LES Applied to Low-Temperature, Diesel and Hydrogen Engine Combustion Research

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Sponsor: DOE EERE Office of Vehicle Technologies
Program Manager: Gurpreet Singh, Team Leader, EECT

DOE Office of Vehicle Technologies Annual Review Meeting
February 25-29, 2008, Bethesda, Maryland
Session: Combustion Research (Gurpreet Singh),
Monday, February 25, White Flint Amphitheater, 1:00-4:50 PM

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Perspective … Project provides significant link between DOE Office of Science and Office of Vehicle Technologies

- **High-performance computing (HPC) offers new opportunities for advances in modeling and simulation**
- **Project combines three unique capabilities to maximize benefits of HPC for advanced engine research**
  - **Specialized theoretical-numerical framework**
  - **Access to "capability-class" computers**
  - **Portable massively-parallel software**

- **Objective: Combine state-of-the-art capability based on Large Eddy Simulation (LES) with key engine experiments**
  - **Detailed simulations that identically match optical engines**
  - **Joint experimental-computational benchmark data**
- **Benefits: Reaches beyond resources, time-constraints of industry by providing high-fidelity benchmarks**
  - **Fundamental insights not available anywhere else**
  - **Foundation for advanced model development**

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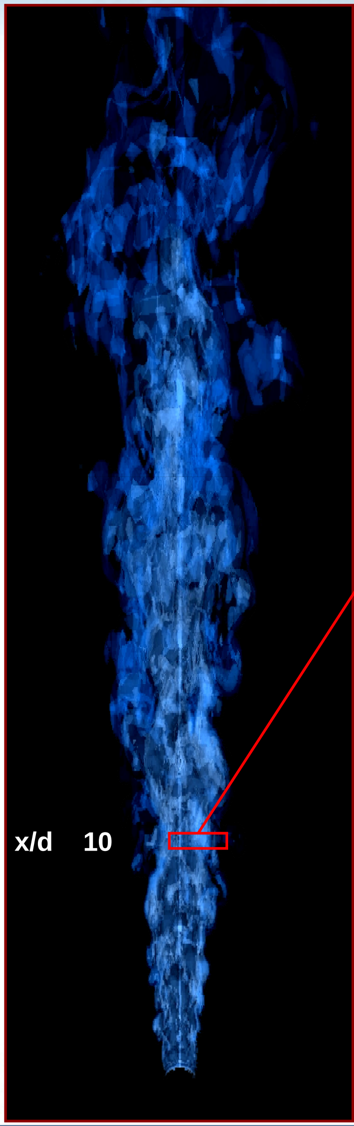
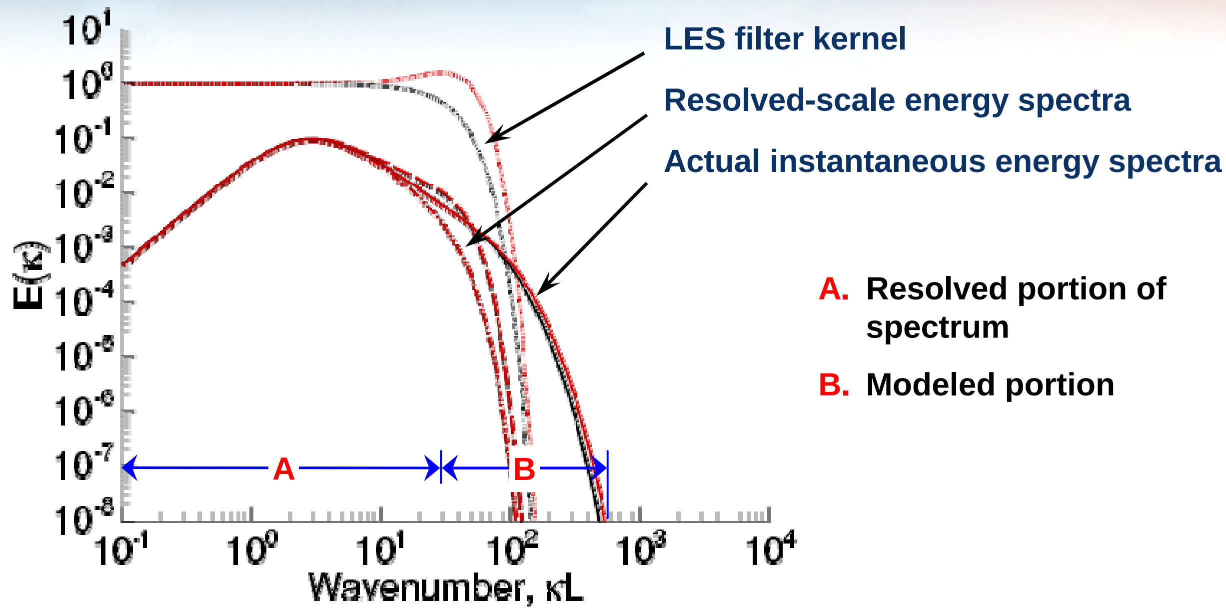
Why LES?





- **Provides mathematical formalism to treat full range of multidimensional scales in a turbulent reacting flow**
  - Large energetic-scales are resolved directly
  - Small "subgrid-scales" are modeled
- **Used when direct numerical simulations are not feasible**
  - Inhomogeneous (i.e., "real") turbulence characteristics
  - Device-scale geometries, engineering relevant conditions
- **Implemented as tool for both "science" and "engineering"**

Purpose of Work (FY08 Milestones)

Current directive is to focus on H_2ICE experiment, extend to LTC applications

- **Continue leveraging between DOE Office of Science and Office of Vehicle Technologies (Ongoing)**
  - **Access to "leadership-class" computers**
  - **Detailed model validation (Basic Energy Sciences)**
- **Develop improved high-pressure models for time-accurate treatment of direct-injection processes (January 2008)**
  - **Focus on high-pressure hydrogen injectors (collaboration with Petersen and Ghandhi, U. Wisconsin)**
  - **Ensure model extendable to liquid jets for LTC and Diesel applications (collaboration with Pickett *et al*., www.ca.sandia.gov/ECN)**
- **Perform detailed analysis of DI H_2-ICE engine and joint comparisons with experimental data (July 2008)**

Guidance from FY07 Review

- **Strengths:**
  - Connection with DOE Office of Science
  - Coupling simulations with engine experiments
  - Foundational for future model development
- **Weaknesses:**
  - Does not address near term goals for industry (emphasis on H_2)
  - No direct emphasis on simplified models
  - Rate of progress

