SAND2011-3325P

Workshop on Predictive Simulation of Internal Combustion Engine (PreSICE)

Wayne Eckerle Co-Chair

Cummins

BESAC March 18, 2011

Jointly sponsored by:

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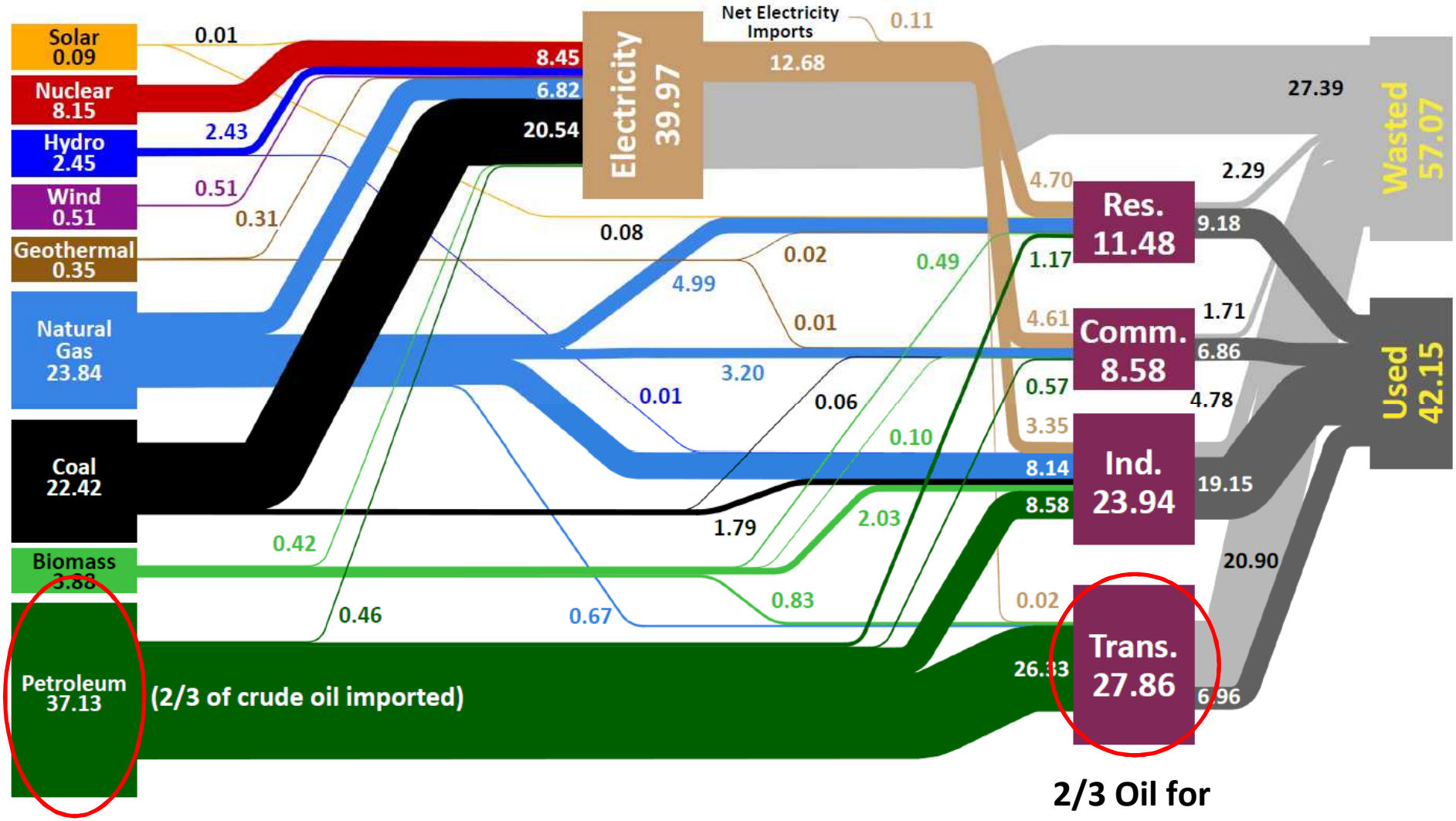
Energy Security Tied to Transportation



Source: Lawrence Livermore National Laboratory and the Department of Energy, Energy Information Administration, 2009 (based on data from DOE/EIA-0384(2008), June 2009).

Reducing Fuel Use Through Enhancing Engine Efficiency

- Internal combustion engines thermodynamic limit 60%
- Average current gasoline engine efficiency: 30%
- Improvements to >45% thermal efficiency achievable
- Fuel economy improvements >50%
  - Potential for 50% reduction of fuel use from cars

