Large Eddy Simulation (LES) Applied to Low-Temperature and Diesel Engine Combustion Research

Joseph C. Oefelein
Sandia National Laboratories
Livermore, California 94551-9051

May 10, 2011

Support provided by the DOE EERE Vehicle Technologies Program is gratefully acknowledged

Project ID: ACE007

Overview

Timeline

- Project provides fundamental research that supports advanced engine development
- Focused on next generation simulation capabilities using "capability class" computers
- Project scope, directions and continuation evaluated annually

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 range)
  2. – Requirements for efficient and routine use of high-performance (exascale) computers, development of predictive <u>and</u> affordable models for advanced engine combustion research

Budget

- Project funded by DOE/OVT:
  FY10 – $450K
  FY11 – $450K

Partners

- PI's in the Engine Combustion Group at Sandia, Wisconsin, Penn State, Michigan, TU Darmstadt, GM (most recent)
- Project lead: Joe Oefelein

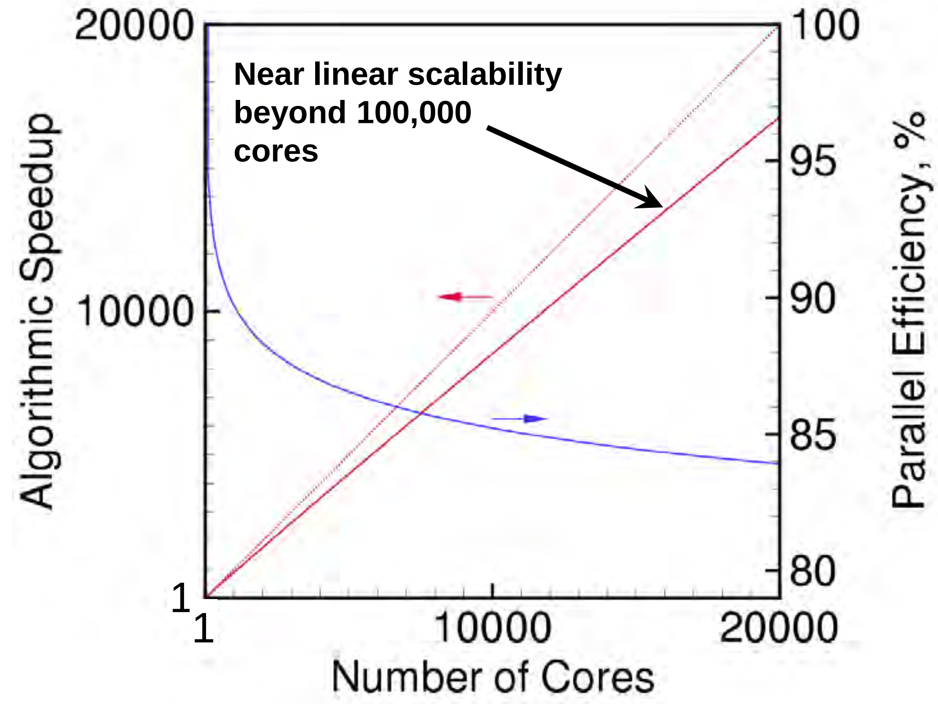
Objective … maximize benefits of high performance computing for AEC research

- Apply unique capabilities that complement 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
  - Access to DOE Office of Science (OS) supercomputer facilities
    - LBNL NERSC (www.nersc.gov)
    - ORNL NCCS (www.nccs.gov)
    - INCITE program (… Innovative and Novel Computational Impact on Theory and Experiment)
  - Synergy between CRF OS-BES and EERE-VT programs
- Establish dedicated facilities, resources
  - Mid-scale computer clusters and storage
  - Enhanced collaborative interactions

Relevance

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

- **Theoretical framework**
  - 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**
  - All-Mach-number formulation
  - Non-dissipative, conservative
  - Complex geometry
  - Adaptive mesh (ALE)
  - Massively-parallel
- **Extensively validated, ported to all major platforms**



- Strong (fine-grain) scaling attributes exhibited on the ORNL NCCS 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

Oefelein, J. C. (2006). Large eddy simulation of turbulent combustion processes in propulsion and power systems. *Progress in Aerospace Sciences*, 42: 2-37.

Relevance

New project related facilities and resources

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

Image courtesy of Oak Ridge National Laboratory

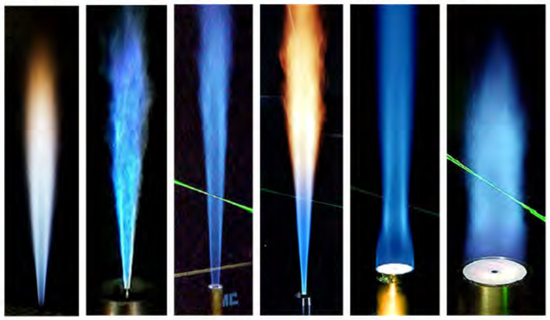
- CRF Combustion Research and Computational Visualization Facility (Joint support from BES – OVT)
  - 9000 sq-ft building for computational combustion
  - Computer room, visualization, office/visitor space
  - Collaborations welcome!
- New multiyear INCITE grant entitled High-Fidelity Simulations for Advanced Engine Combustion Research on "Jaguar" (ORNL Cray XT5 2.33 petaflop system, 224,256 cores, 60-million CPU-HRS in 2011)

Relevance

Approach … bridge gap between basic and applied research programs

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

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

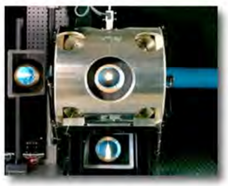


TNF Workshop
www.ca.sandia.gov/TNF

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

Detailed measurements but relatively limited due to complex geometry, flow and fuels →

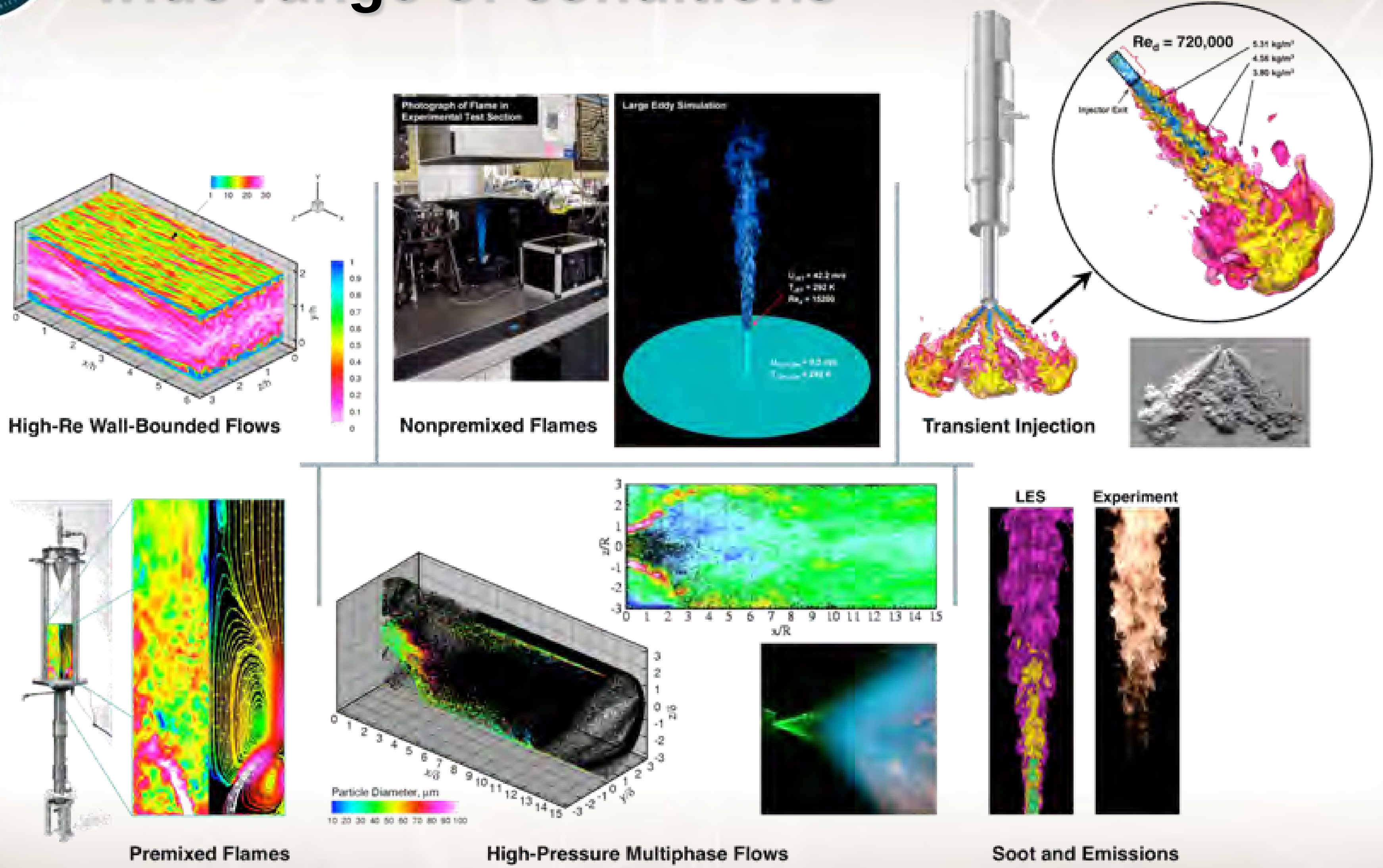
LES of High-Pressure, Low-Temperature Engine Combustion Processes
DOE Office of Vehicle Technologies



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

- **Combine state-of-the-art LES with AEC experimental efforts**
  - Benchmark calculations that identically match operating conditions
  - Detailed treatment of geometry, high-quality grid generation
  - Science-based models for subgrid-scale closure
- **Perform hierarchal model development using high-fidelity benchmarks**
  - Fundamental insights not available anywhere else
  - Model performance and implementation requirements
  - Collaborative model development for engineering design

Progressive validation performed over a wide range of conditions



Approach

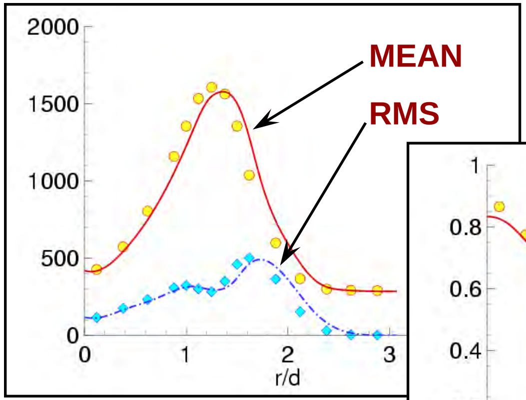
BES target flames provide detailed data for model development