- **<u>Recommendations</u>: Shift away from H_2ICE, clarify approach and technology transfer aspect**
  - We are placing more emphasis on LTC and Diesel applications
    - H_2ICE work has direct extensions
    - Model development is general, not specific to H_2
  - Issues related to progress, technology transfer linked to initial barriers
    - Three sets of technical barriers (only one mentioned in past reviews)

      Engine R&D ↔ Model Development & HPC ↔ Staffing

Engine R&D Barriers

- **High-Efficiency Hydrogen-Fueled Engines**
  - **Thermal efficiency, emissions goals requires increased power density**
    - **Direct injection offers highest power density**
    - **Dilute LTC with high levels of EGR (50%) required to control NO_X**
  - **Improved understanding of small-scale turbulent mixing, optimization of injection-valve timing required**

- **Advanced Low-Temperature Combustion Technology**
  - **Operation limited to moderate and low-load**
    - **HC/CO emissions, combustion inefficiencies at low loads**
    - **Unacceptable noise, engine damage at high loads**
  - **Improved understanding of mixture preparation strategies and loss mechanisms required**

Advanced simulations of in-cylinder processes will provide insights into:

- **Effects of timing, load, engine speed, heat transfer on mixture preparation**
- **Effects of fuel injection and engine geometry on mixing, combustion, emissions**
- **Tolerance of combustion to high EGR and mechanisms for controlling ignition timing, etc.**

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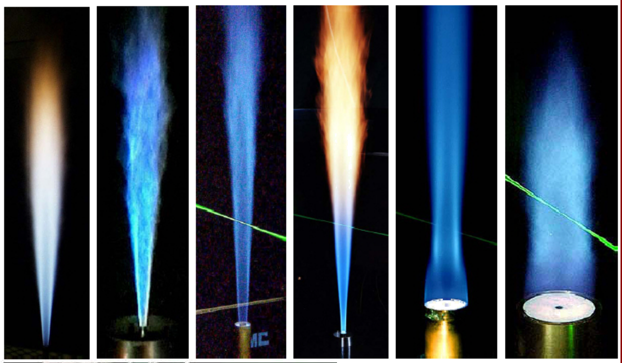
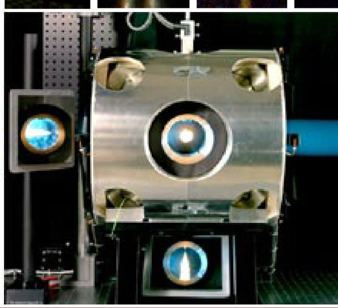
Model Development & HPC Barriers (Several Simultaneous Requirements)

Extensive subgrid-scale model development and validation





- Fuel injection, breakup, sprays
- Turbulent mixed-mode combustion
- Detailed thermo and transport
- Detailed chemistry
- Heat transfer

TNF Workshop
www.ca.sandia.gov/TNF

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

Verification of high quality numeric's for LES

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Highly-scalable parallel performance and I/O

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High-quality grids in complex geometry

↓

Advanced treatment of boundary conditions

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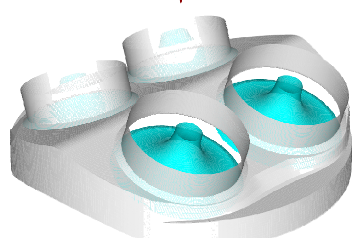
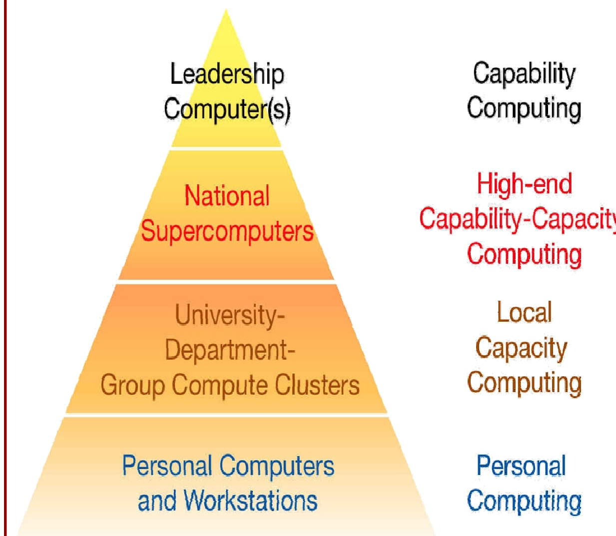


Detailed Analysis of In-Cylinder Processes

Hierarchy of computer resources, portable software



"Opportunities for Discovery: Theory and Computation in Basic Energy Sciences," U. S. DOE report, January 2005

CRF Computational Combustion and Chemistry Laboratory

National Center for Computational Sciences
www.nccs.gov

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Approach

- **Adhere to <u>strict algorithmic and implementation requirements</u>**
  - **Non-dissipative spatial stencils, no explicit artificial dissipation**
  - **High-quality grids, minimal stretching, cell deformation**
  - **High-level models for subgrid-scale closure**
- **Incorporate <u>level of physics beyond conventional approaches</u>**
  - **Complex geometries with high-accuracy**
  - **Direct treatment of finite-rate chemistry**
  - **Detailed turbulent, molecular transport**
- **Address <u>critical needs, challenges in key target experiments</u>**
  (i.e., effects of **<u>small-scale</u>**, **<u>unsteady</u>**, **<u>intricately-coupled</u>** processes)

Accomplishments

Office of Science

INCITE

Advancing America's Science and Industrial Competitiveness

"High-Fidelity Simulations for Clean and Efficient Combustion of Alternative Fuels"

1. **Awarded grand-challenge grant for CPU time on capability class computers based on this projects objectives**
   - **Multiyear (2008 – 2010) at National Center for Computational Sciences, ORNL (www.nccs.gov)**
     - **18-million hours in 2008 (CRAY XT4, 32,000 cores)**
     - **24-million hours in 2009**
     - **30-million hours in 2010**
2. **New combustion model shown to be capable of reconstructing important small-scale combustion processes**
3. **Developed new tabulation approach for treatment of complex hydrocarbon fuels based on the Linear Eddy Model**
4. **Developed and validated a general use high-fidelity model to simulate high-pressure fuel injection processes**
5. **Performed series of comparisons between LES and PIV data taken from the CRF hydrogen-fueled IC-engine**

