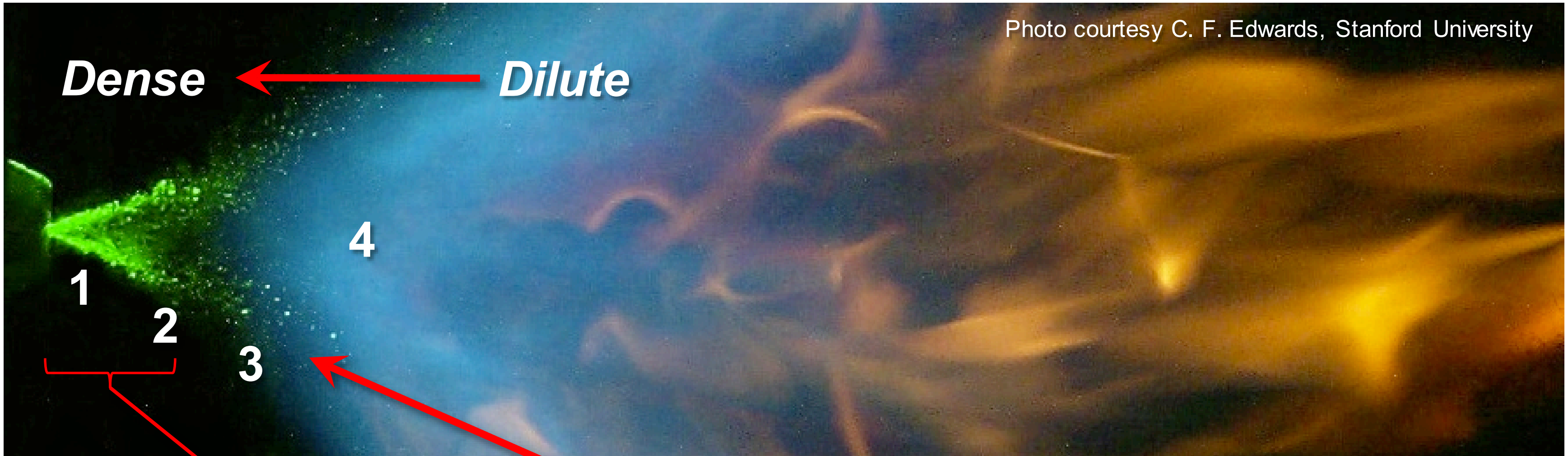
- Continue detailed analysis of direct-injection processes for both Diesel and Gasoline in collaboration with ECN activities
  - Perform detailed analysis of injector geometry and wall surface anomalies to determine effect on nozzle exit condition
  - Begin parallel effort aimed at treatment of classical GDI spray phenomena following (Lagrangian-Eulerian drop tracking)
  - Extend combustion closure for n-dodecane system to spark-ignited GDI with iso-octane
- Following the approach outlined above, expand the current focus on optical engines (e.g. CRF LTGC, UM TCC engines)
  - Proficiency and workflow for high-quality grid generation and interface with RAPTOR code framework has been significantly improved
  - Systematically establish high-fidelity benchmarks by adding detailed physics and wall treatments (e.g., thermodynamics, transport, combustion, radiation, and wall heat transfer)
- Establish close working collaborations with engineering code teams (e.g., S. Som et al. at ANL) with emphasis on joint comparisons and analysis of selected target cases



- Needle wobble
- Wall profile anomalies
- Wall roughness and heat transfer
- Compressibility effects and cavitation
- Geometric asymmetries, boundary layer dynamics
- Initial condition inside sac, cycle to cycle variations

e.g., to what degree can the cut-cell technique used in CONVERGE^{TM} reproduce important wall effects, etc.