DLR-A Flame: Re_d = 15,200

Fuel: 22.1% CH_4, 33.2% H_2, 44.7% N_2

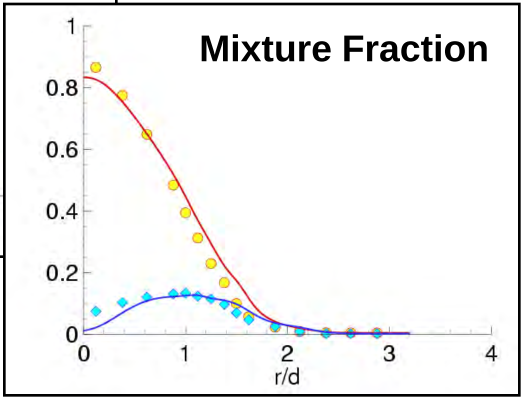
Coflow: 99.2% Air, 0.8% H_2O

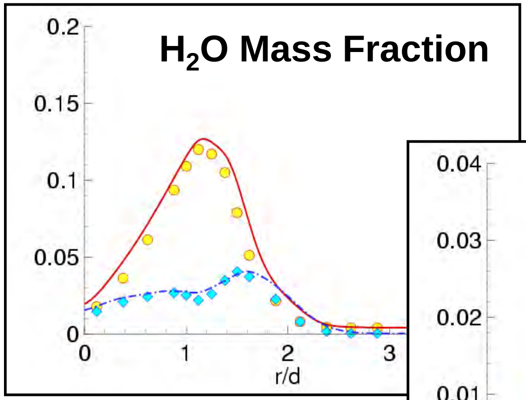
Detailed Chemistry and Transport: 12-Step Mechanism (J.-Y. Chen, UC Berkeley)

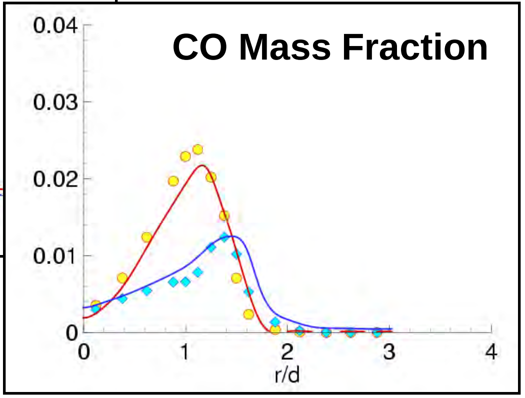


Temperature

Comparisons with 1D Raman/Rayleigh/CO-LIF line images (Barlow et al.)







Milestones have been synchronized with DOE INCITE grants …

- LES of DI processes for high-pressure LTC engine applications with emphasis on hydrocarbon fuels (Musculus, Pickett et al.)
  - Work in FY10 focused on transient jet dynamics and entrainment associated with Diesel injection processes
  - In FY11, model extended to include complex injector geometries using Pickett's ECN baseline n-heptane cases for validation
- CRF Homogeneous-Charge Compression-Ignition (HCCI) engine with emphasis on in-cylinder thermal stratification (Dec et al.)
  - Work in FY10 demonstrated LES can capture basic physics
  - In FY11, the goal is to improve fidelity (advanced gridding)
    - Treatment of intake flow by including anti-swirl plate
    - Valve seat indentations and piston crevice
    - Detailed heat transfer model for walls
  - Baseline validation and analysis of thermal stratification at operating conditions identical to the experiment to be completed by August 2011
- University of Michigan Common Engine Platform with emphasis on cyclic variability and stochastic nature of in-cylinder flows
  - LES working group (GM, U Mich, U Wisc, PSU, TUD, Sandia)

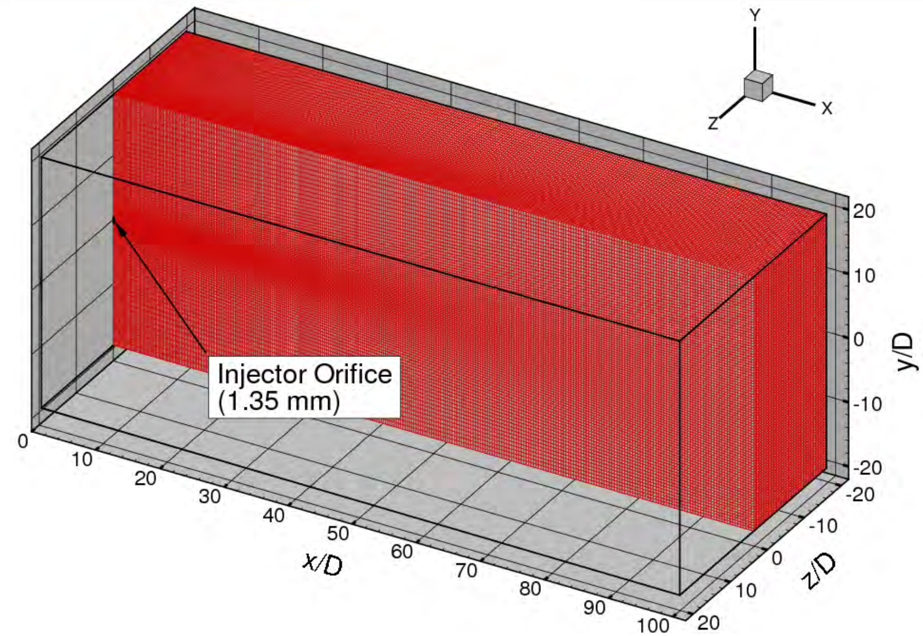
Transient jet dynamics and entrainment with emphasis on Diesel injection

- **Diesel jets involve quasi-steady and transient (decelerating) phases**
- **Decelerating phase important for LTC engines due to greater mixing**
  - Lean mixture decreases tendency for soot formation … desirable
  - Over-lean mixture increases tendency for UHC emissions … undesirable
- **Entrainment rate-controlling process**

- **Objective: Understand entrainment processes in transient jets at Diesel like injection conditions**
  - Quantify unsteady characteristics as function of entrainment coefficients
  - Understand governing processes during jet deceleration

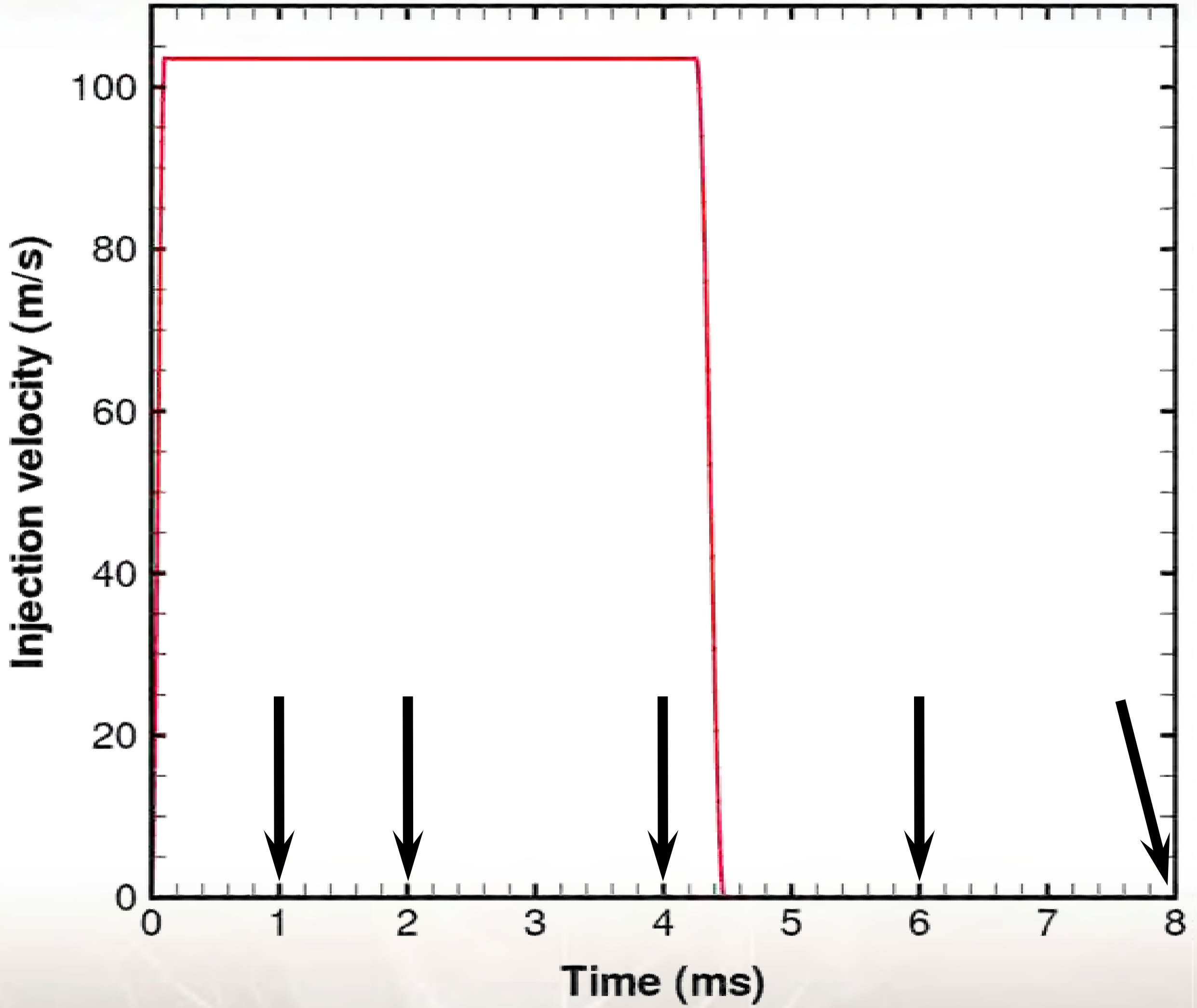
B. Hu, M. P. Musculus, and J. C. Oefelein. Large eddy simulation of a transient gas jet with emphasis on entrainment during deceleration. SAE World Congress, Paper 2010-01-1133, April 13-15 2010.