OVT cluster critical for both production runs and staging to DOE platforms

mputational Combustion and Chemistry Laboratory

Visualization Cluster:

34 Opteron™ processors with high-end graphics cards, Gigabyte Ethernet, 50 terabyte parallel file system.

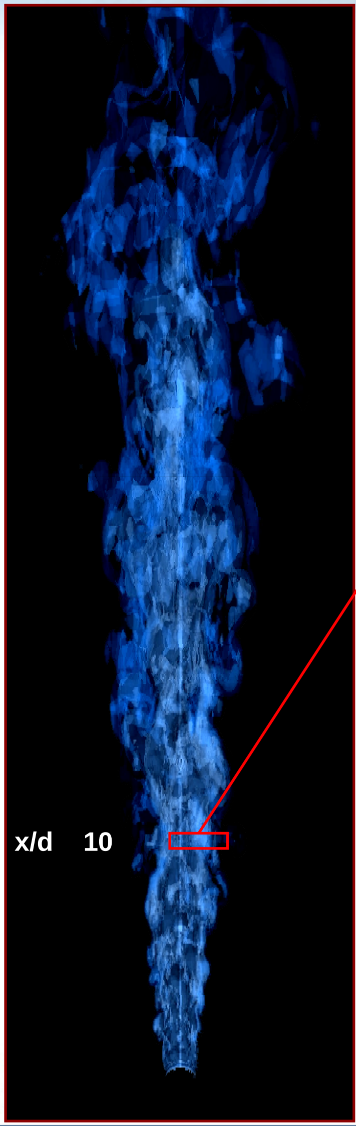
OVT System:

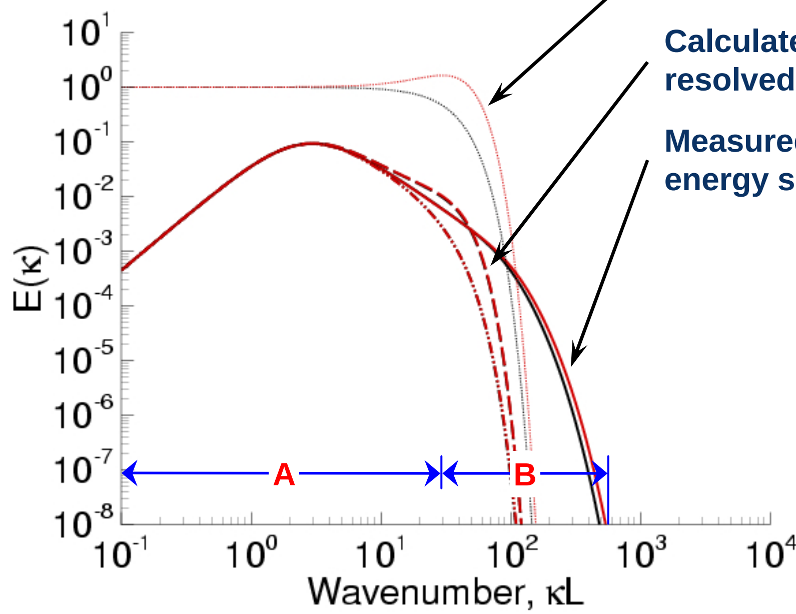
256 Opteron™ processors, InfiniBand, 10 terabytes NFS disk storage.

BES System:

284 Opteron™ processors, InfiniBand, 15 terabytes NFS disk storage.

Accomplishment 2 … New combustion model shown to be capable of reconstructing subgrid-scale structures





Specified (black) and corrected (red) LES filter kernel

Calculated (dash-dot), corrected (dashed) resolved-scale energy spectra

Measured (black) and reconstructed (red) energy spectra

A. **Resolved portion of spectrum**

B. **Stochastically reconstructed portion**

Turbulent Jet Flame:

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

Coflow: 99.2% Air, 0.8% H_2O

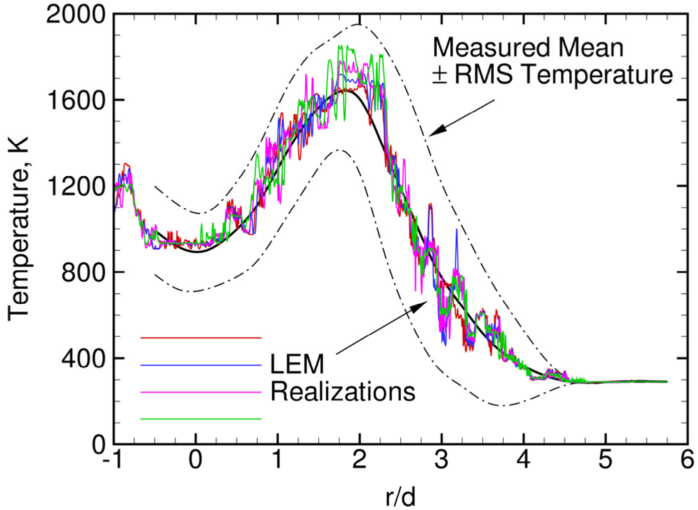
Detailed Chemistry and Transport: 12-Step Mechanism (J.-Y. Chen, UC Berkeley)