Remaining challenges and barriers 1/2 … treatment of classical GDI sprays



Current LDRD (Arienti/Oefelein/Doisneau)

- Liquid fuel injection and multiphase flow processes are prevalent in many combustion devices
- Liquid injection controls fuel-air mixture formation, which ultimately sets conditions for combustion
- Lack of accurate models is a major barrier toward design of high-efficiency, low-emissions systems

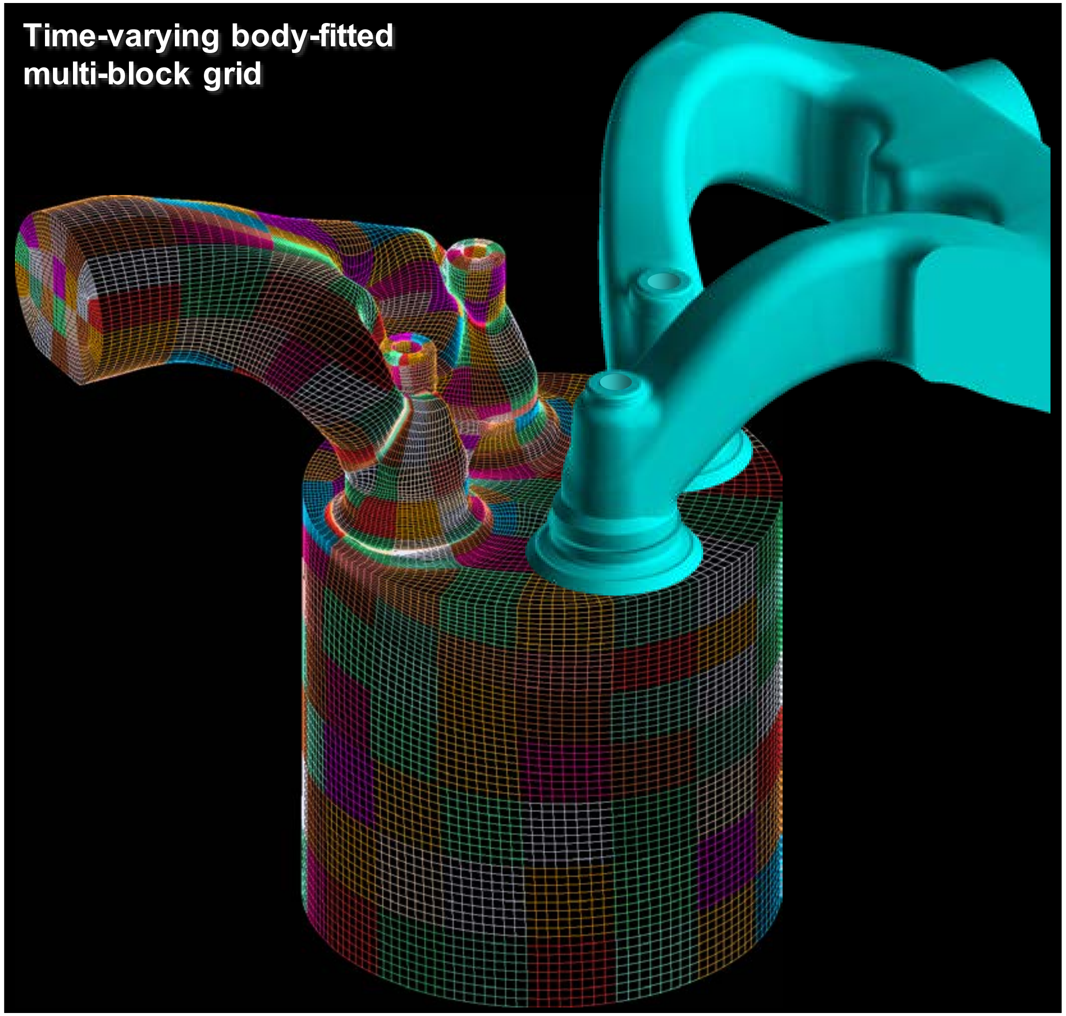
1. **Primary atomization (sheet, filament and lattice formation)**
2. **Secondary breakup (particle deformation and coalescence processes)**
3. **Dilute spray dynamics**
   a. Drop dispersion
   b. Multicomponent drop vaporization
   c. Two-way coupling between gas and dispersed liquid phase
      − Turbulence modulation (damping of turbulence due to particle drag effects)
      − Turbulence generation (production of turbulence due to particle wakes)
4. **Turbulent mixed-mode combustion**
   a. Complex hydrocarbon chemistry
   b. High-pressure chemical kinetics
5. **High-pressure supercritical phenomena (not shown)**
   a. Real-fluid equations of state, detailed thermodynamics and transport
   b. Multicomponent mixtures, extreme property gradients, preferential transport

Early Career LDRD (Dahms/Oefelein)

Remaining challenges and barriers 2/2 … enhancing workflow for HPC

- **RAPTOR is designed to facilitate complex time-varying geometries with high accuracy**
  - Hexahedral grids with staggered spatial stencils provide optimal numerics for LES
  - Multi-block decomposition with generalized connectivity provide optimal treatment of surfaces
- **Refactoring for hybrid multi-core systems required for optimal use of Leadership Class Computers**
  - MPI tasks at block/node level
  - OpenMP at flux/operator level
  - OpenACC for GPU acceleration, e.g., property, chemistry, SGS-model kernels
- **Routine use of *O*(100,000) cores for AEC research is game changer**

HPC = High Performance Computing



CRF optical LTGC engine, Dec et al.