Computational Domain



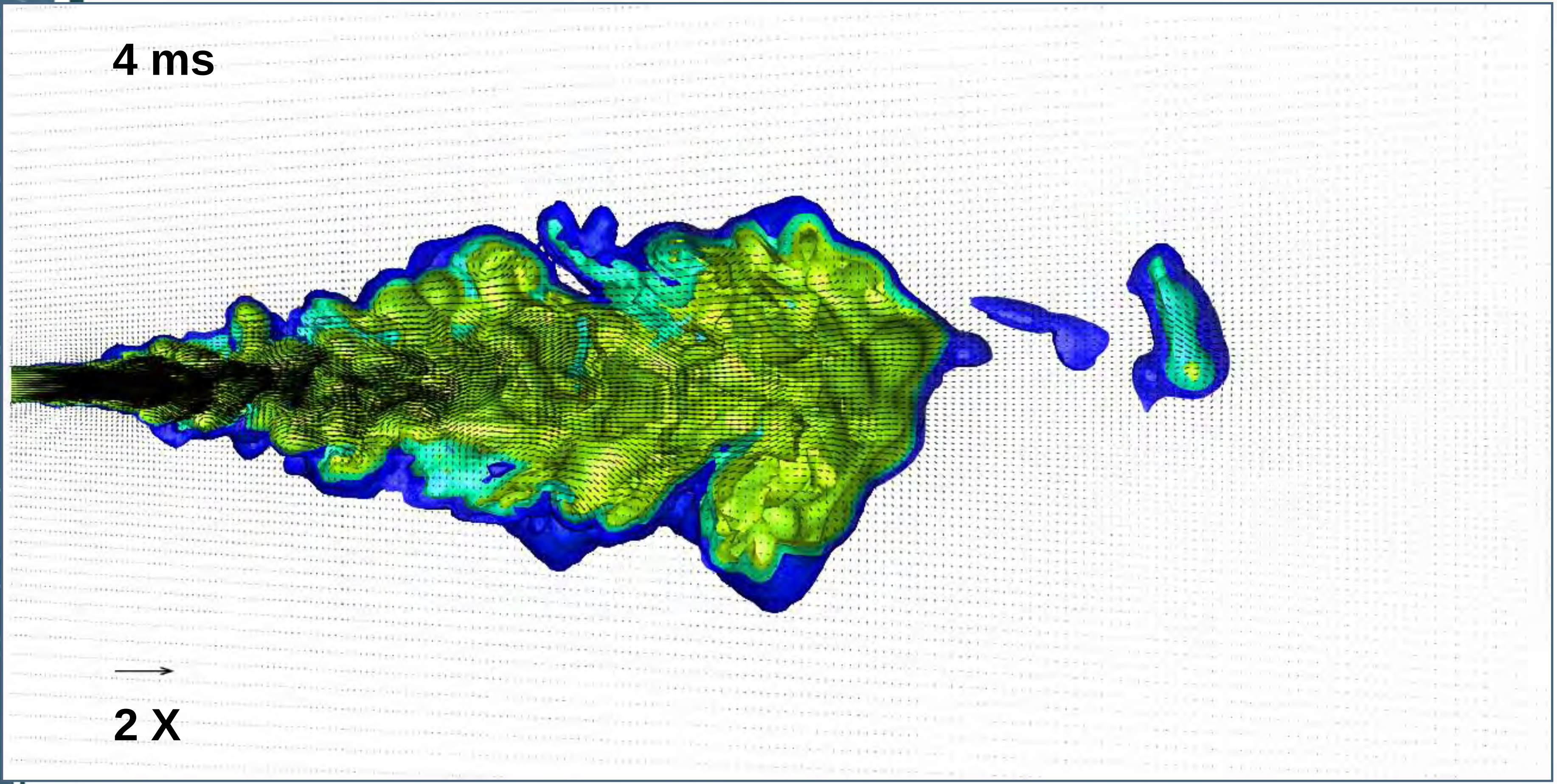
- **Multiblock grid, 3-million cells, optimal stretching (130-million CPU hrs)**
- **Time step 160 ns with correlated fluctuations imposed at inflow boundary**
- **Injected fluid marked using passive scalar ($Z_{JET} = 1$)**

Injection profile … Witze et al.



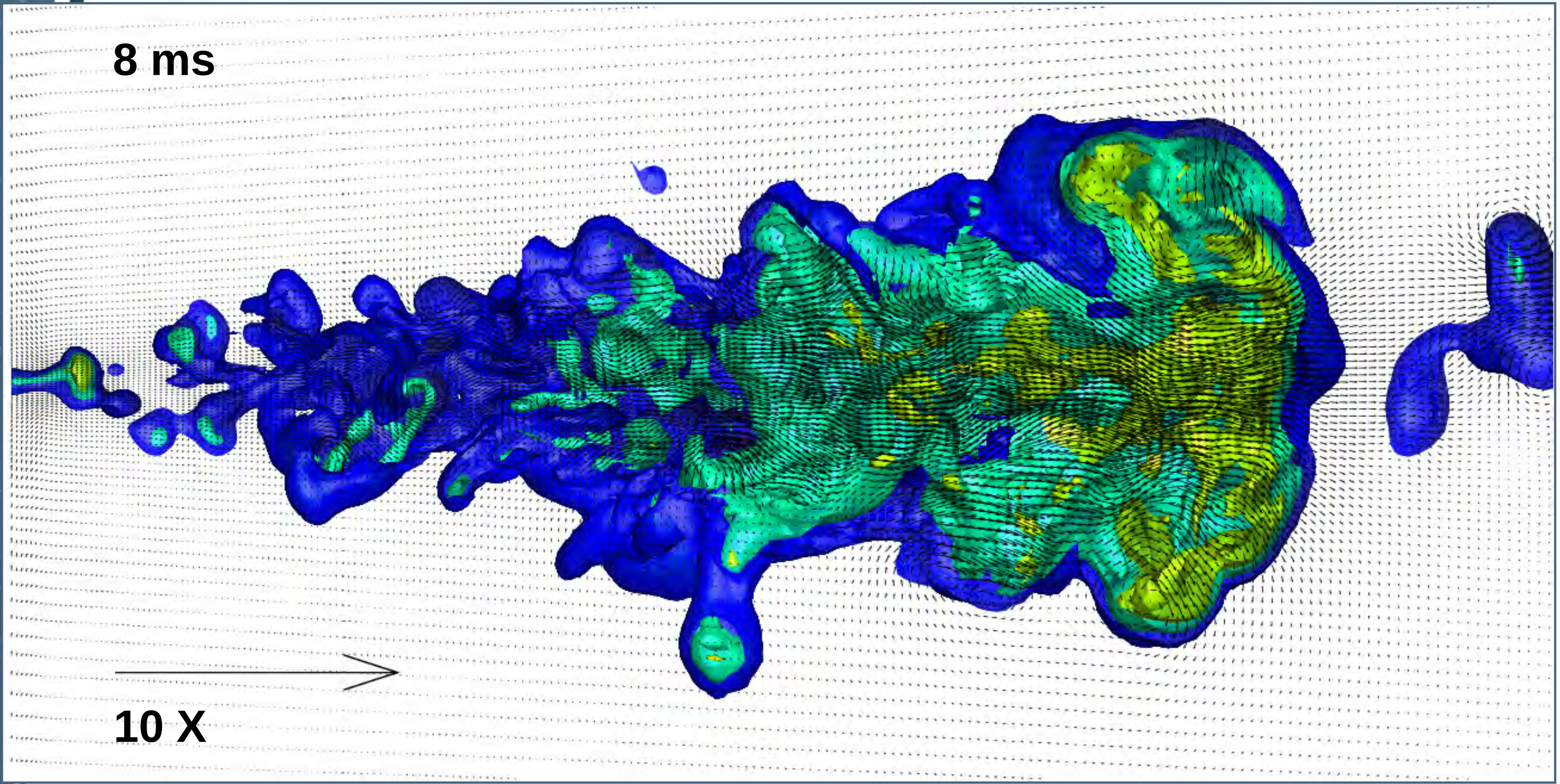
Accomplishments and Progress

Transient jet evolution (4 ms)



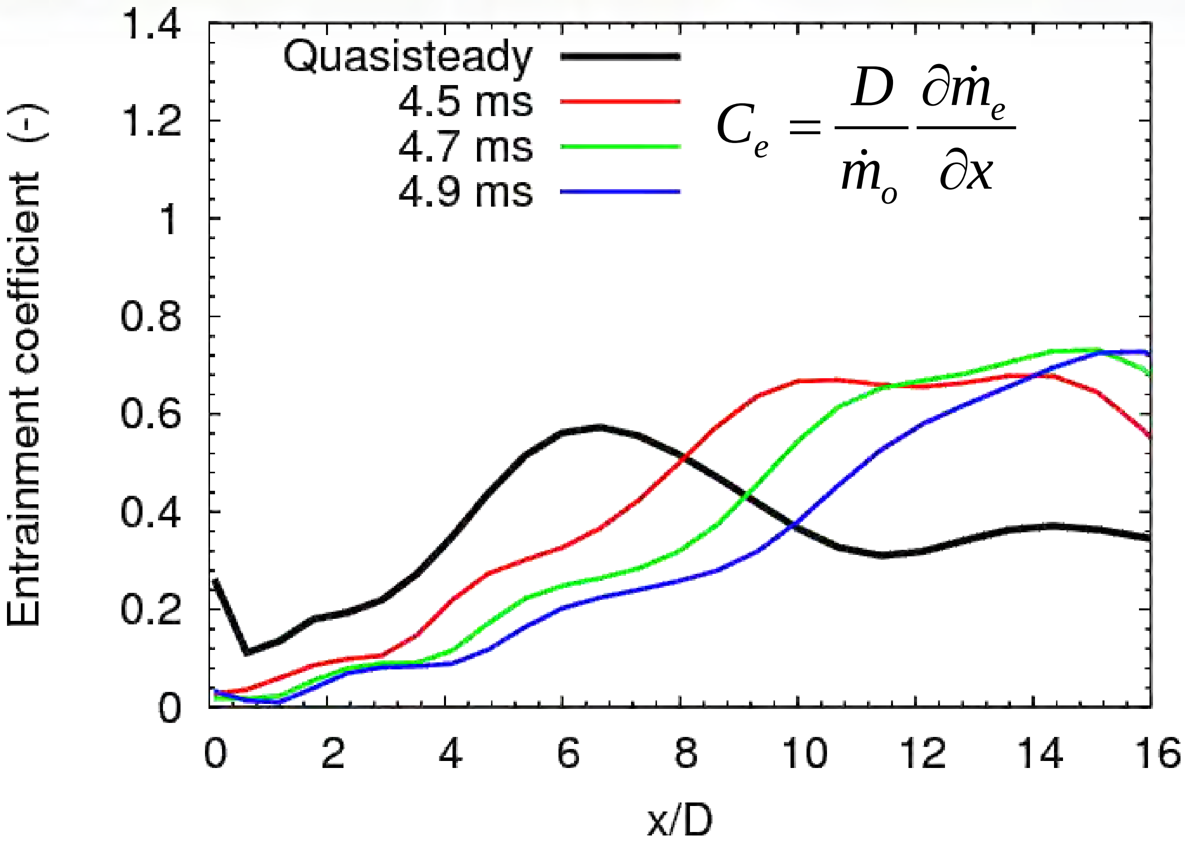
Iso-surfaces of passive scalar with the corresponding velocity vectors

Transient jet evolution (8 ms)