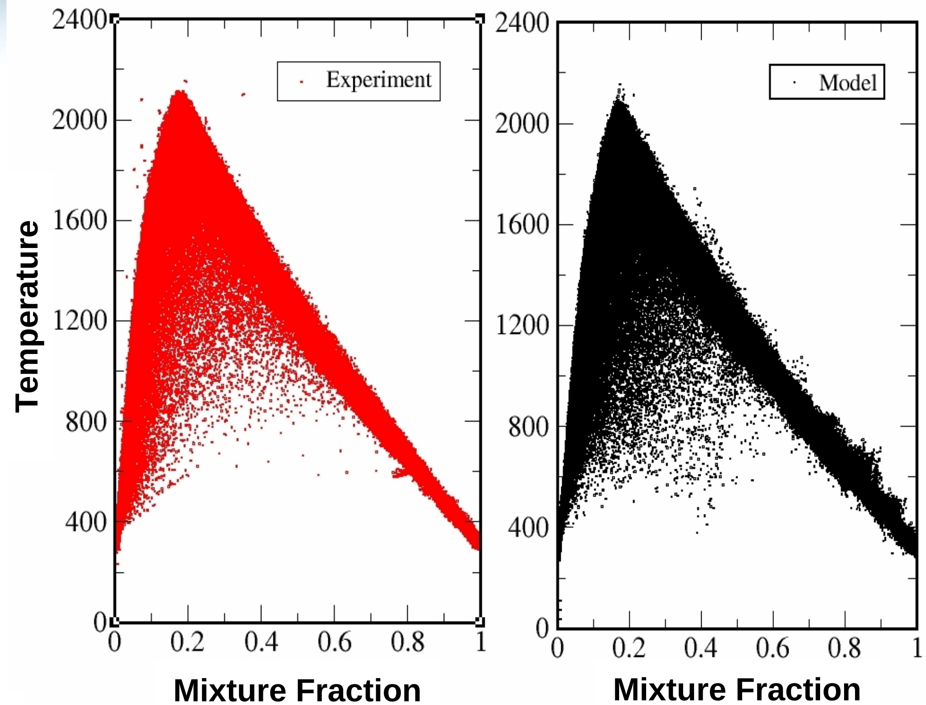
Reconstruction Model

dies suggest that model can be used to reconstruct energy and dissipation spectra accurately

Accomplishment 3 … Development of Tabulated Linear Eddy Model (for both LES and standalone)

- **Uses LEM to build thermo-chemical state library (i.e., "turbulent flamelet")**
  - **Provides 1D turbulent signal as a function of Mixture Fraction, Scalar Dissipation, Turbulent Re**
  - **Direct relevance to treatment of alternative fuels (complex hydrocarbons) and high-Re turbulence**





Model validated using flame data from TNF workshop (www.ca.sandia.gov/TNF)

Two Relevant Publications

ankaran, V., Drozda, T. G. and Oefelein, J. C. (2008).A tabulated closure for turbulent nonpremixed combustion based on the linear eddy model. Proceedings ofth e CombustionIn stitute, 32: (Submitted)

Steeper,R . R., Sankaran, V., Oefelein, J.C . an Hessel R. P. (2007). Simulation of the effect of spatial fuel distribution using a linear eddy model. Paper 2007-01-4131, SAE Powertrain & Fluid Systems Conference and Exhibition, October 29-November1, Chicago, IL.

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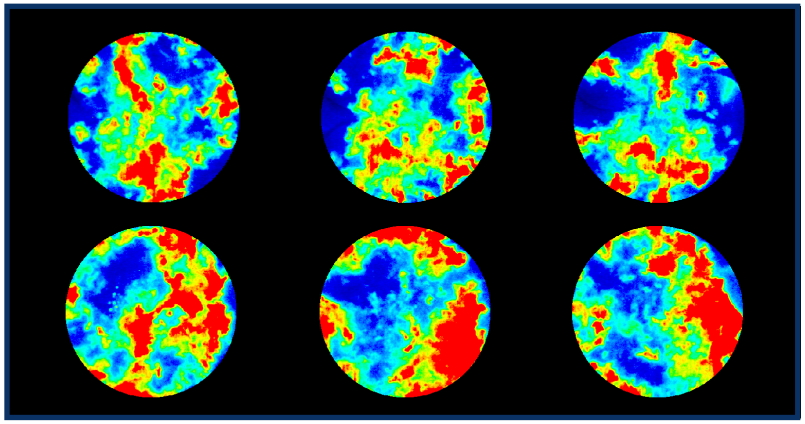
LEM provides fully resolved spatial and temporal representation of turbulent flow along a line in the locally predominant direction of scalar transport

Combining LEM with KIVA provides fine scale details of turbulent fuel/air mixing

LIF images of fuel distribution

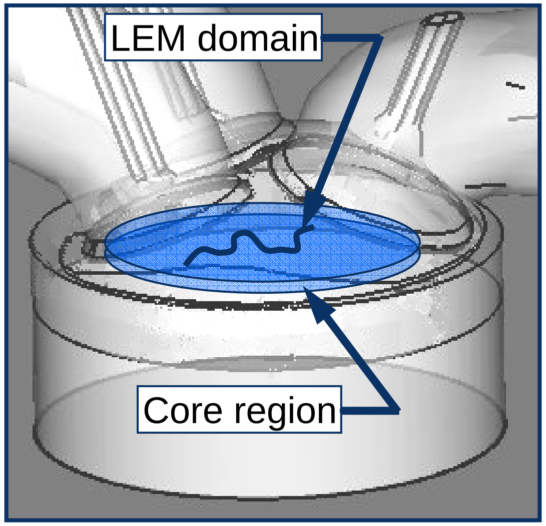
Injector A series

Injector B series



- **LEM predicts mixing to have significant effect when fuel distribution length scales match turbulence scales**
  - Results show that measurements should be analyzed using both spatial and PDF statistics
  - Both needed to understand how turbulent mixing affects HCCI combustion performance
  - Turbulent mixing affects combustion phasing and pressure-rise rates
  - Randomness of turbulence causes significant cycle-to-cycle variation of combustion

- **Similarities**
  - Same fueling, same operating conditions
  - Same pressure & heat release traces
  - Similar PDF statistics
- **Differences**
  - Spatial fuel statistics (coarse vs. fine)
  - NO_X emission performance
- **Typical PDF analysis discards spatial information that may influence combustion**