Response to previous year reviewer comments

- **Widespread agreement expressed that project supports overall DOE objectives, approach is good, well integrated with others, and appropriate technical barriers are being addressed.**
  - "Crucially important work to provide benchmarks against commercially useful codes. Need to investigate speeding up simulation turn-around time and reducing cost."
  - "If pathway for migrating this understanding into engineering models is established this reviewer would rate the approach as outstanding (instead of very good)."
  - "The PI made great use of a modest amount of funding (relative to other projects)."
  - **RESPONSE:** We agree that a key challenge/need now is to accelerate the rate at which we can perform these types of calculations and to establish a pathway for migrating this understanding into affordable engineering models. We are approaching this challenge by 1) optimizing our staffing plan, 2) enhancing the workflow associated with the RAPTOR code framework (e.g., toward exascale), and 3) expanding our collaborative interactions within the ECN and with industry partners as tools mature.
- **Technical accomplishments provide unique insights and the scope should be expanded to include gasoline-direct-injection (GDI), spark-ignition (SI), and related in-cylinder flows. More direct collaboration with industry partners is also desirable.**
  - "The interface with the ECN is an excellent and important collaboration."
  - "It will be important to tie improvements in understanding the detailed physics to the capability of predicting combustion processes and what advantages these bring to applied teams."
  - "It will be nice to see a prediction of when this type of computing could be used by the OEMs (i.e., will these types of simulations ever be affordable enough to use directly for design)."
  - **RESPONSE:** We agree that we should build on the ECN collaboration, move toward studies of GDI, SI, and in-cylinder calculations with emphasis on detailed physics, complex geometry, and incorporation of wall effects and heat-transfer. The steps being taken to accelerate our efficiency (e.g., man-power, code-performance, workflow) will have a direct impact on the viability of these types of calculations for design (e.g., computers have gotten bigger, models have not changed yet and need to "catch up").

Collaboration and coordination with other institutions

- CRF Departments 8351, 8353, 8362, 8365 (Arienti, Barlow, Chen, Dahms, Debusschere, Frank, Lacaze, Miles, Musculus, Najm, Pickett, Shaddix, Siebers, Templeton)
  - 8351 Reacting Flow Research
  - 8353 Combustion Chemistry
  - 8362 Engine Combustion
  - 8365 Thermal/Fluid Science and Engineering

- Professor W. Anderson, Purdue
- Professor J. -Y. Chen, UC Berkeley
- Professor B. Cuenot, CERFACS, France
- Professor R. Davis, UC Davis
- Professor A. Dreizler, TU Darmstadt, Germany
- Professor D. Haworth, The Pennsylvania State University*
- Professor O. Haidn, TU Munich, Germany
- Professor B. Helenbrook, Clarkson
- Professor M. Ihme, Stanford*
- Professor A. Kempf, Duisburg-Essen University, Germany
- Professor M. Linne, Chalmers, Sweden
- Professor T. Lieuwen, Georgia Institute of Technology
- Professor S. Menon, Georgia Institute of Technology
- Professor M. Modest, UC Merced*
- Professor T. Poinsot, CERFACS, France
- Professor S. Pope, Cornell
- Professor C. Rutland, University of Wisconsin, Madison
- Professor V. Sick, Michigan*
- Professor J. Sutton, Ohio State
- Professor V. Yang, Georgia Institute of Technology

*NSF/DOE Advanced Combustion Engines Collaborations:

Development of a Dynamic Wall Layer Model for LES of Internal Combustion Engines

Radiation Heat Transfer and Turbulent Fluctuations in IC Engines – Toward Predictive Models to Enable High Efficiency