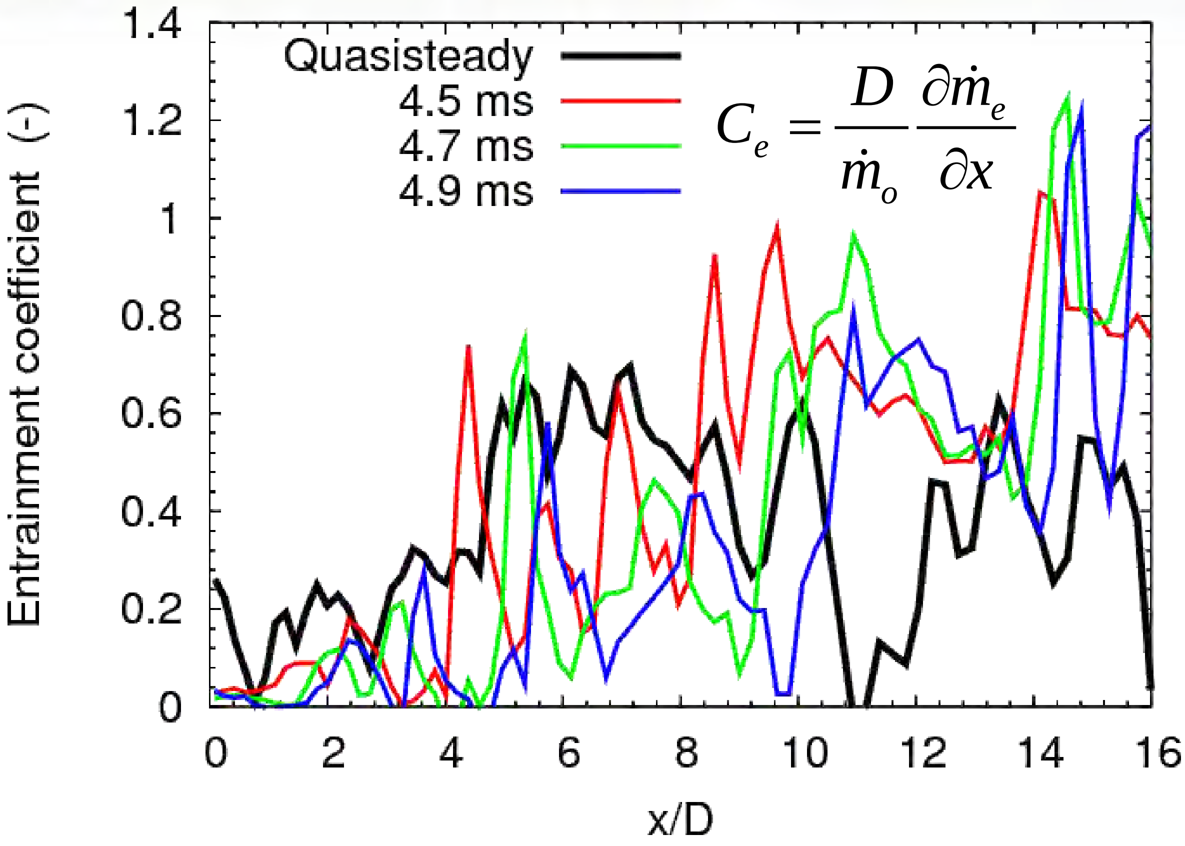
Iso-surfaces of passive scalar with the corresponding velocity vectors

Decelerating jet shows increased entrainment compared to quasi-steady jet



- **Entrainment coefficient describes entrained mass per unit axial distance**
- **Decelerating jet shows increased entrainment in downstream region**
- **Increased entrainment leads to a much leaner mixture**

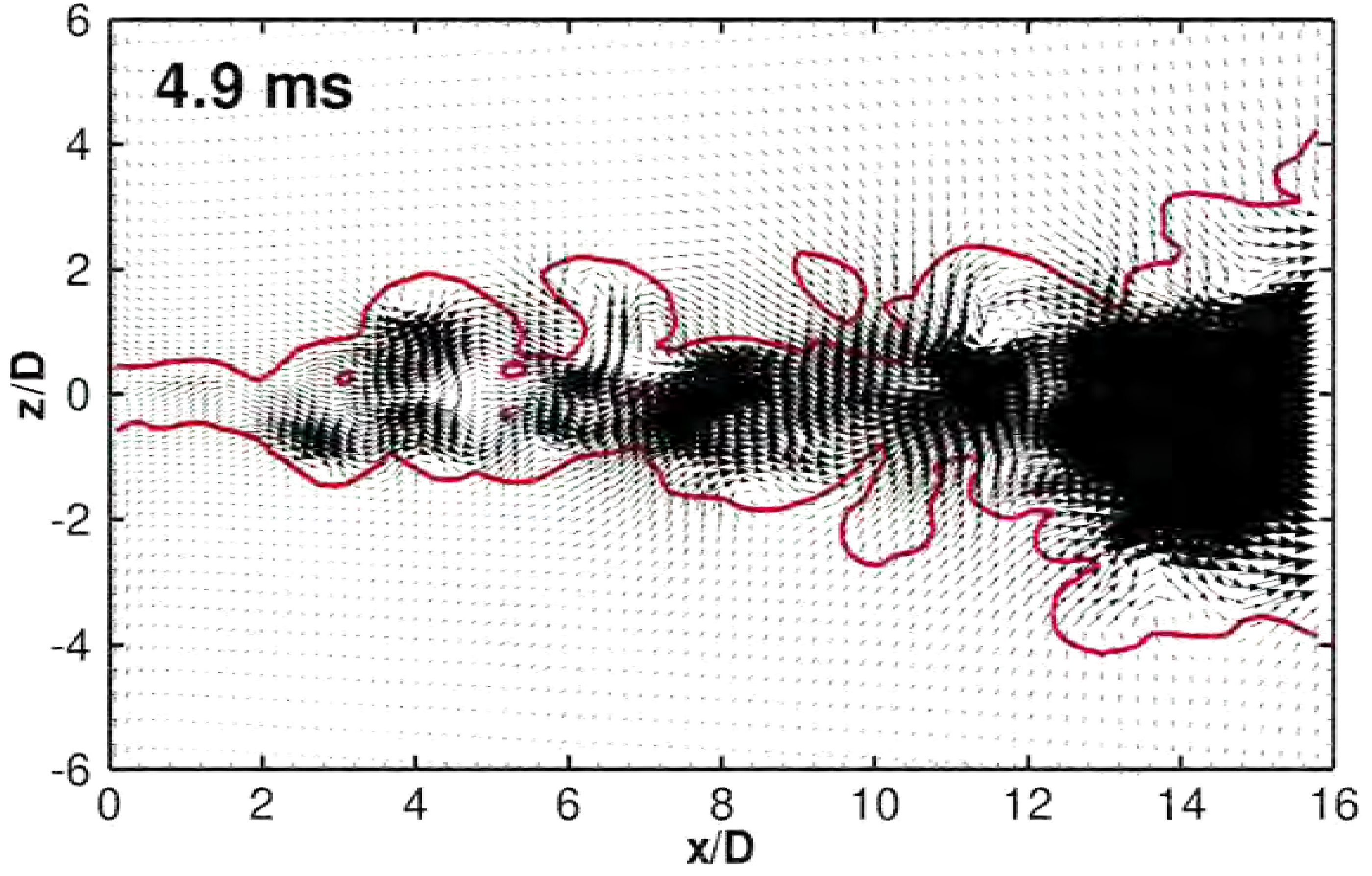
Analysis of unsteady effects illuminates broadband dynamics



- **Entrainment coefficient describes entrained mass per unit axial distance**
- **Decelerating jet shows increased entrainment in downstream region**
- **Increased entrainment leads to a much leaner mixture**

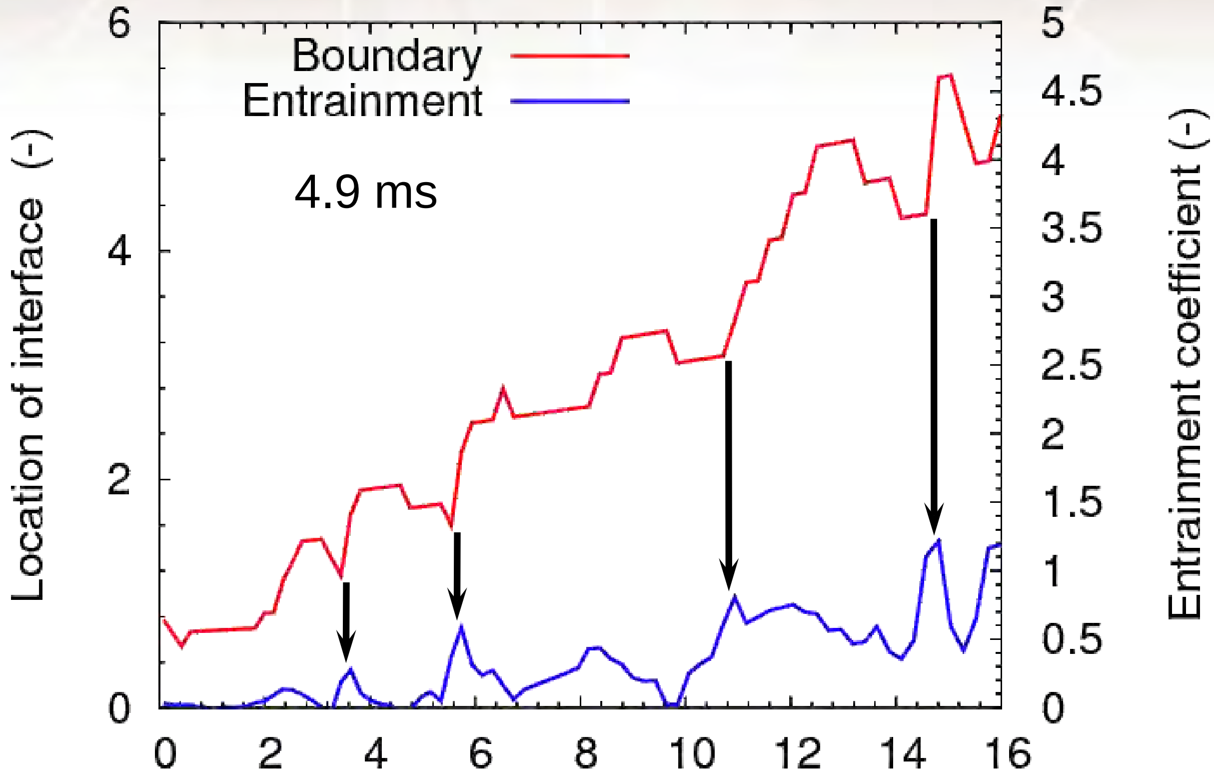
Accomplishments and Progress

Does formation of interface indentations induce increased entrainment?



