Lawrence Livermore National Laboratory

Modeling of high efficiency clean combustion engines

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DOE National Laboratory Advanced Combustion Engine R&D
Merit Review and Peer Evaluation
Washington, DC

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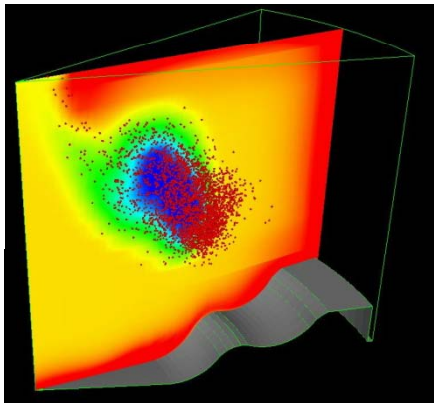
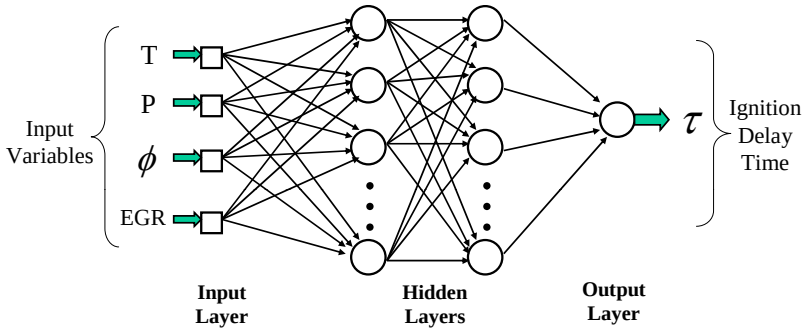
Goals/Objectives: collaborate with industry, academia and national labs in the development of analysis tools enabling clean, efficient engines

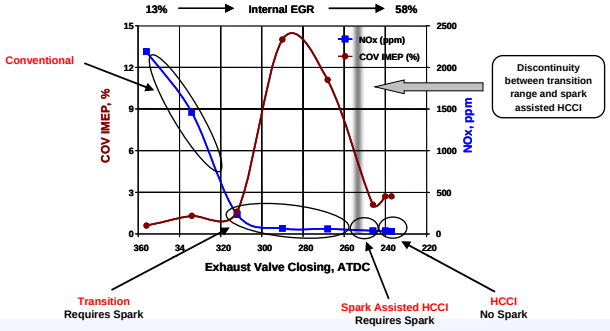
- **We are demonstrating our modeling tools for partially stratified combustion**



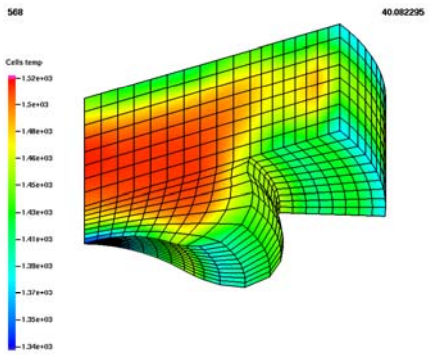
- **Our Artificial Neural Network-based KIVA-ANN provides computationally inexpensive analysis capability for HCCI/PCCI**



- **We are working with ORNL in analyzing HCCI-SI transition experiments**



- **We are working with LANL on KIVA4MZ, a multi-zone version of KIVA4**



FY2007 Reviewer's Comments and Response

- ***Relevance is good, but the scope should include a broad view of low temperature combustion, so it is not narrowly focused on HCCI.*** **Most of our activity is now focused on partially stratified combustion and SI-HCCI transition.**

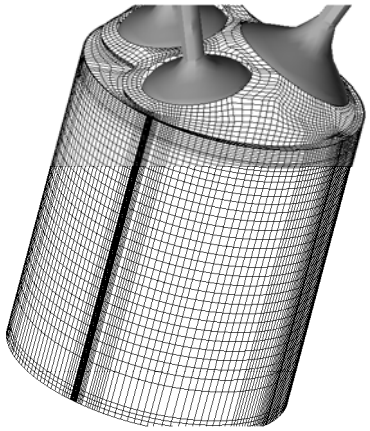
- ***Multiple injections are a "fact of life" and will eventually have to be fully incorporated in modeling and lab work*****.** **We are currently dedicating most of our effort to direct-injected, partially stratified engine analysis**

- ***It has been difficult to develop commercial IP agreements with the LLNL industrial partnership office. Dan et al. are excellent to work with at the technical level, but at the "commercial level" we have struggled.*** **Codes and models have been transferred to industry and they are available to industrial collaborators and researchers.**