- Dr. R. Balakrishnan, Argonne National Laboratory
- Dr. A. Dord, General Electric Global Research
- Dr. T. Drozda, NASA LaRC
- Dr. S.-Y. Hsieh, General Electric Aviation
- Dr. I. Leyva, Air Force Research Laboratory, EAFB
- Dr. M. Oschwald, The German Aerospace Center (DLR), Germany
- Dr. R. Sankaran, Oak Ridge National Laboratory
- Dr. V. Sankaran, Air Force Research Laboratory, EAFB
- Dr. S. Som, Argonne National Laboratory
- Dr. K. Tucker, NASA MSFC
- Dr. D. Talley, Air Force Research Laboratory, EAFB
- Dr. D. Walker, General Electric Global Research

Postdoc's and Students

- J. Segura, Doctoral Committee, 2004 (Stanford); T. Drozda, Oct 2005 - Oct 2008 (NASA LaRC); V. Lee, Intern 2006, 2007 (California Polytechnic State University); V. Sankaran, Feb 2006 - Oct 2008 (UTRC); R. Knaus, Intern 2007, 2008 (UIUC); J. Smith, Doctoral Committee, 2007 (University of Adelaide, Australia); J. Doom, Jan 2009 - Aug 2010 (Minnesota State); B. Hu, Jan 2009 - Sep 2011 (Cummins); G. Lacaze, Aug 2009 - Nov 2012 (Sandia); V. Vuorinen, Doctoral Committee, 2009 (Helsinki University of Technology, Finland); R. Dahms, Jul 2010 - Dec 2012 (Sandia); R. Mari, Intern Apr 2011 - Sep 2011 (CERFACS, France); M. Masquelet, Doctoral Committee, 2012 (Georgia Institute of Technology); A. DeFilippo, Sep 2011 - Dec 2012 (UC Berkeley); J. Quinlan, Intern May 2013 - Jun 2013 (NASA LaRC); A. Misdariis, Intern Jun 2013 - Sep 2013 (CERFACS, France); A. Ruiz, June 2012 - Present (Sandia);
- L. Hakim, April 2014 - Present (Sandia) … DI Ignition/Combustion
- F. Doisneau, April 2014 - Present (Sandia) … Primary Atomization

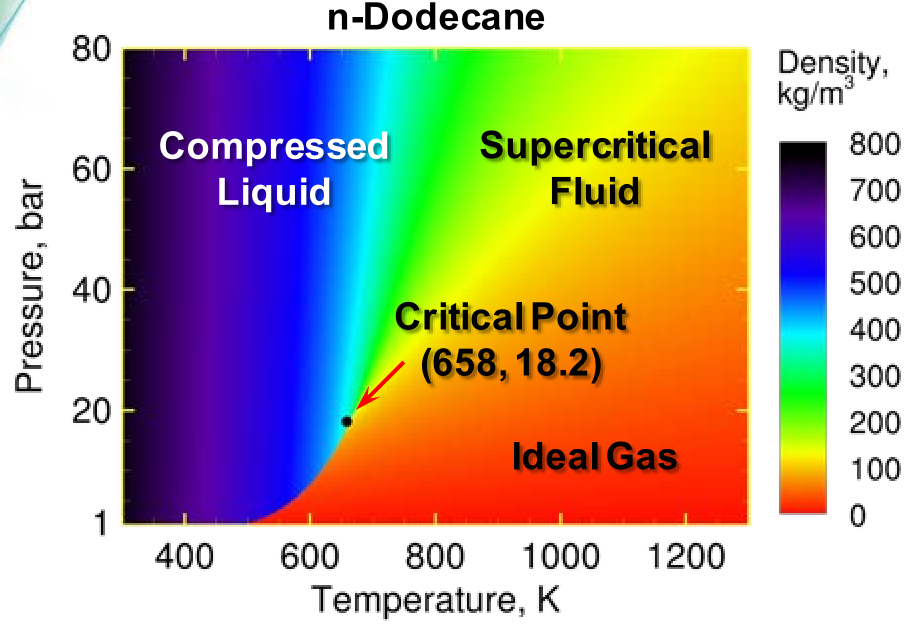
New Postdoctoral Appointees who will focus on DI Ignition and Combustion (this project) and development of advanced models for primary atomization (Sandia LDRD)

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

Technical Back-Up Slides

Advanced framework for treatment of complex fuels ("Real-Fluid Model")