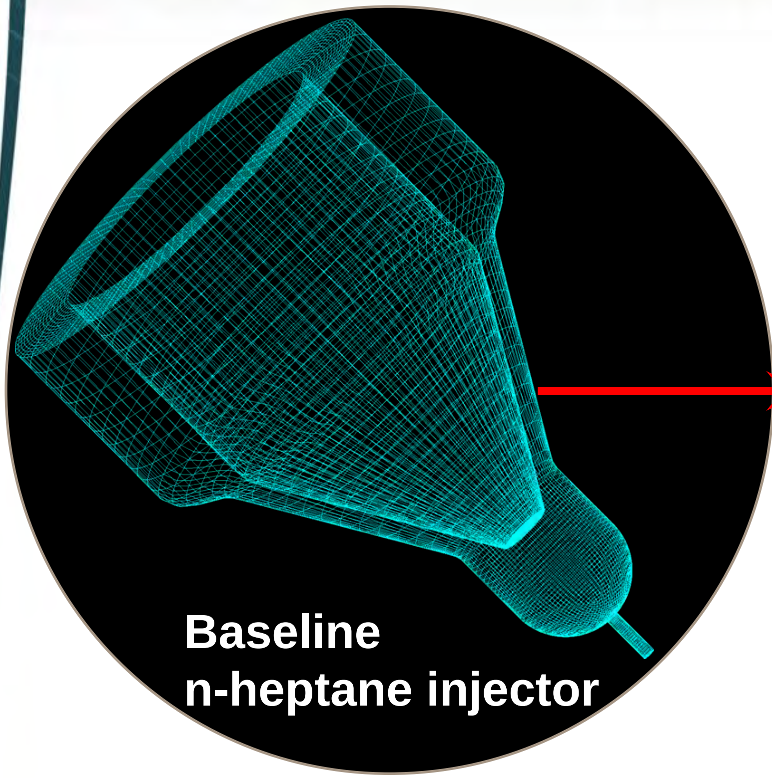
Accomplishments and Progress

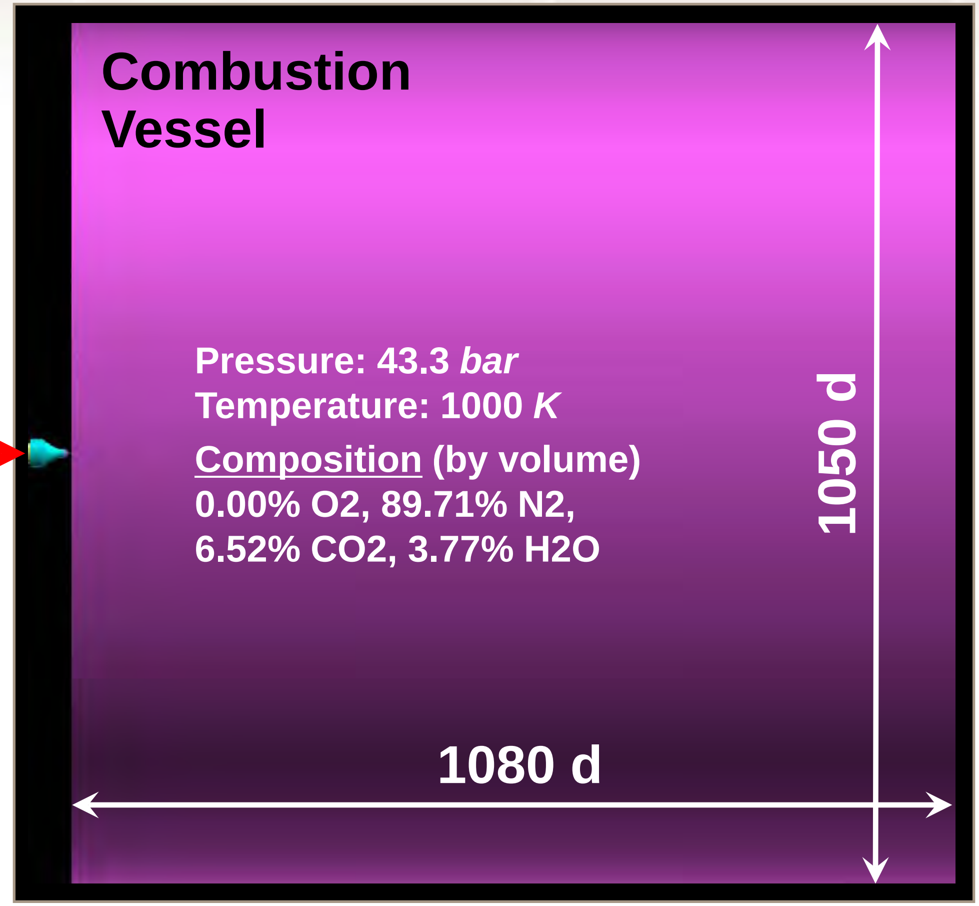
Analysis reveals correlation between indentations and entrainment



- **Interface indentations induced by flow instabilities accompany increased entrainment (… primary enhancement mechanism)**
  - **Indentations form engulfment regions which contain packets of ambient fluid**
  - **Packets have higher probability to cross jet boundary (i.e., to be entrained)**
- **Implies manipulation of instabilities as part of injection strategy can be used to control downstream mixing**

Extension to n-heptane combustion using Pickett's ECN target cases



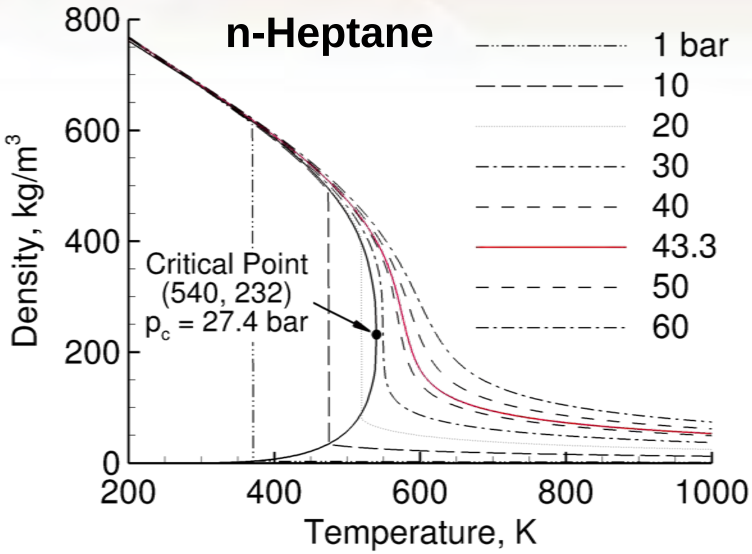


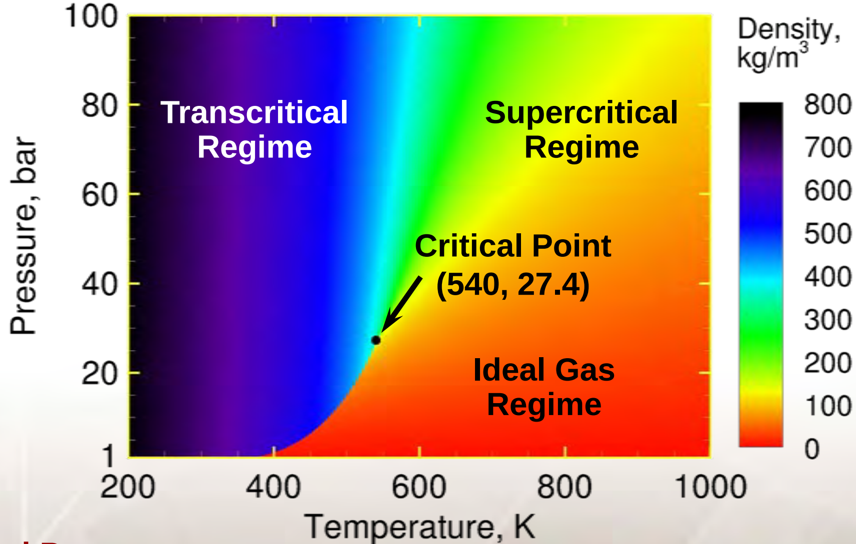
Nominal Injection Conditions

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

New dense fluid model for simulation of Diesel fuel injection

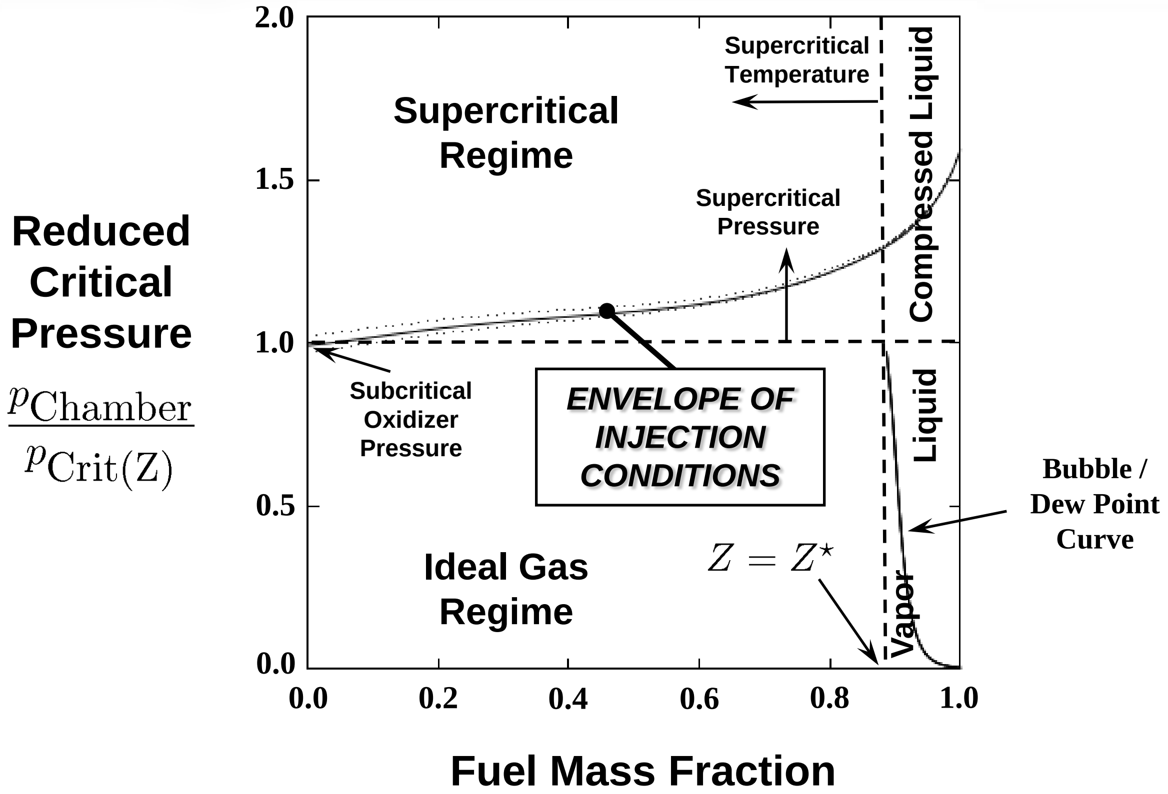
- **Fuel typically injected at transcritical thermodynamic conditions**
  - Supercritical with respect to pressure, subcritical with respect to temperature
  - Substantial thermodynamic nonidealities and transport anomalies
  - Mixture properties exhibit liquid-like densities, gas-like diffusivities
  - Heat of vaporization and surface tension (i.e., gas-liquid interface) diminish
  - Classical view of spray atomization as appropriate model comes into question
- **To account for these phenomena, we apply a dense fluid approximation that applies to arbitrary hydrocarbon mixtures**
  - 32-term BWR equation of state
  - Nonlinear mixing rules to account for multi-component mixture states
  - Applies to any arbitrary hydrocarbon fuel/oxidizer/product mixture