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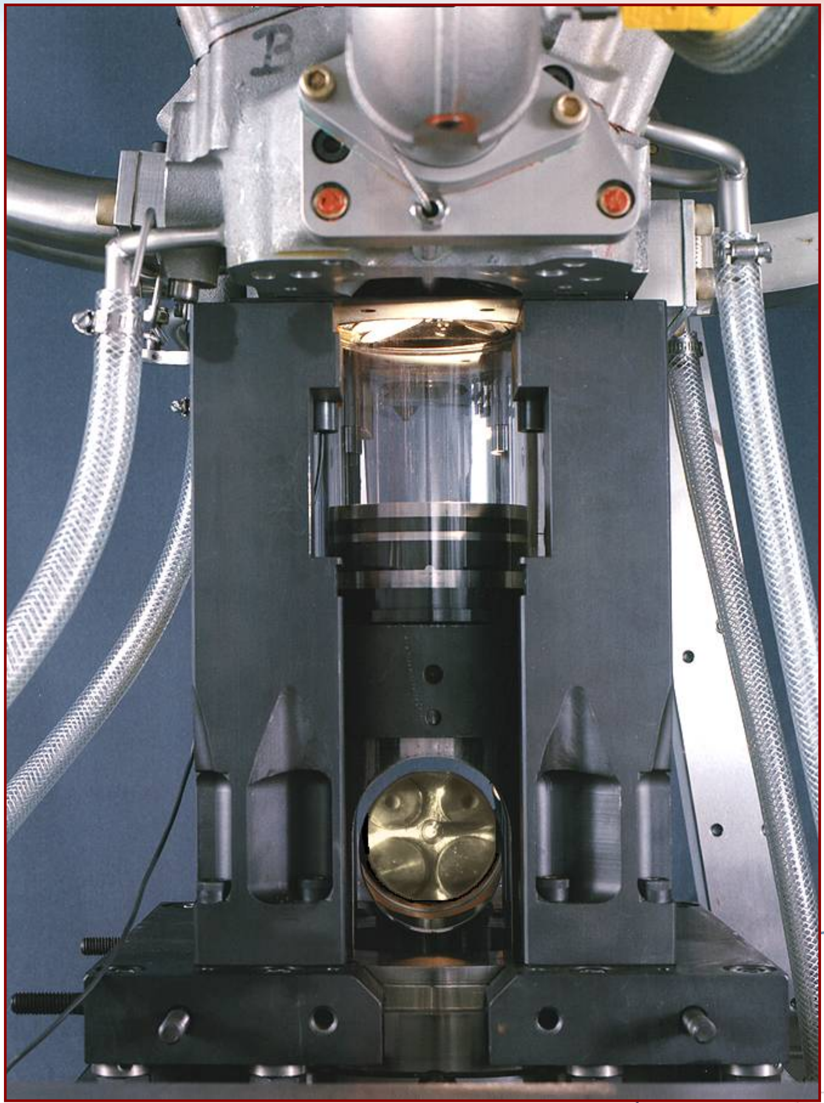
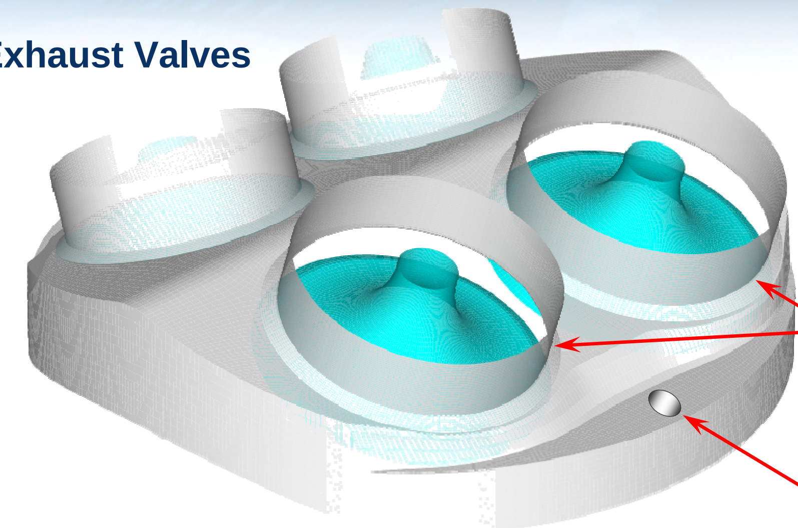
CRF Optically Accessible Hydrogen-Fueled IC-Engine

Typical In-Cylinder Turbulence Scales in an IC-Engine at TDC (start of combustion)	
Compression Ratio	9.1
Bore	92 *mm*
Stroke	85 *mm*
Cylinder Volume at BDC	634.81 cm^3
Cylinder Volume at TDC	69.759 cm^3
Peak Turbulence Intensity	2.85 *m/s*
Integral Length Scale	2 *mm*
Thermal Layer Thickness	6.3 μm
Reaction Zone Thickness	3.9 μm
Kolmogorov Length Scale	5.6 μm
Turbulent Reynolds Number	2550



Detailed Treatment of Geometry (Including High-Pressure Injector)

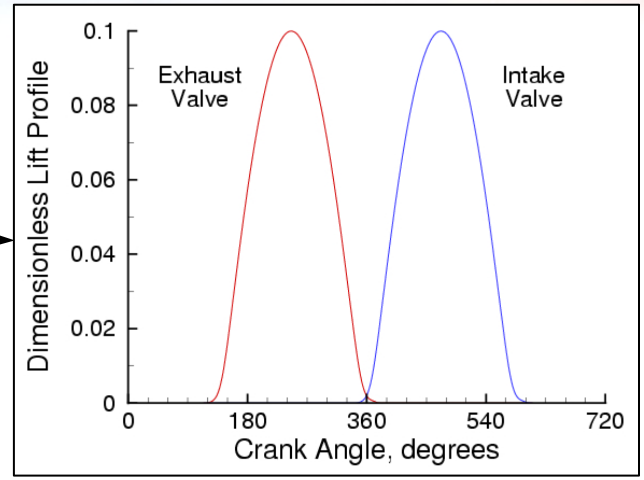
Exhaust Valves



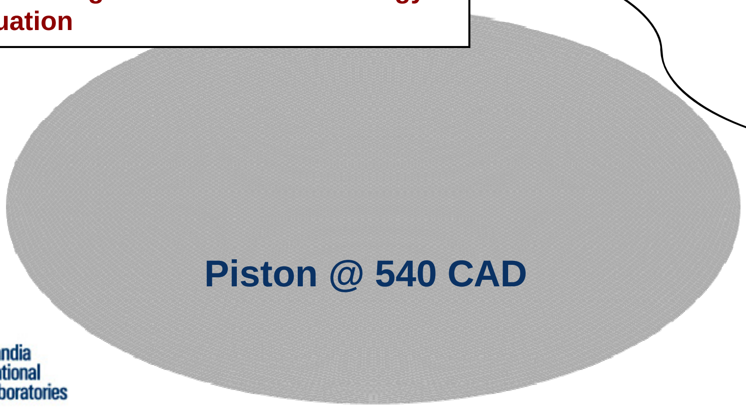
Intake Valves

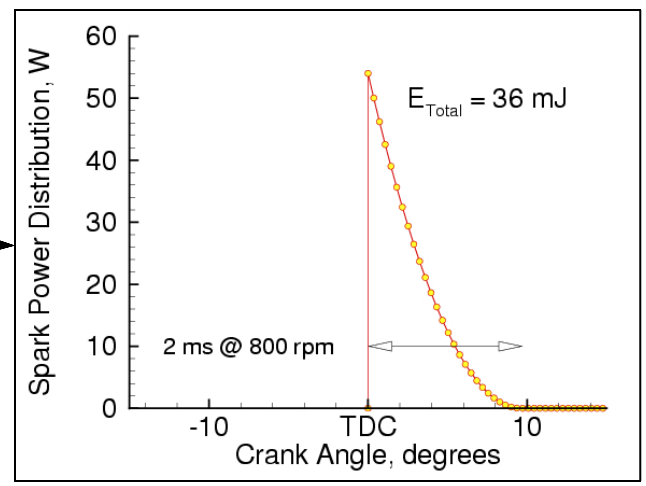
High-Pressure Injector

Valve lift profiles measured directly from camshaft



Spark ignition simulated by distributing total integrated energy over defined spark volume (1 mm^3) and adding as source to total energy equation