The Washington Post March 9, 2011

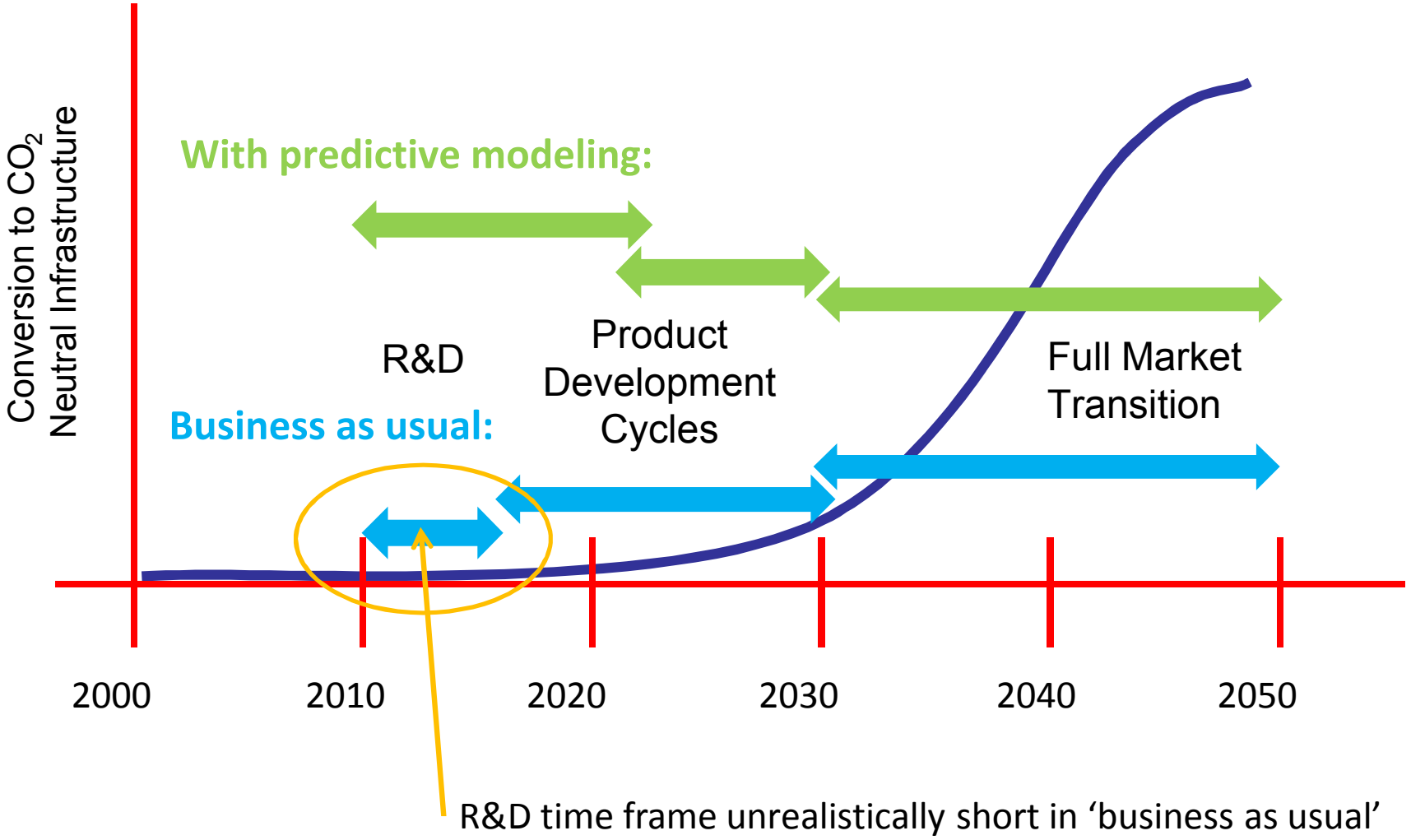
"Conventional gas-powered cars starting to match hybrids in fuel efficiency"

"The new Chevrolet Cruze Eco can reach eye-popping fuel economy levels of more than **50 miles per gallon** on the highway, which even in this era of hybrid-electric cars stands among the best.

"But here's the real trick: The Cruze Eco is neither a hybrid nor electric. It runs on that "old" technology, the **conventional gasoline engine**. "

Potential to save 4 M barrels per day ($400 M per day)

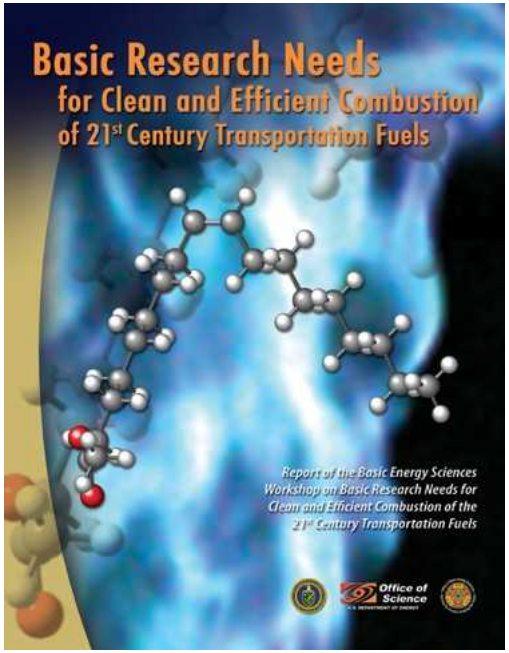
Product Development Must Be Accelerated To Meet Energy Goals



Advanced Combustion Research-Development-Deployment Critical to Achieving CO_2 and Fuel Reduction Goals

- Realizing thermodynamic limits with clean operation
- Maintain clean fleet operation with evolving fuel streams
- Optimize IC engines for PHEV use

Grand Challenge: Predictive Simulation of Combustion Engine Performance in an Evolving Fuel Environment



Predictive modeling is the key to rapid combustion optimization in a non-linear parameter space

Science-Based Engine Design
An early example

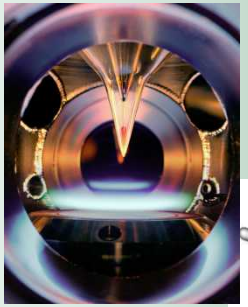
Basic Science

Applied R&D

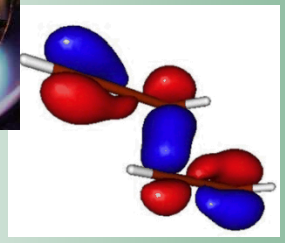
Manufacturing/ Commercialization

BES
Sustained support in 2 areas

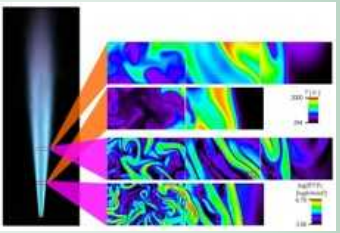
Development of predictive chemistry in model flames



Computational kinetics and experiments

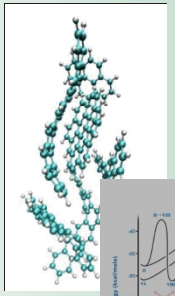


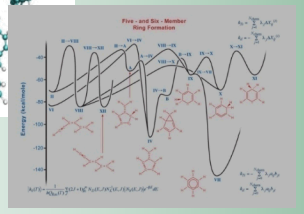
Advance laser diagnostics applied to model flames



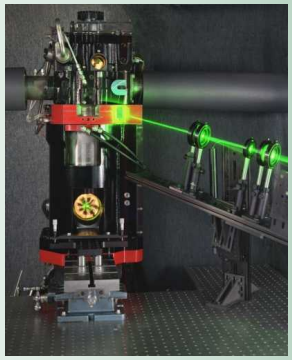
Laser-based chemical imaging

BES → EERE
Applications of chemistry and diagnostics to engines





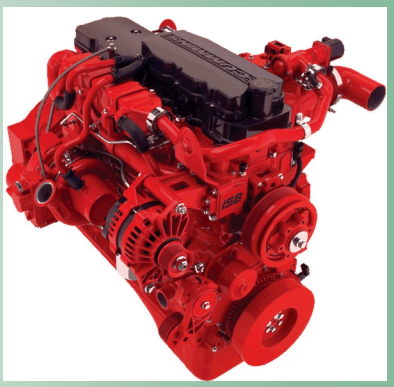
Predictive chemical models under realistic conditions



Laser diagnostics of diesel fuel sprays in engine cylinders

Cummins and Dodge

Cummins used simulation tools and improved understanding of diesel fuel sprays to design a new diesel engine with reduced development time and cost and improved fuel efficiency.