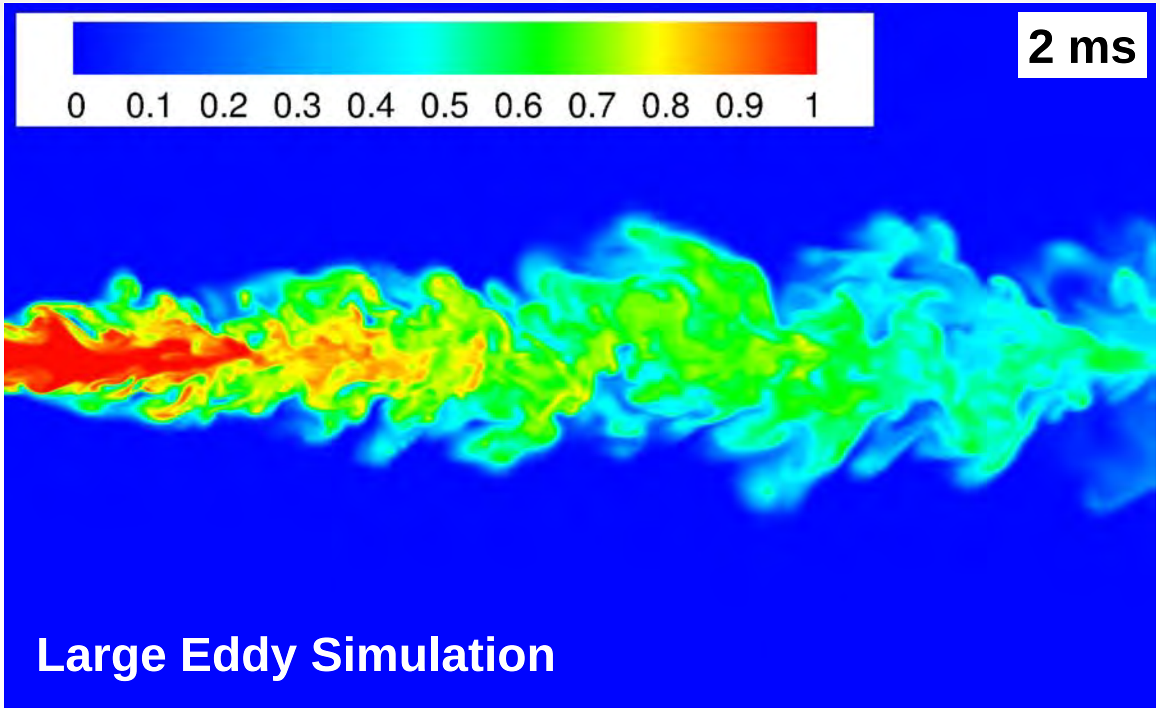


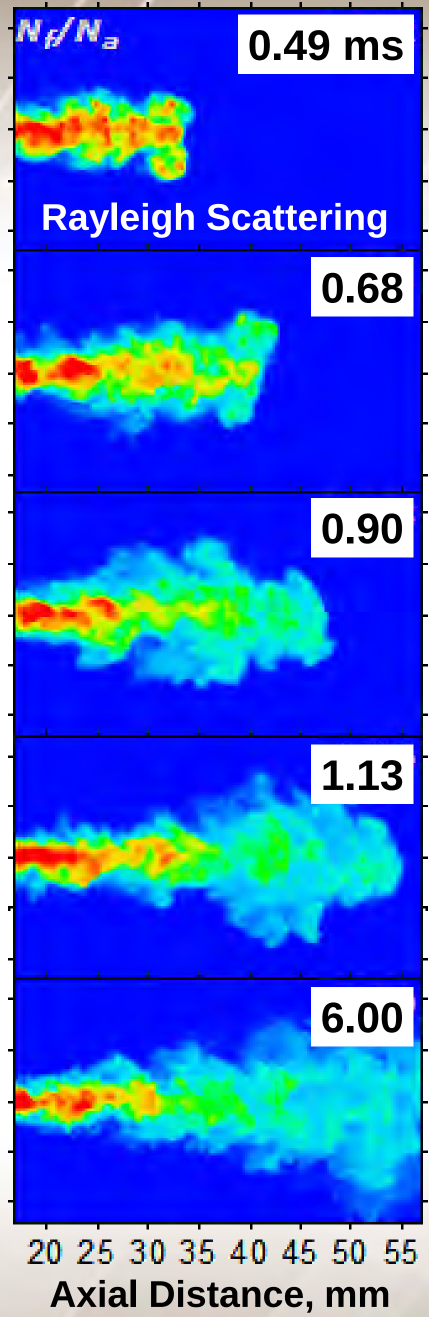
Accomplishments and Progress

Thermodynamic mixture states associated with baseline n-heptane case



Instantaneous distribution of mixture fraction



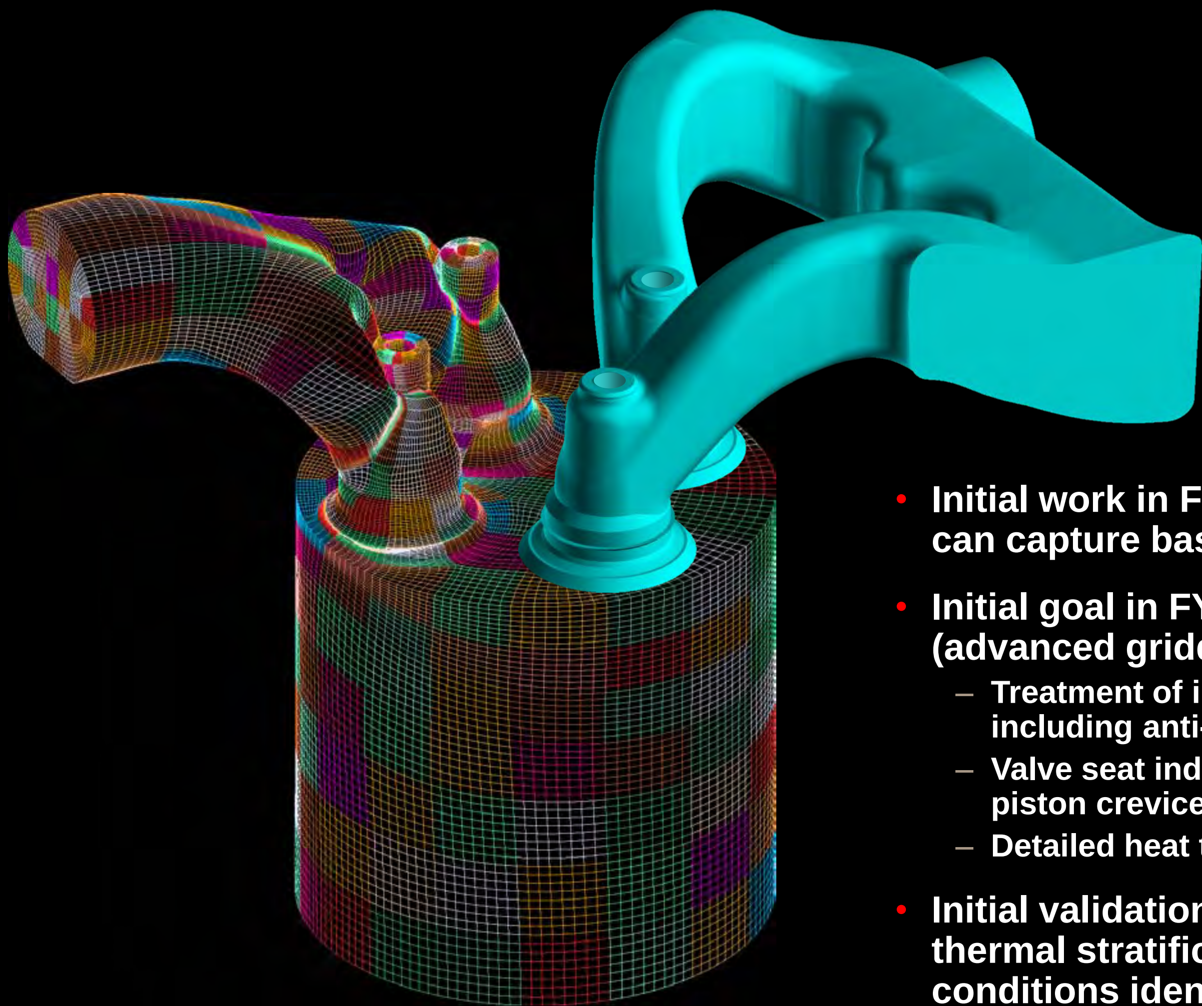


Data Available from ECN

Rate of injection
Liquid length versus time
Vapor penetration versus time
Rayleigh scattering images
Shadowgraphs

- **Systematic validation in close collaboration with Pickett et al. in progress**
- **Detailed results to be presented at upcoming ECN workshop and ILASS**

LES of optically assessable HCCI engine



- Initial work in FY10 demonstrated LES can capture basic physics
- Initial goal in FY11 to improve fidelity (advanced gridding)
  - Treatment of intake flow by including anti-swirl plate
  - Valve seat indentations and piston crevice
  - Detailed heat transfer model for walls
- Initial validation and analysis of thermal stratification at operating conditions identical to the experiment to be completed by August 2011

Collaborators ... special thanks to Dr. Bing Hu and Dr. Rainer Dahms

- CRF Departments 8351, 8353, 8362, 8367, 8963 (Barlow, Chen, Dec, Frank, Kerstein, Miles, Musculus, Najm, Pickett, Rouson, Settersten, Shaddix, Siebers, Steeper).
  - 8353: Combustion Chemistry
  - 8362: Engine Combustion
  - 8367: Hydrogen & Combustion Technology
  - 8963: Scalable Modeling & Analysis

- Professor W. Anderson, Purdue University.
- Professor J.-Y. Chen, University of California, Berkeley.
- Professor J. Doom, Minnesota State University.
- 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 C. Merkle, Purdue University.
- 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. J. Bell, Lawrence Berkeley National Laboratory.
- Dr. J. Bellan, NASA Jet Propulsion Laboratory.
- Dr. C. Carter, Air Force Research Laboratory, WPAFB, OH.
- Dr. T. Drozda, Rolls Royce Aircraft Engines.
- Dr. O. Haidn, The German Aerospace Center (DLR).
- Dr. D. Kothe, Oak Ridge National Laboratory.
- Dr. T.-W. Kuo, General Motors R&D Center.
- Dr. M. Oschwald, The German Aerospace Center (DLR).
- Dr. S. Rahman, NASA Stennis Space Center.
- Dr. M. Roquemore, Air Force Research Laboratory, WPAFB, OH.
- 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

- Postdoc's and Students
- 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.
- Bing Hu, University of Wisconsin, Madison, Jan 2009 – Present.
- Jeffrey Doom, University of Minnesota, Jan 2009 – Aug 2010.
- 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.