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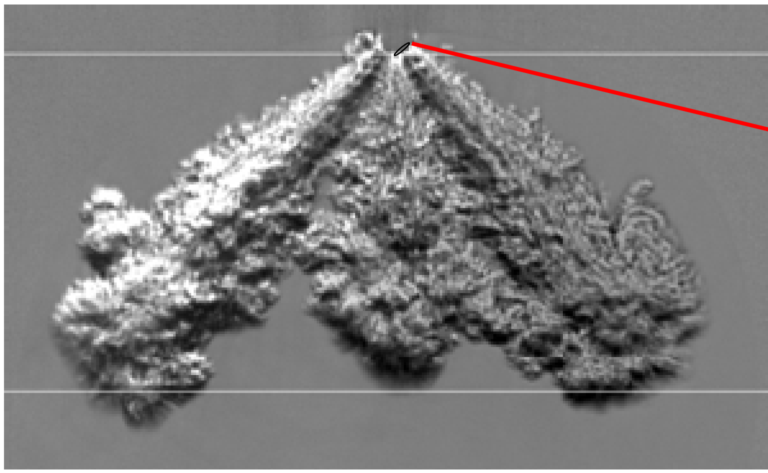
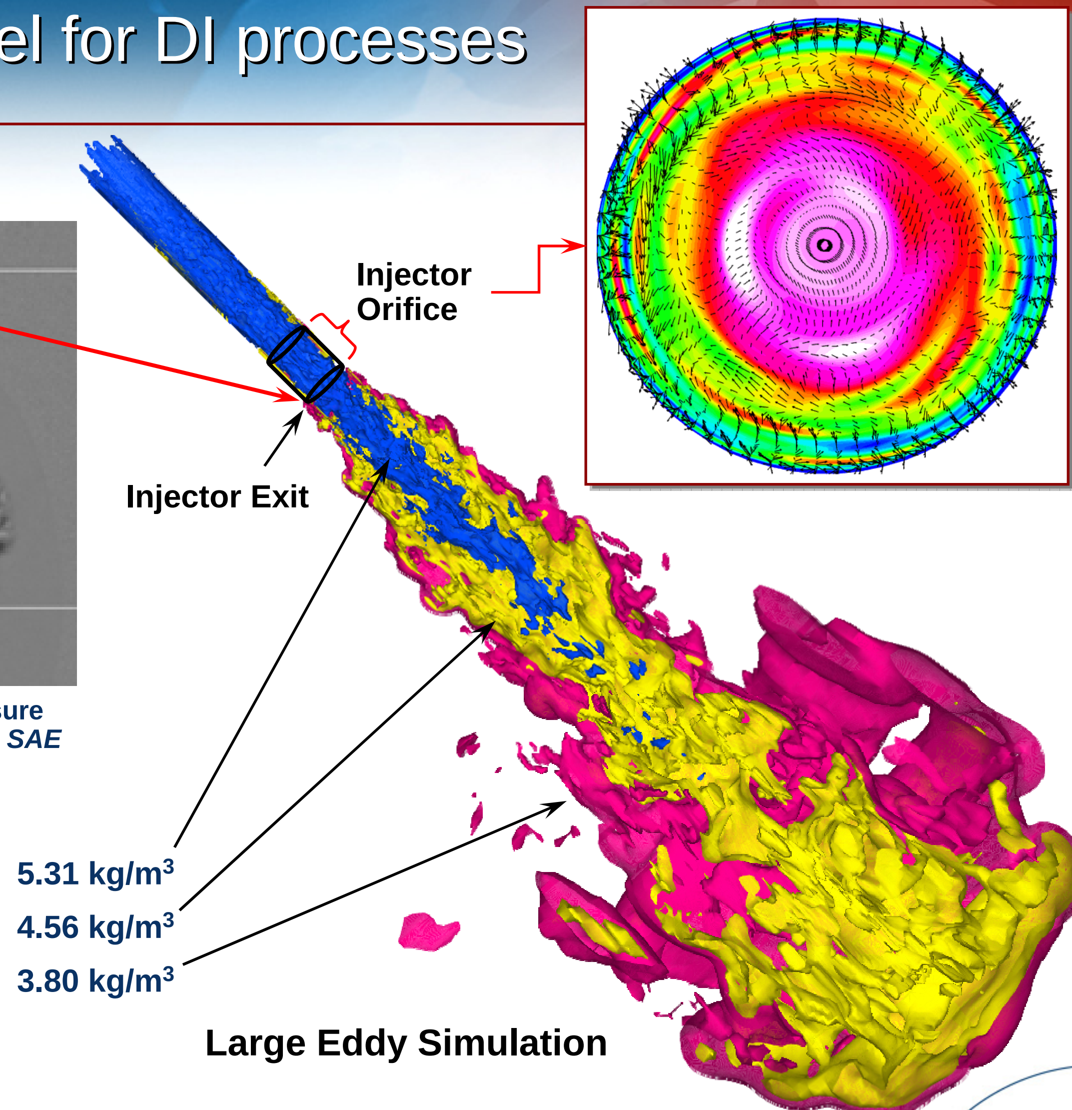
Accomplishment 4 … Developed and validated general high-fidelity model for DI processes

Shadowgraph (U. Wisconsin)



B. R. Petersen and J. B. Ghandhi. Transient High-Pressure Hydrogen Jet Measurements, *SAE Paper 2006-01-0652, SAE World Congress*, April 3-6, Detroit, Michigan.