ISB 6.7 liter Cummins diesel engine first marketed in the 2007 Dodge Ram pickup truck; more than 200,000 sold

PreSICE Workshop Culmination of Year-Long DOE-Community Engagement

Workshop for national laboratories
Sandia National Laboratories, Livermore CA
January 20, 2010

Combustion Research Facility Advisory Board
Sandia National Laboratories, Livermore CA
January 22, 2010

Workshop for industry and academia
University of Michigan, Ann Arbor, MI
February 11, 2010

Workshop on near term priorities
O'Hare Airport Hilton, Chicago, IL
March 23, 2010

Argonne National Laboratory
Lawrence Berkeley National Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
Oak Ridge National Laboratory
Pacific Northwest National Laboratory
Sandia National Laboratories
U.S. Department of Energy
U.S. Department of Treasury

University of Michigan
University of Sydney
University of Wisconsin-Madison
UC Berkeley
University of Illinois
Purdue University
Massachusetts Institute of Technology
Sawyer Associates/UC Berkeley
Chevron
BP

Caterpillar
Cummins Inc.
General Electric
Chrysler Group LLC
Ford Motor Company
General Motors
ConocoPhillips
IBM
Cray Inc
Intel

Identified Industry Barriers For Advanced Engines

Highest priorities – PreSICE workshop focus

1. **Effect of stochastic nature of in-cylinder flow on engine combustion, performance and emissions**
2. **Spray modeling and experimentation in dense spray and nozzle internal flow regions, including physics like cavitation and flash boiling**
3. **Surface chemistry and physics for high-efficiency, low-temperature catalysis and filtration**
4. **Fundamental understanding of near-wall processes (e.g., flow, heat transfer, diffusion, chemistry, wall films)**
5. **High-pressure, dilute combustion including turbulence-chemistry interaction and extremes of equivalence ratio, dilution, and turbulence**

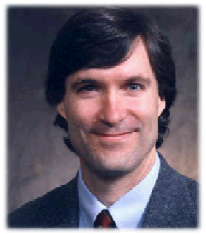
All can be mitigated or overcome through science-based modeling

PreSICE Workshop Charge: Answer 4 Questions

- ***Why*** **is investment in pre-competitive R&D for predictive engine simulation needed?**
- ***Why*** **is *now* the opportune time to develop predictive simulation tools for advanced engine design?**
- ***What*** **are the critical needs in basic and applied R&D in chemistry, physics, and engineering required for the successful realization of predictive combustion simulation for engines?**
- ***What*** **is the potential impact on the U.S. automotive and engine industries *if* new simulation tools are developed?**

PreSICE Workshop

- **March 3, 2011**
- **Sheraton National, Arlington, VA**
- **Chairs:**
  - Wayne Eckerle, Cummins
  - Chris Rutland, University of Wisconsin

- **Breakout Chairs:**
  - Sprays
    - Caroline Genzale, Georgia Tech
    - Joe Oefelein, Sandia
  - Stochastic In-Cylinder Processes
    - Dan Haworth, Penn State
    - Volker Sick, University of Michigan




PreSICE Workshop Agenda & Attendees

A Workshop to Identify Research Needs and Impacts in Predictive Simulation for Internal Combustion Engines (PreSICE)

Sheraton National Hotel • 900 South Orme Street • Arlington, VA 222044 • 703-521-1900

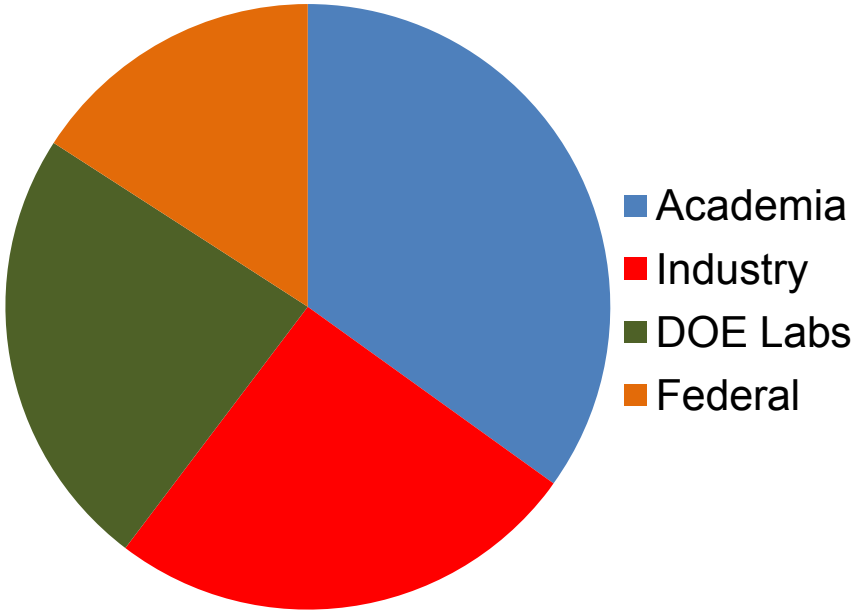
Chairs: Wayne Eckerle, Cummins, Chris Rutland, University of Wisconsin

DOE Sponsors: Eric Rohlfing, Office of Science, Gurpreet Singh, Office of Energy Efficiency and Renewable Energy