*Names in red are Postdoctoral Appointees assigned to this project

Collaborators … LES working group

Dr. Tang-Wei Kuo,
Dr. Xiaofeng Yang
GM – LES Applications
CONVERGE

Prof. Volker Sick
Dr. Dave Reuss
UM CRL – High Speed PIV
Optical Diagnostics

Prof. Chris Rutland
UW CRL – LES Model Development
KIVA

Objectives

- **Coordinated LES model development**
- **Strategic direction on experiments**
- **Effective global information exchange**
- **Effective deployment of tools**

Prof. Dan Haworth
PSU – LES Model Development
Star-CD

Dr. Martin Freitag
GMPT-Eu – LES Applications
Star-CD

Prof. J. Janicka
TUD – LES Model Development,
Optical Diagnostics

Dr. Joe Oefelein
Sandia – LES Model Development
RAPTOR

Common engine platform for model development and validation

Future Work

- **Continue to work toward routine treatment of**
  - Direct injection processes for LTC engine applications (Musculus, Pickett et al., Engine Combustion Network for validation)
  - In-cylinder HCCI with emphasis on thermal stratification (Dec et al., extend to reacting flow over full engine cycles)
  - University of Michigan Common Engine Platform with emphasis on cyclic variability (LES working group)
- **Continue leveraging between DOE Office of Science and Energy Efficiency and Renewable Energy activities**
  - Access to DOE high-performance “capability-class” computers
  - Development of turbulent multiphase combustion models

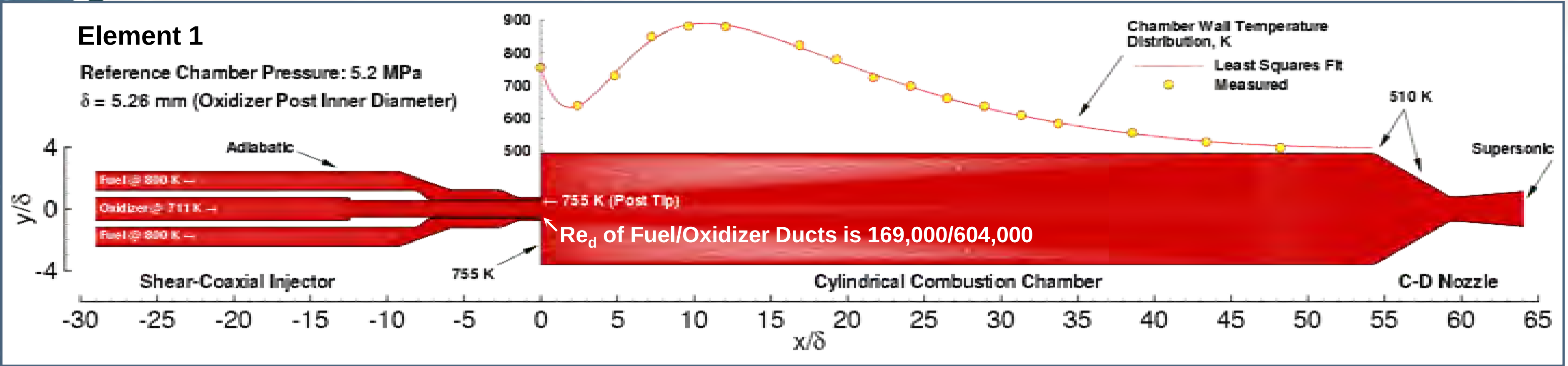
Proposed Future Work

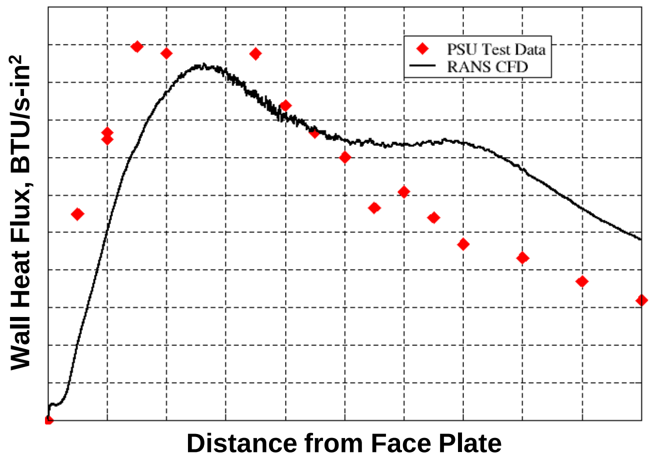
Summary

- **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 different models at identical conditions
  - Joint analysis to understand model performance, limitations
    - Critical trade-off's between cost and accuracy
    - Uncertainties as a function of fidelity and method
    - Implementation requirements as function of model

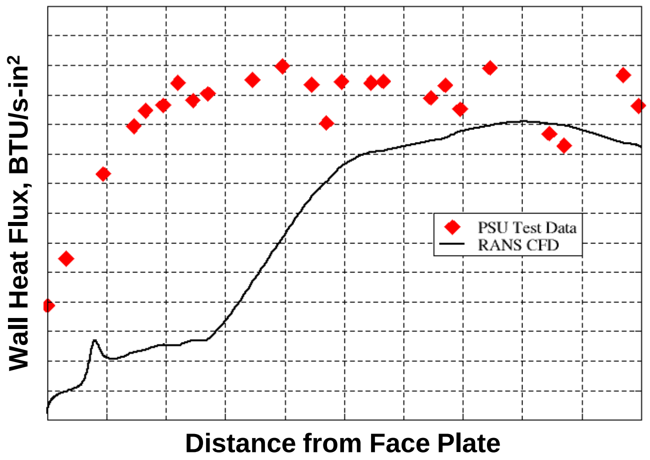
Technical Back-Up Slides

Role of high-fidelity LES … example
(NASA/PennState high-pressure uni-element rocket)





Element 1: Shear coaxial injector with GO_2/GH_2 propellants

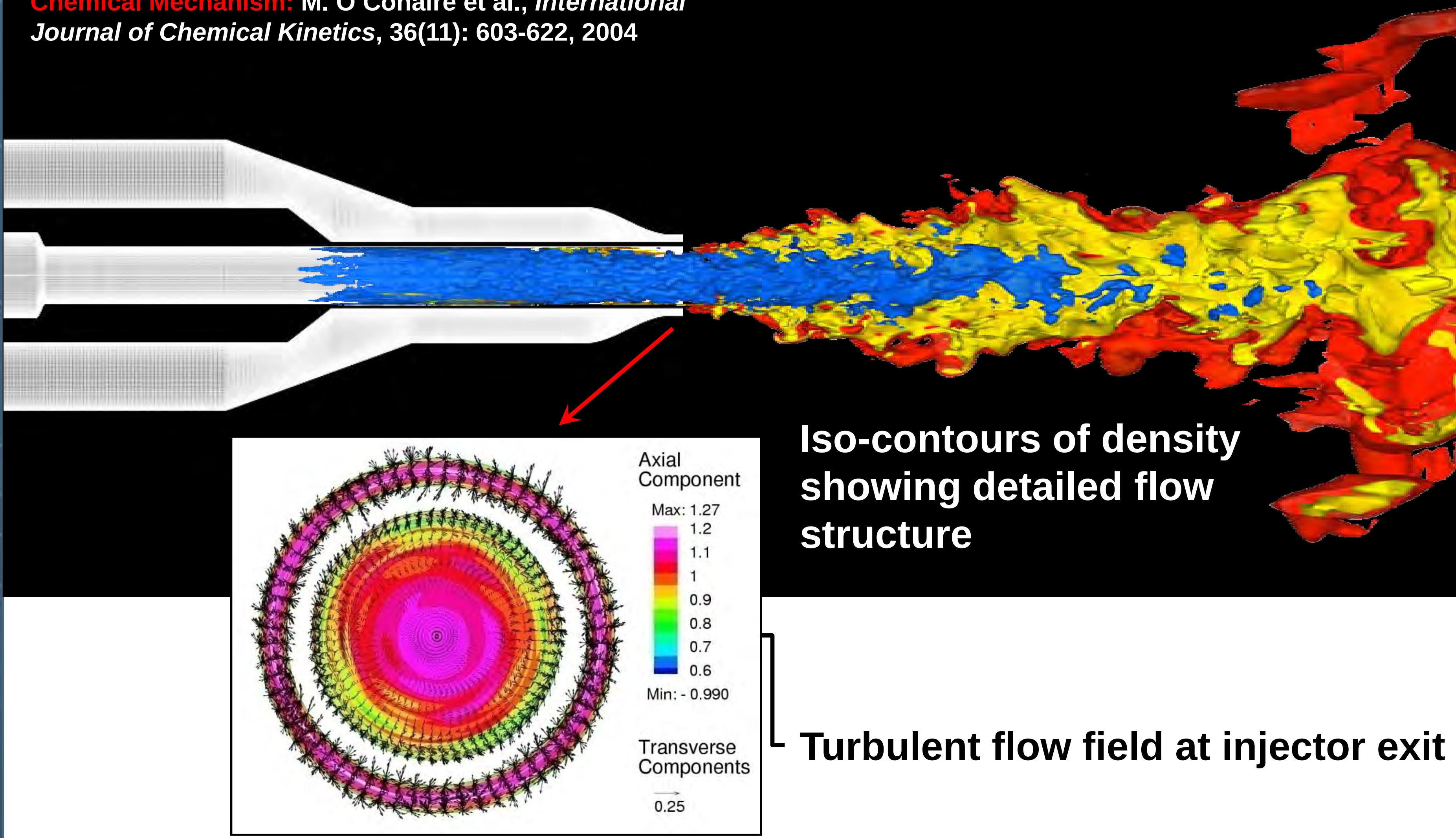


Element 2: Shear coaxial injector with LO_2/GH_2 propellants

- RANS (and other simulations) have demonstrated insufficient accuracy for injector design
- Accuracy must be improved to have major impact in the design process … how?