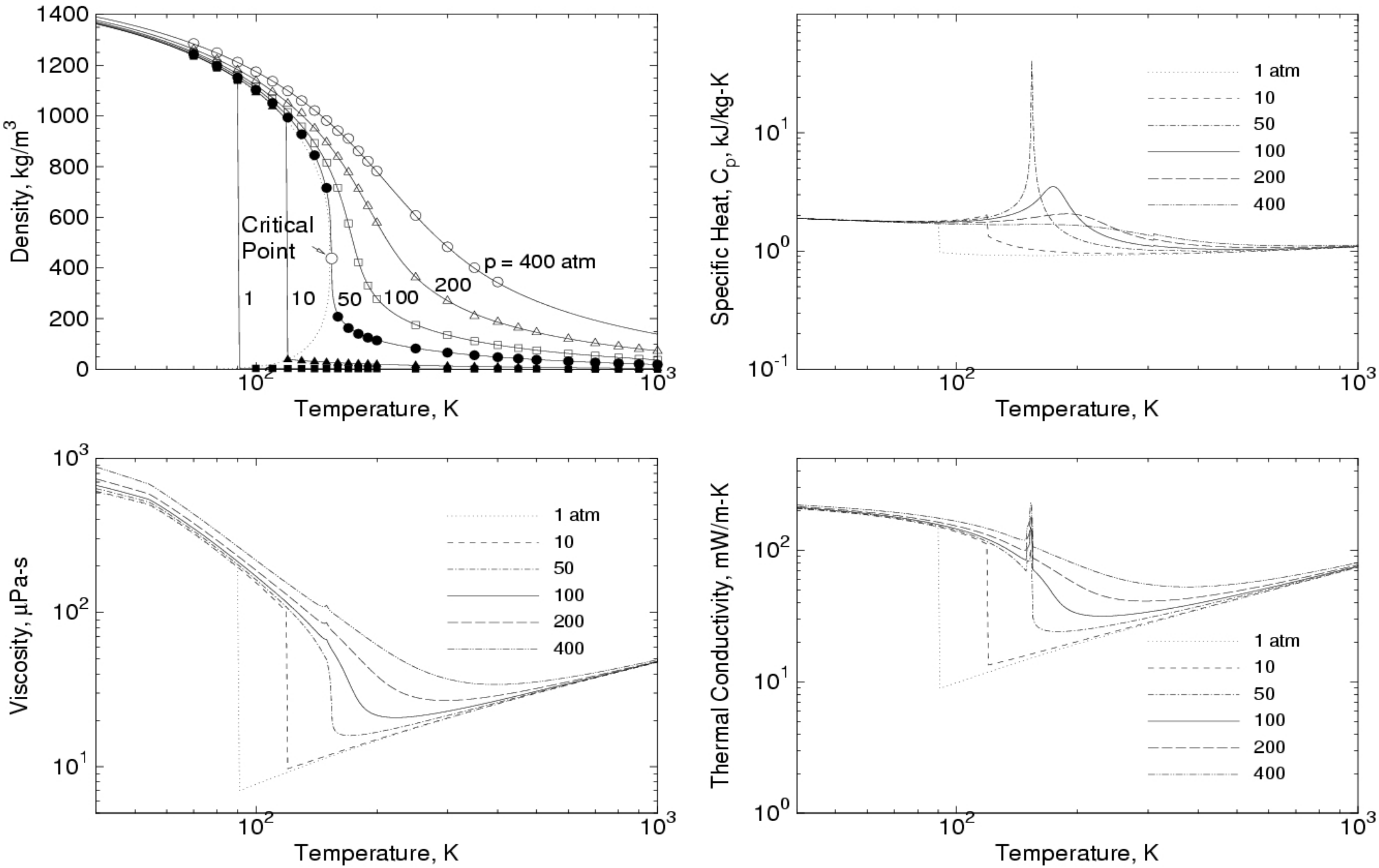
- Real-fluid mixture properties obtained using extended corresponding states model
- Provides detailed representation of gas/liquid EOS, thermodynamics, and transport
- Generalized to treat wide range of hydrocarbon mixtures (Fuel/Oxidizer/Products)

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

J. C. Oefelein (2014). General package for evaluation of multicomponent real-gas and liquid mixture states at all pressures. *SAND Report*.

Provides exact treatment of multicomponent mixture properties



Workflow for collaborative model development