Thursday, March 3, 2011

Time	Agenda	Location
7:00 – 8:00	**Continental Breakfast/Registration**	Concourse Room
8:00 – 8:30	**Welcome** *Chairs, DOE and Under Secretary Steve Koonin*	Concourse Room
8:30 – 9:15	**PreSICE Background** *Andy McIlroy, Sandia National Lab*	Concourse Room
9:15 – 10:00	**Predictive Simulation Enabling Industry** *John Deur, Cummins*	Concourse Room
10:00 – 10:15	**Breakout Charge** *Chairs*	Concourse Room
10:15 – 10:30	**BREAK**	Concourse Room
10:30 – 12:00	**Breakout Panel 1: Sprays**	Cavalier B
	Breakout Panel 2: Stochastic In-cylinder Behavior	Cavalier C
12:00 – 1:00	**Lunch with panel progress and questions**	Concourse Room
1:00 – 5:00	**Breakout Panel 1: Sprays**	Cavalier B
	Breakout Panel 2: Stochastic In-cylinder Behavior	Cavalier C
5:00 – 5:40	**Panel Report Outs**	Concourse Room
5:40 – 6:00	**Summary** *Chairs, DOE*	Concourse Room

- **Invitation only – 63 participants.**
- **Significant industrial participation (Cummins, GM, Ford, Chrysler, Caterpillar, GE, Navistar..)**



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PreSICE Workshop Report

Executive Summary (1 page)

Introduction (3 pages)

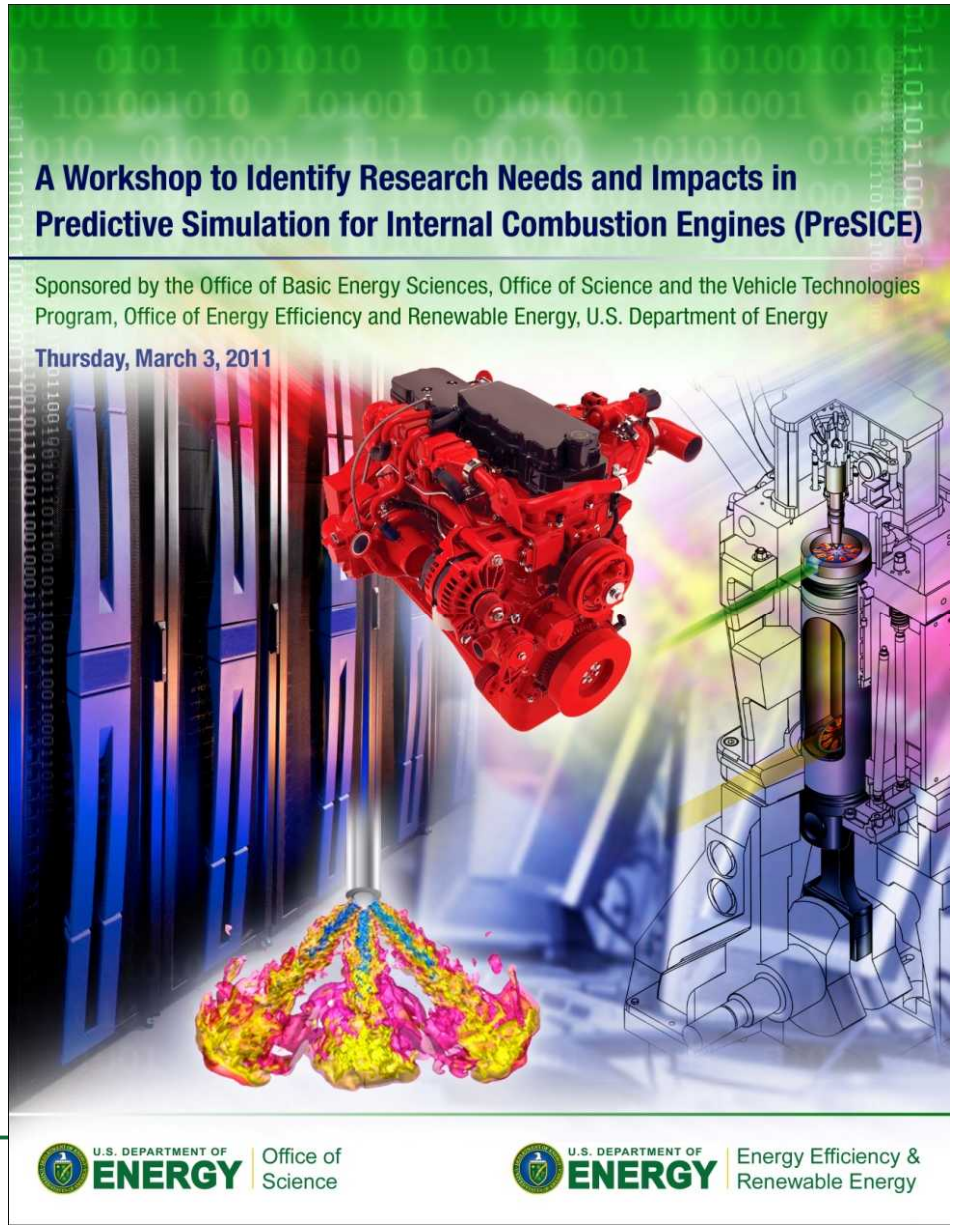
Research and Development Foci:

- **Sprays**
  - Research needs (4 pages)
  - Expected software tools (1 page)
  - Impact on future vehicles (1 page)

- **Stochastic In-cylinder Processes**
  - Research needs (4 pages)
  - Expected software tools (1 page)
  - Impact on future vehicles (1 page)

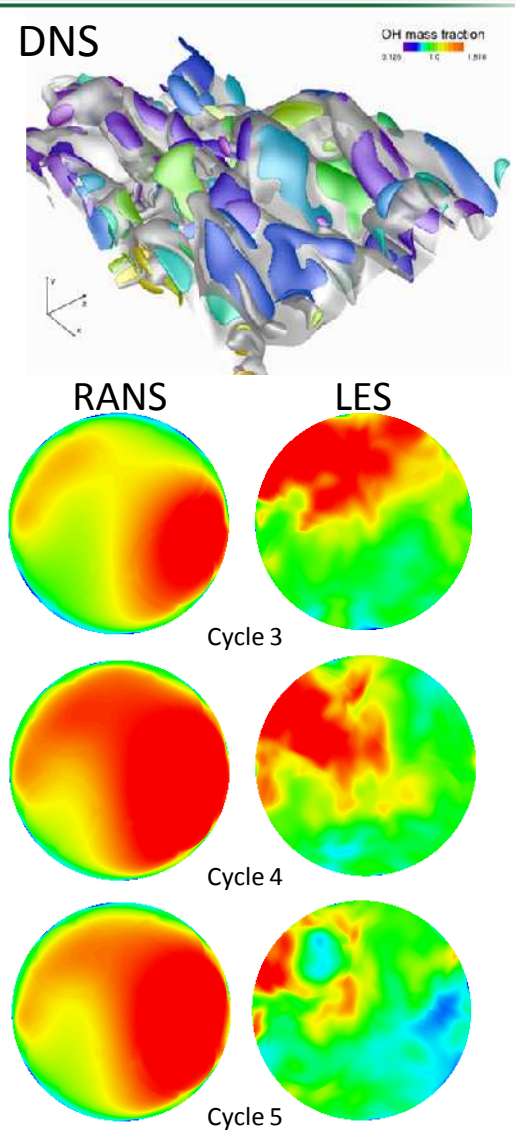
Conclusion (1 page)

Report complete by March 31!