Large Eddy Simulation

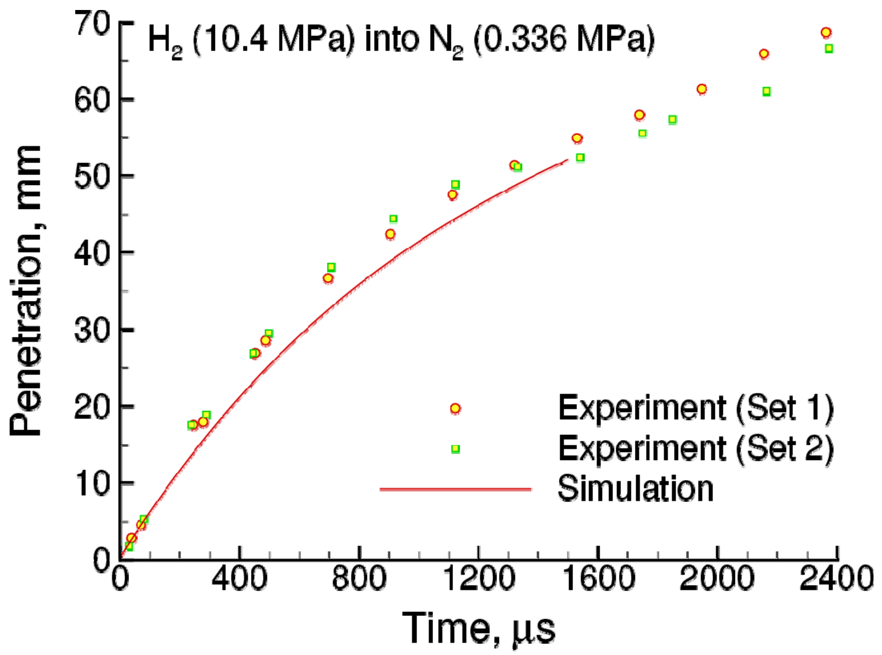
Iso-Contours of Density (H_2 – N_2):

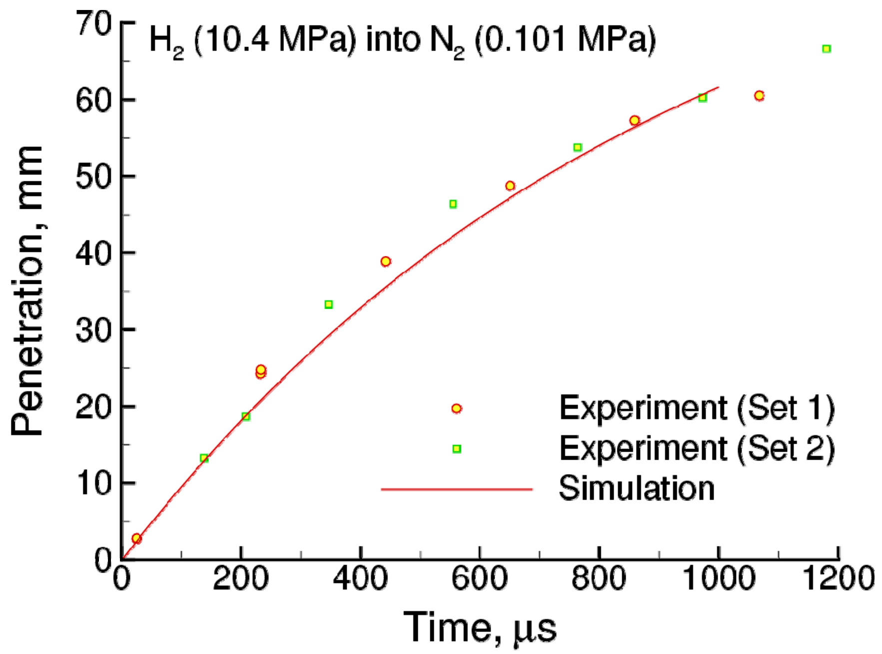
- $d_{orifice}$ = 0.8 *mm*
- $p_{injector}$ = 10.4 *MPa*, $T_{injector}$ = 298 *K*
- $p_{chamber}$ = 0.34 *MPa*, $T_{chamber}$ = 298 *K*

Publication

Drozda, T. G. and Oefelein, J. C. (2008). Large eddy simulation of direct injection processes for hydrogen and LTC engine applications, Paper 2008-01-0939, SAE World Congress, April 14-17, Detroit, Michigan.

Jet Penetration Compared to Experiments of Petersen and Ghandhi (U. Wisconsin)





Progress to-date provides both short- and long-term benefits:

- Have validated ability to handle injection process accurately in the in-cylinder calculations
- Can provided information beyond the experimental database for development of simpler models
- Have established a foundational capability for detailed studies of liquid hydrocarbon fuels

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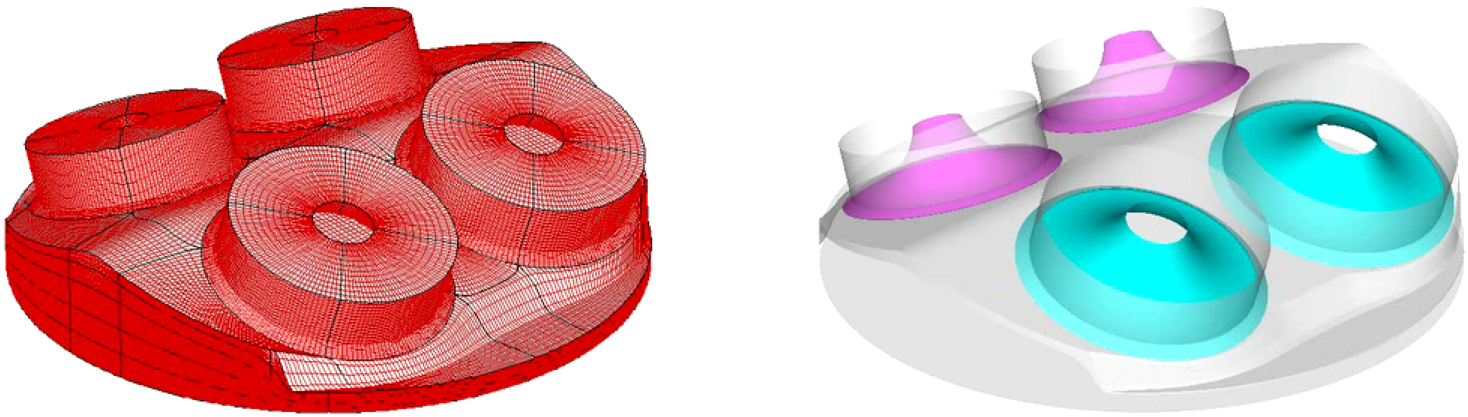
Accomplishment 5 …