Sandia contribution … near DNS benchmark compared to 4 engineering RANS/LES cases

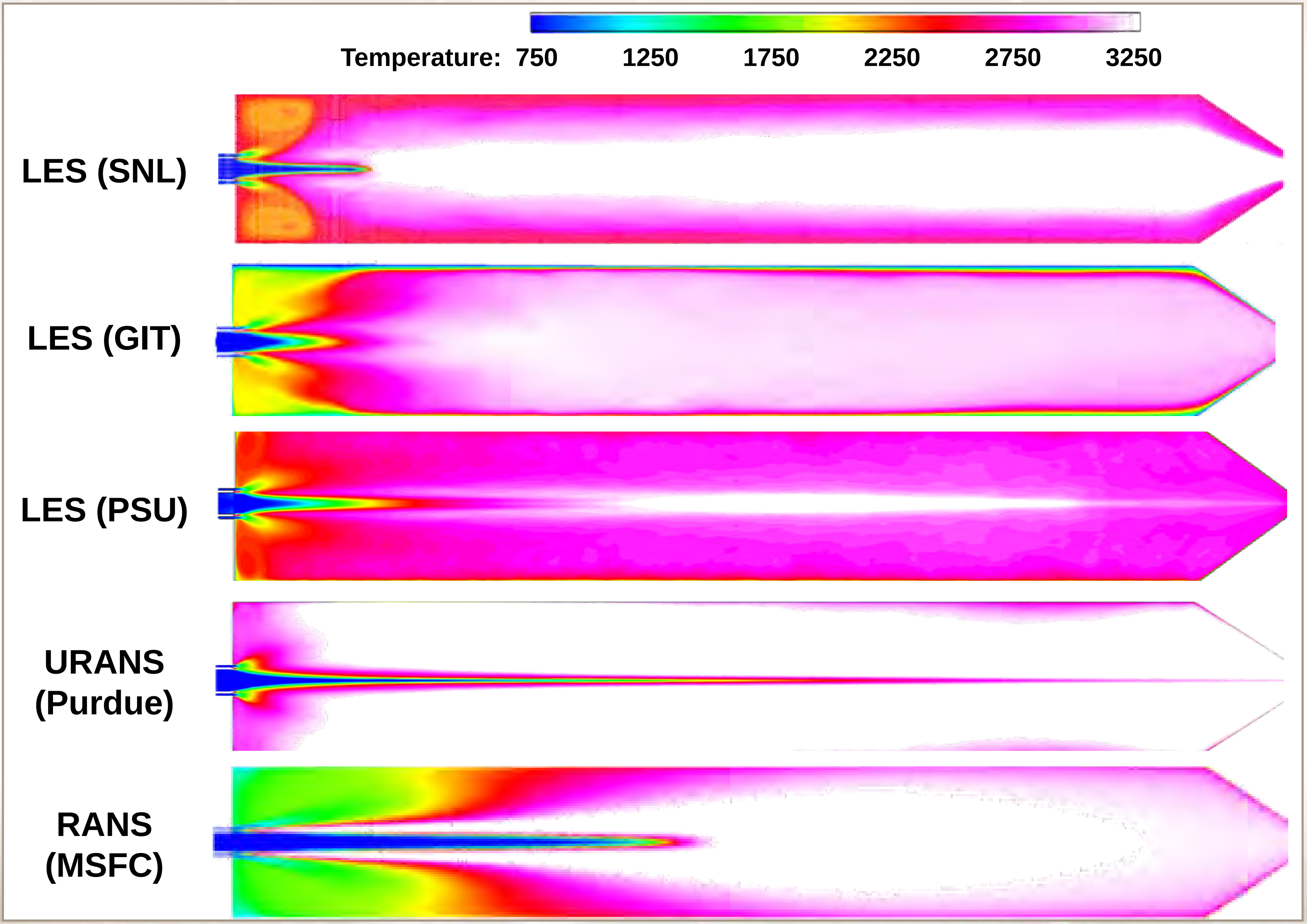
Chemical Mechanism: M. Ó Conaire et al., *International Journal of Chemical Kinetics*, 36(11): 603-622, 2004



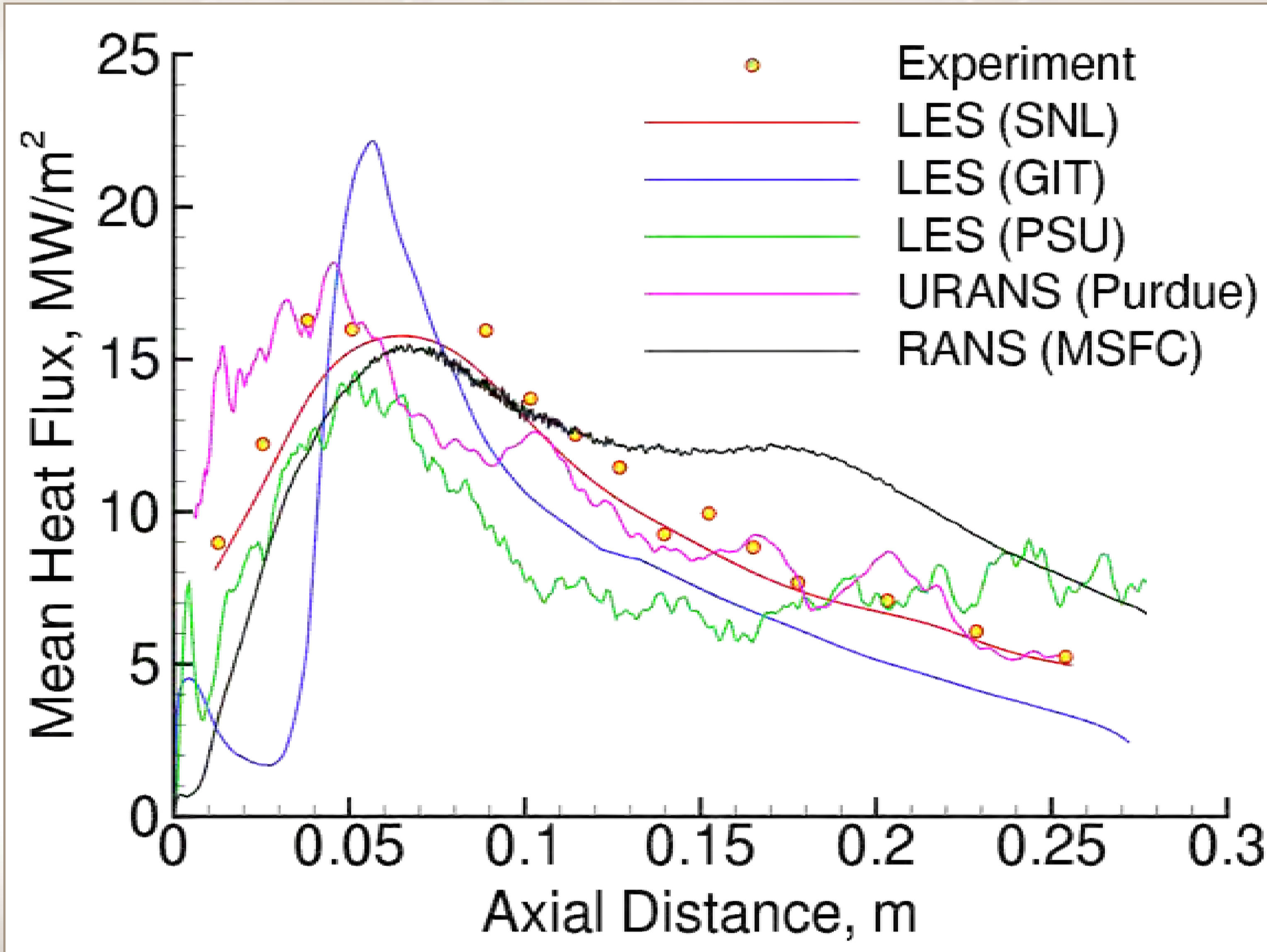
Iso-contours of density showing detailed flow structure

Turbulent flow field at injector exit

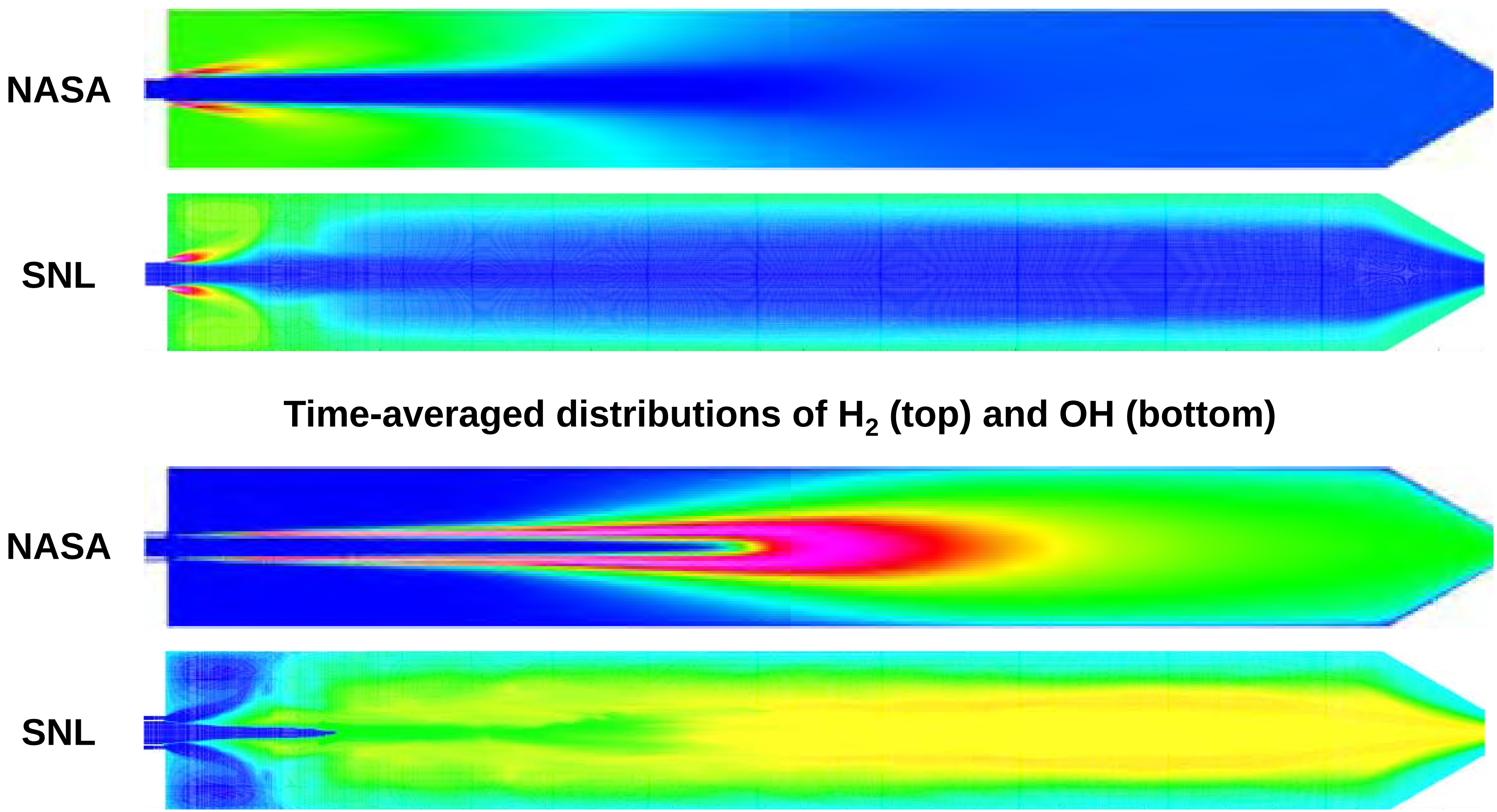
Same domain BC's and chemistry, different codes resolution and models … why?



Heat flux at chamber wall … why?



Validated high-fidelity LES provides revealing insights beyond available experimental data



Time-averaged distributions of H_2 (top) and OH (bottom)

Critical trade-off's between cost and accuracy, uncertainties as a function of fidelity and method