Hierarchy of software tools is needed

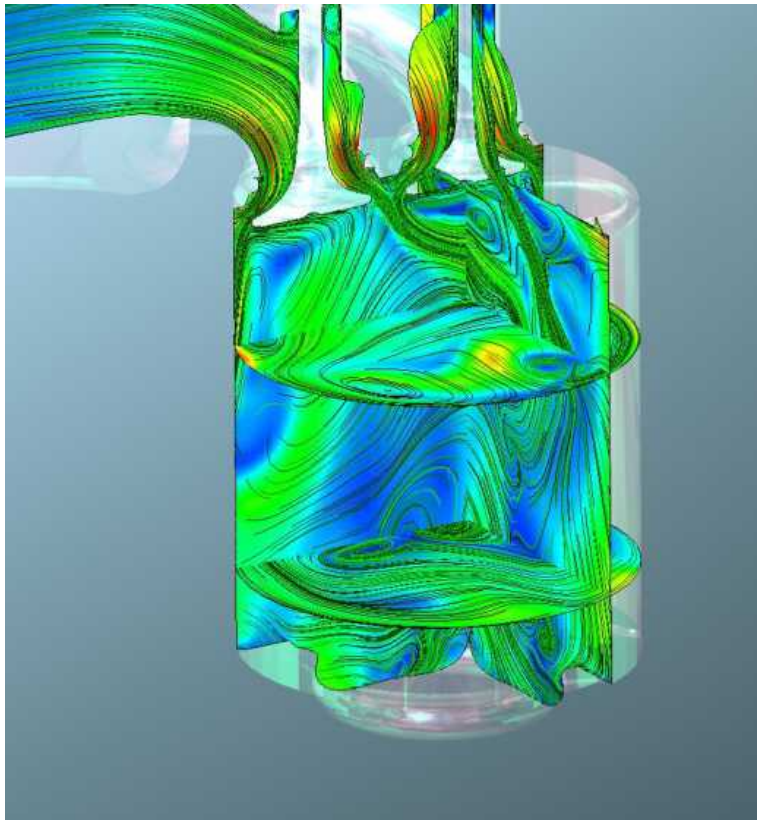
- **Direct Numerical Simulation (DNS)** – Extremely high fidelity simulation tools that enable scientific discovery
- **High-Fidelity Large Eddy Simulation (LES)** – Fine resolution and stringent error control will provide insight for modeling and the bench-mark for computations encompassing the full complexity of stochastic engine flows and sprays
- **Engineering LES** – The design tool for minimizing cyclic variability. Less demanding computationally to allow simulations of many cycles or design optimization, but modeling of small scale processes needs refinement
- **Reynolds-Averaged Navier Stokes (RANS) approaches** – The current workhorse of industry will continue to play a dominant role in multi-parameter optimization. Improved sub-model accuracy will lead to more optimum designs



Temperature at Start of Injection

What are the critical needs?
Stochastic Processes Priority Research Directions

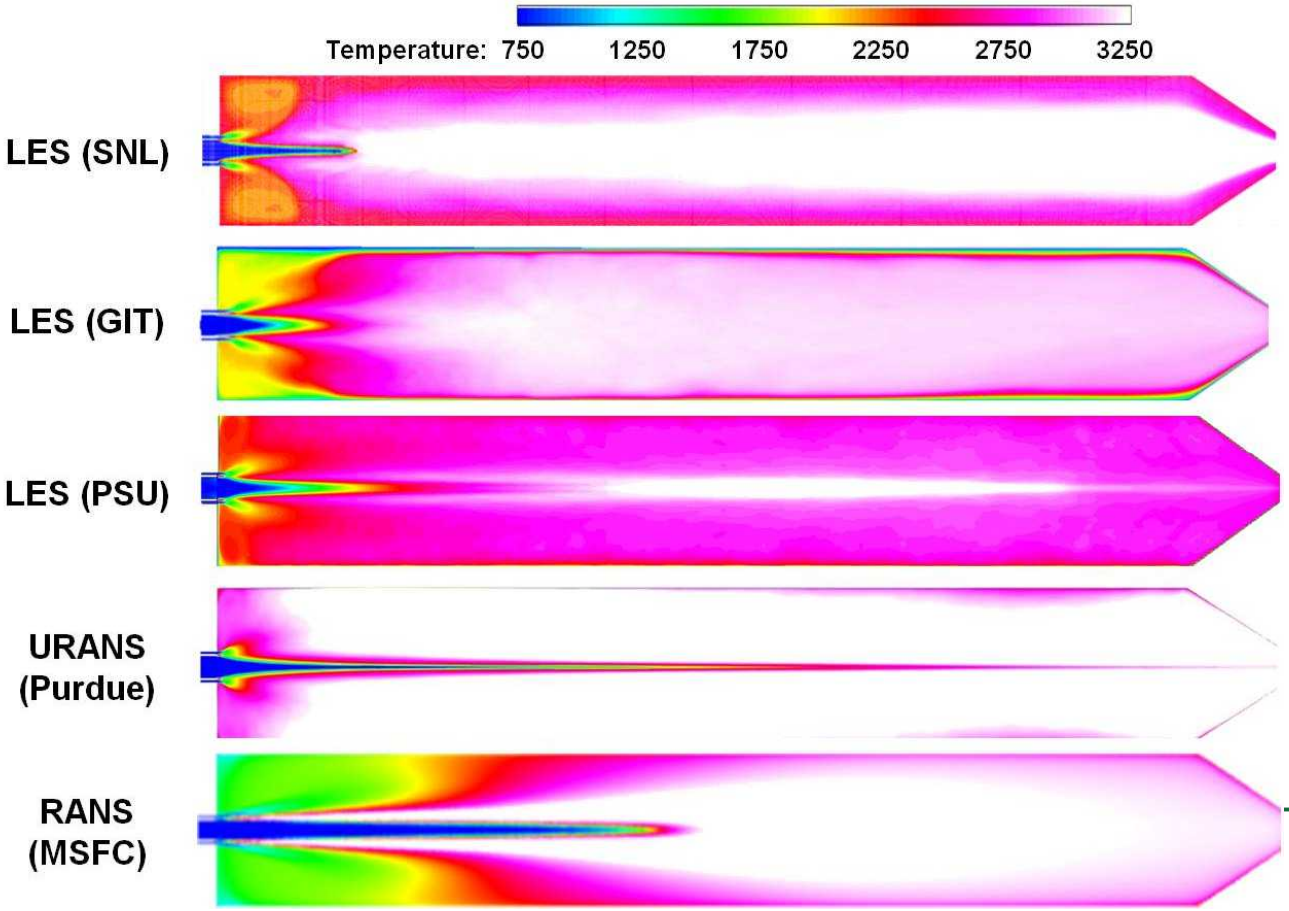
- **Development and validation of models to enable simulation of stochastic processes**
  - Sub-grid scale models for unresolved processes
  - Reduced chemical kinetic mechanisms
  - New theoretical frameworks / efficient numerical approaches