Comparisons of LES with PIV data

H_2ICE Engine Configuration:

- **Baseline: 3-million cells, 137 blocks**
- **Production: *O*(10)-million cells**
- **ANSYS ICEM now fully integrated**



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Technology Transfer

- **Merging HPC, unique simulation capabilities, and advanced experiments provides four new conduits for tech-transfer**
  - **High-fidelity benchmark data from simulations**
  - **Mechanism for collaborative model development**
  - **Better bridging between science and engineering**
  - **Approach toward development of next generation tools**
- **Current Collaborators:**
  - **Boyer *et al*., Ford Motor Company on issues related to H_2ICE**
  - **Ghandhi *et al*., U. Wisconsin on validation of HP-injection model**
  - **Rutland *et al*., U. Wisconsin on comparing KIVA LES to detailed LES**
  - **Abraham *et al*., Purdue University on development of injection models**
  - **Najt *et al*., General Motors on further applications of LEM (pending)**
- **Institutions**
  - **DOE Office of Science, Basic Energy Sciences**
  - **ORNL National Center for Computational Sciences**

Future Work

- **Continue high-fidelity simulations of optical H_2-ICE**
  - **Direct-injection with new head, match experimental activities**
  - **Validation through comparison of measured, simulated results**
    - Chemiluminescence Imaging and Particle Image Velocimetry (PIV)
    - Planar Laser Induced Fluorescence (PLIF)
  - **Joint analysis of data extracted from validated simulations**
    - Enhance basic understanding
    - Improve engineering models
  - **H_2-injector pattern optimization studies**
- **Systematically extend to HCCI engine experiments**
  - **Detailed studies of low temperature combustion processes**
  - **Work toward treatment of complex hydrocarbon processes**
- **Continue leveraging between DOE Office of Science and Energy Efficiency and Renewable Energy activities**
  - **Detailed validation, analysis of key combustion phenomena**
  - **Access to high-performance "leadership-class" computers**

Summary

- **Project provides significant link between DOE Office of Science and Office of Vehicle Technologies**
  - **Objective: Merge state-of-the-art LES capability with key experiments**
  - **Benefits: Moves beyond current models, additional source of detailed data**
  - **Focus: Barriers related to both Advanced Engine R&D and Development of Advanced Simulation Capabilities using high-performance computing**
- **Five major accomplishments since last review**
  - **Grand-challenge grant for time on DOE capability class computers**
  - **New combustion model that treats important small-scale interactions**
  - **New simplified model for treatment of complex fuels using LEM**
  - **Developed and validated general model for high-pressure fuel injection**
  - **Comparisons of simulations and PIV data in CRF H_2ICE**
- **Have begun to establish technology transfer through collaborations with industry and academia with emphasis on**
  - **Developing a validated suite of benchmark simulations and sub-models**
    - **High-pressure phenomena (chemistry, thermodynamics, transport …)**
    - **Multiphase flow and combustion (atomization, jet breakup …)**
    - **Clean and efficient combustion of alternative fuels …**

Publications

- V. Sankaran, T. G. Drozda and J. C. Oefelein (2008). A tabulated closure for turbulent nonpremixed combustion based on the linear eddy model. *Proceedings of the Combustion Institute*, **32**: (Submitted).
- T. G. Drozda, G. Wang, V. Sankaran, J. R. Mayo, J. C. Oefelein and R. S. Barlow (2007). Scalar filtered mass density functions in nonpremixed turbulent jet flames. *Combustion and Flame* (Submitted).
- T. G. Drozda and J. C. Oefelein (2008). Large eddy simulation of direct injection processes for hydrogen and LTC engine applications. *Paper 2008-01-0939, SAE World Congress*, April 14-17, Detroit, MI.
- R. R. Steeper, V. Sankaran, J. C. Oefelein and R. P. Hessel (2007). Simulation of the effect of spatial fuel distribution using a linear eddy model. *Paper 2007-01-4131, SAE Powertrain & Fluid Systems Conference and Exhibition*, October 29-November 1, Chicago, IL.
- P. K. Tucker, S. Menon, C. L. Merkle, J. C. Oefelein and V. Yang (2007). An approach to improved credibility of CFD simulations for rocket injector design. *Paper 2007-5572, 43rd AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit*, July 8-11, Cincinnati, OH.
- T. G. Drozda, G. Wang, V. Sankaran, J. R. Mayo, J. C. Oefelein and R. S. Barlow (2007). Scalar filtered mass density functions in nonpremixed turbulent jet flames. *Proceedings of the 5th US Joint Meeting of the Combustion Institute*, March 25-28, San Diego, CA.
- V. Sankaran and J. C. Oefelein (2007). Advanced preconditioning strategies for chemically reacting flows. *Paper 2007-1432, 45th AIAA Aerospace Sciences Meeting & Exhibit*, January 8-11, Reno, NV.
- T. C. Williams, R. W. Schefer, J. C. Oefelein and C. R. Shaddix (2007). Idealized gas turbine combustor for performance research and validation of large eddy simulations. *Review of Scientific Instruments*, **78**(035114): 1-9.
- J. C. Oefelein, V. Sankaran and T. G. Drozda (2006). Large eddy simulation of swirling particle-laden flow in a model axisymmetric combustor. *Proceedings of the Combustion Institute*, **31**: 2291-2299.
- J. C. Oefelein (2006). Large Eddy Simulation of mixing and combustion for direct-injection operation. *European Commission HyICE Program: Optimization of a hydrogen powered internal combustion engine*, Project 506604, Chapter **D4.3.G**: 1-18.
- J. C. Oefelein, T. G. Drozda and V. Sankaran (2006). Large Eddy Simulation of Turbulence-Chemistry Interactions in Reacting Flows: The Role of High-Performance Computing and Advanced Experimental Diagnostics. *Journal of Physics*, **46**: 16-27.
- J. C. Oefelein (2006). Large eddy simulation of turbulent combustion processes in propulsion and power systems. *Progress in Aerospace Sciences*, **42**: 2-37.