Complex in-cylinder flow during intake stroke in diesel engine

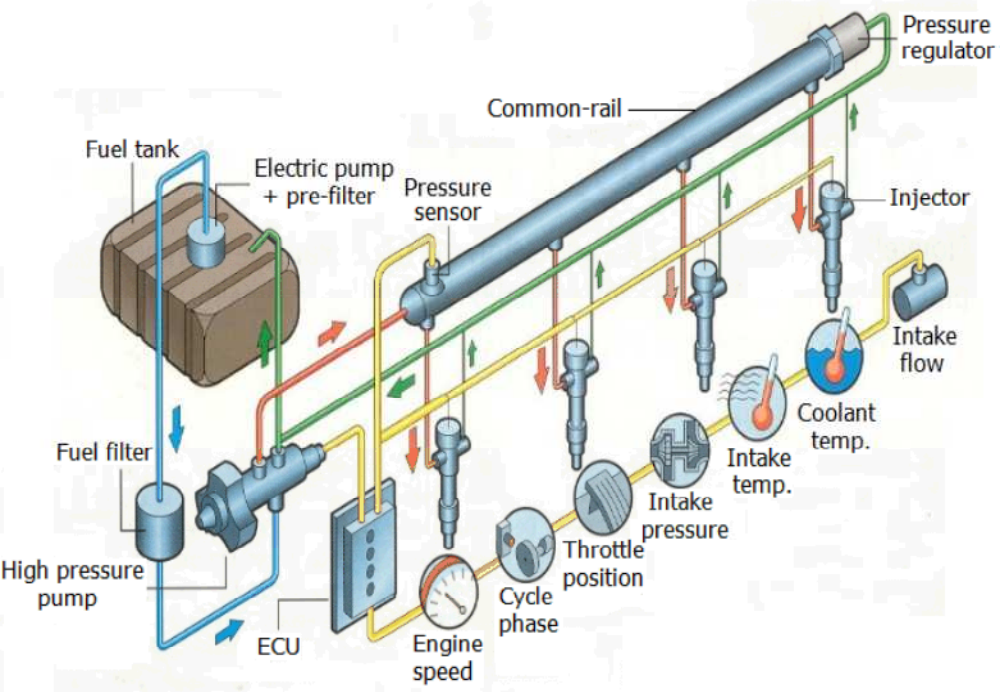
What are the critical needs?
Stochastic Processes Priority Research Directions (cont.)

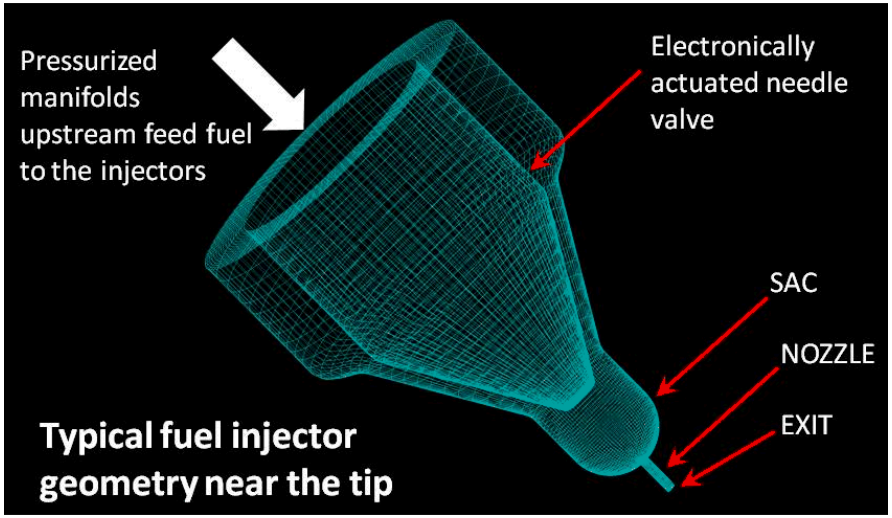
- **Improved accuracy and minimization of uncertainty**
  - Ability to tune model complexity to necessary accuracy level
  - Impact of uncertainty in initial conditions, boundary conditions, parameters
  - Propagation of uncertainties and errors reduction



What are the critical needs?
Spray Dynamics Priority Research Directions

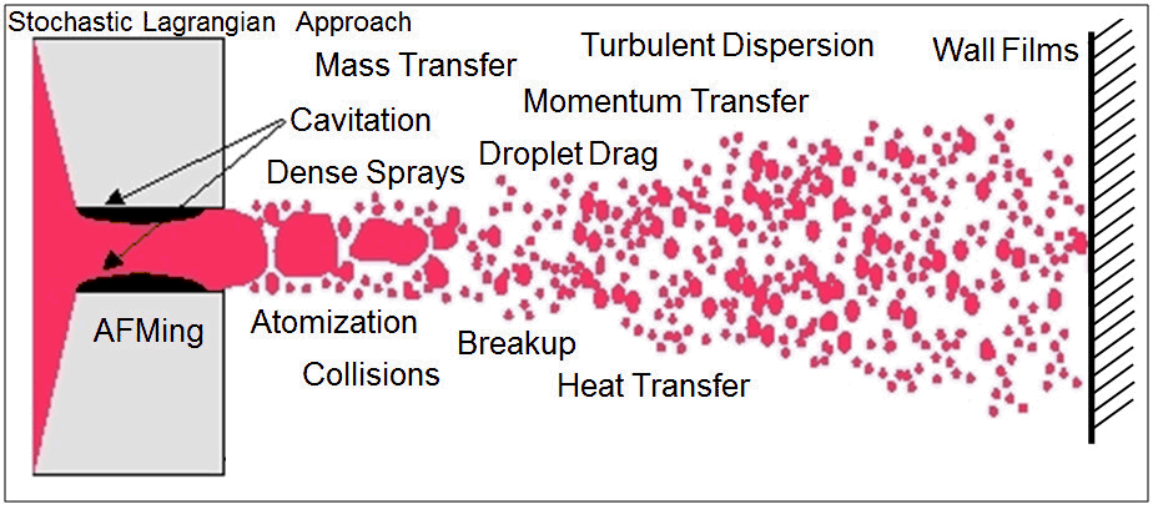
- **Detailed treatment of fuel-delivery systems (fuel rail and internal injector flows)**
  - Geometric complexities of flow passages upstream of injector
  - High pressure internal flow dynamics and transients
  - Turbulence and cavitation within injector sac and nozzle(s)





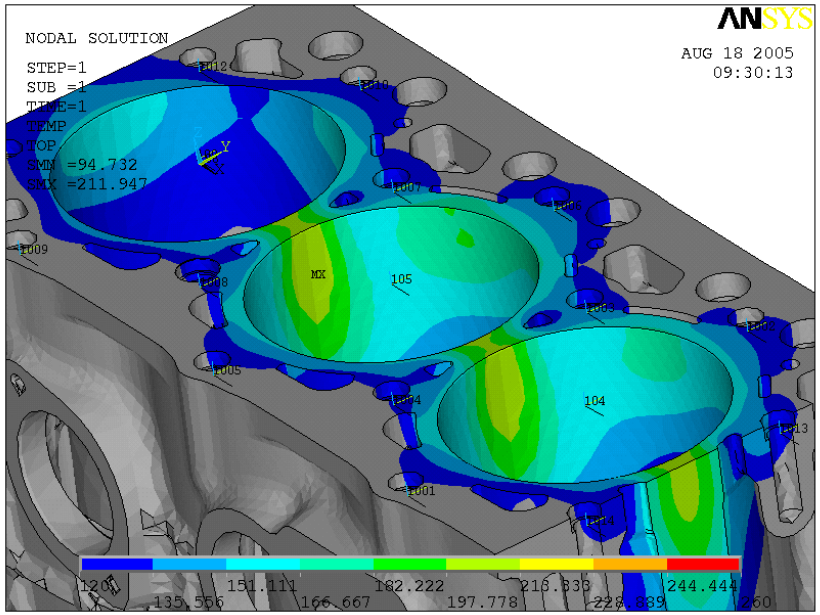
What are the critical needs?
Spray Dynamics Priority Research Directions (cont.)

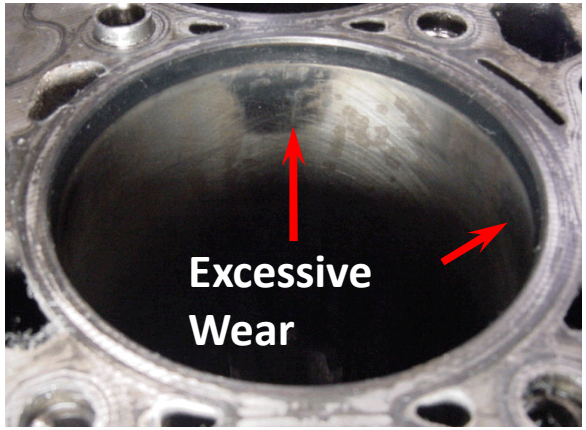
- **Optimization of fuel-preparation strategies (in-cylinder injection, mixing and combustion)**
  - Injection timing and strategy (single/multiple-pulse, etc.)
  - Primary-breakup, atomization, dense spray dynamics
  - Secondary-breakup, particle deformation, coalescence
  - Dilute drop dynamics, vaporization, combustion
  - High-pressure thermodynamically supercritical flow



What are the critical needs?
Spray Dynamics Priority Research Directions (cont.)

- **In-cylinder fluid-wall interactions, heat transfer**
  - Fuel impingement on cylinders degrades performance, emissions and durability
  - Surface temperature variations create similar problems
  - Improved modeling of near-wall effects is required for advanced systems

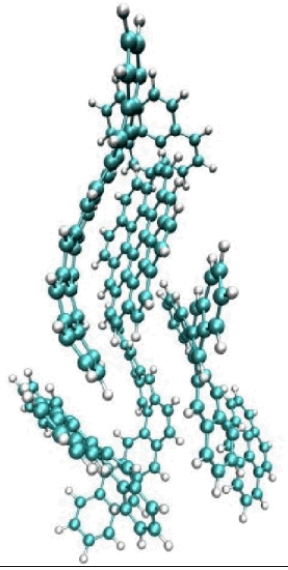




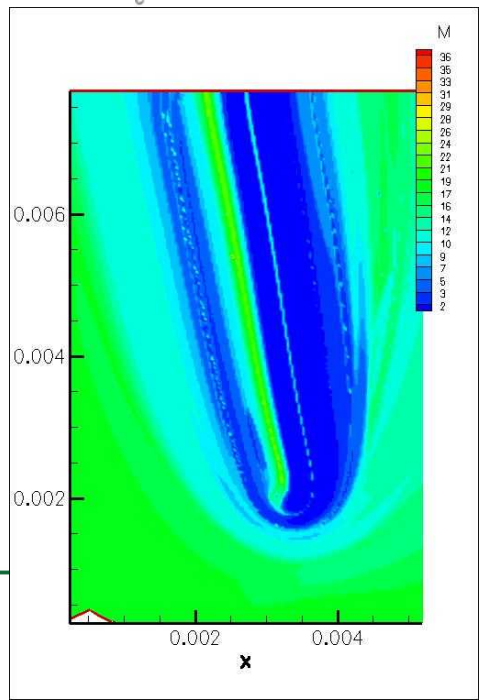
Calculated heat load from wall impingement and observed wear

Cross Cutting Research Needs

- **Chemistry of complex systems**
  - Methods to obtain chemical force fields, rate representations, and automatic mechanism generation
  - Efficient, on-the-fly kinetic mechanism reduction as a function of local conditions will be needed to enable cost-effective simulation of combustion



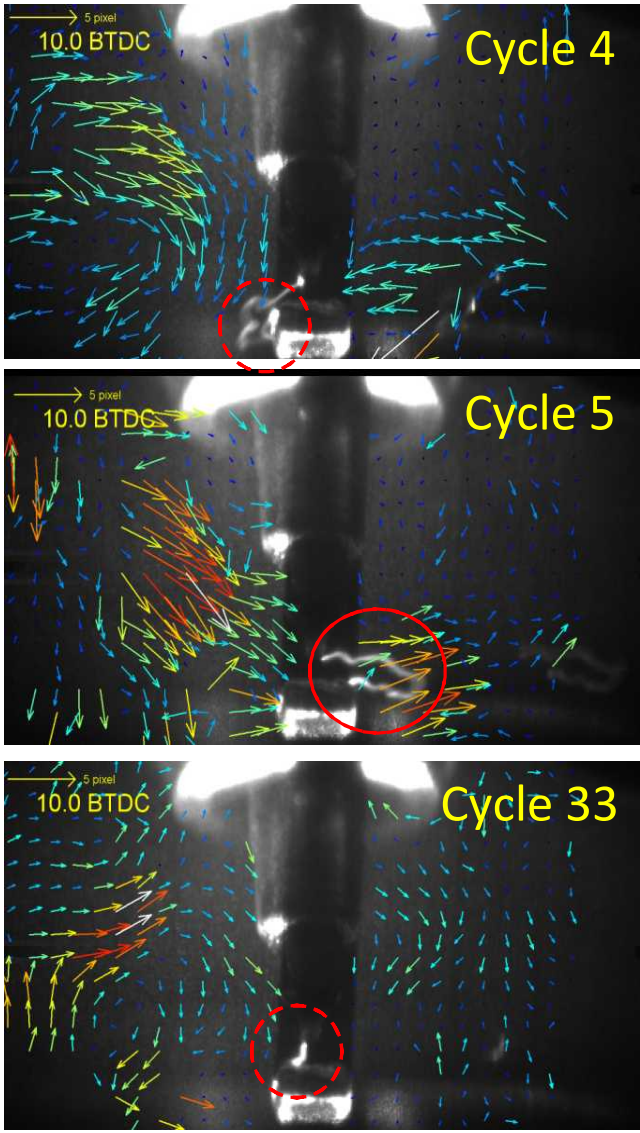
- **Uncertainty quantification**
  - Error (perturbation) propagation tools
  - Sophisticated sensitivity analysis



Computational Singular Perturbation (CSP) theory analysis of edge flame chemistry

Cross Cutting Research Needs (cont.)

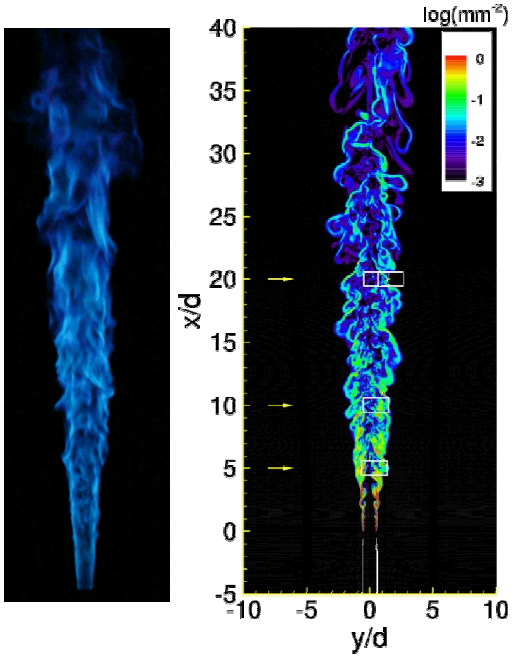
- **Development of tailored discovery and validation experiments**
  - Spatially and temporally-resolved, multi-parameter diagnostics
  - High pressure chemistry of complex mixtures
  - High pressure spray facilities with advanced diagnostics
  - Standard optical engine for advanced combustion strategies

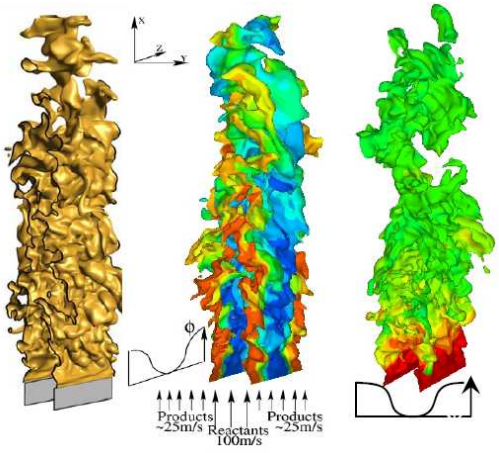


High frame rate, in-cylinder velocity field measurements

Research supporting a hierarchy of software tools is needed

- **Model development, validation and reduction:**
  - Benchmark experiments for validation data
  - Companion high-fidelity LES for detailed model development and reduction (detailed physics)
  - Engineering LES/RANS for engine cycle optimization and analysis (fast solution times)
  - DNS for analysis of small-scale turbulence-chemistry interactions
- **Tool infrastructure development:**
  - Advanced grid generation and grid quality assessment
  - Core solver development (science-based LES and engineering-based LES/RANS)
  - Advanced model reduction and uncertainty quantification
  - Post-processing, visualization, data management for both science and engineering





What is the impact *if* new simulation tools are developed?

- **Design, testing, and calibration portions of the product development cycle can all be shortened**
  - Calibration savings alone could reduce the product development cycle time and cost by 25-50% (industry dependent)
- **Expand design space to broad range of design concepts**
- **Reach the theoretical 60% limit on thermodynamic efficiency**
  - Potential for saving 4 M barrel of petroleum per day

A program based on PreSICE will enhance the competitiveness of and develop the future workforce for US industry, improve US energy security, and promote global environmental security.

Thank you!

Questions?