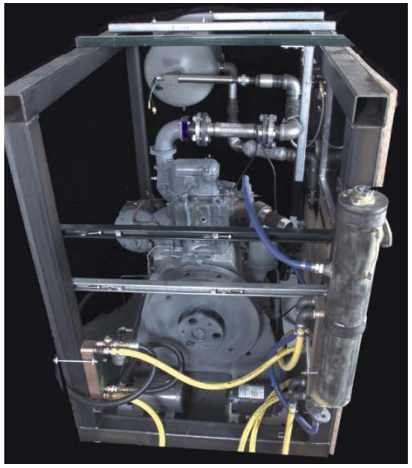
FCVT Barriers: we are contributing to an improved understanding of high efficiency engine regimes

- **Barrier: Increases in engine efficiency and decreases in engine emissions are being inhibited by an inadequate ability to simulate in-cylinder combustion and emission formation processes**
  - **Our Contribution: We focus on improving understanding of advanced combustion processes by developing detailed models of chemical kinetic-fluid mechanic interactions and their effect on engine combustion**

Approach: Fundamental and practical understanding of advanced engine combustion regimes by judicious use of modeling and experiments

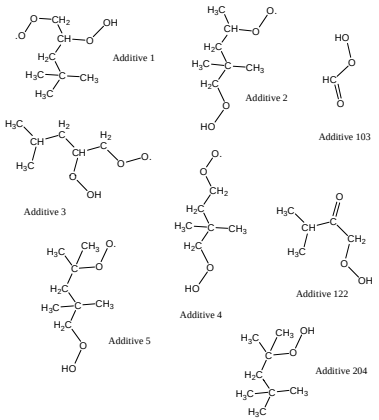


High Resolution CFD



Engine Experiments

Fundamental Understanding + Design Guidance

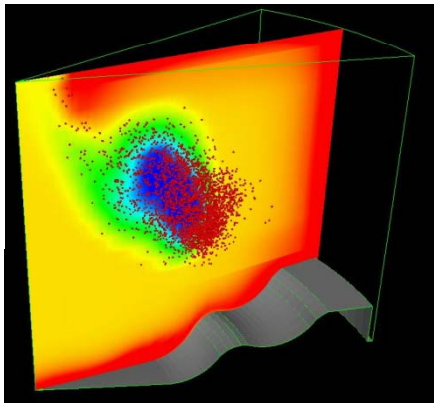


Chemical kinetics

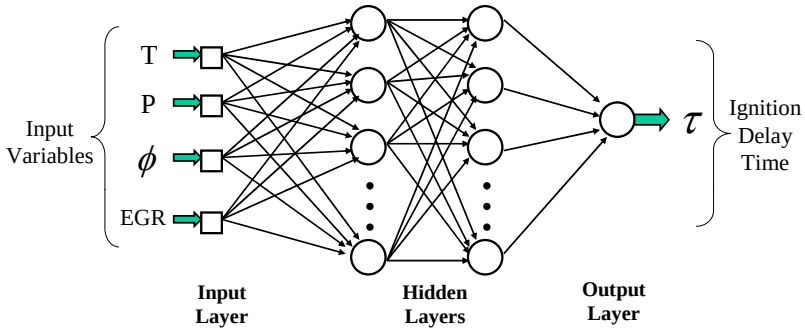
Advanced diagnostics

Technical accomplishment summary: we are working at demonstrating advanced analysis tools for challenging engine combustion problems

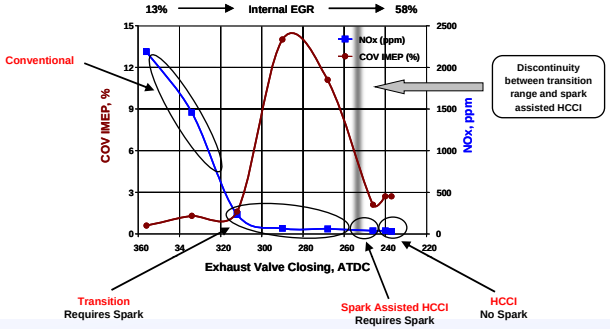
- **KIVA3V-MZ-MPI is running in direct injected mode and producing results**



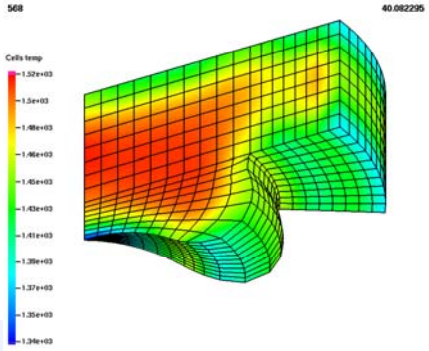
- **KIVA-ANN has demonstrated good performance in PCCI analysis**



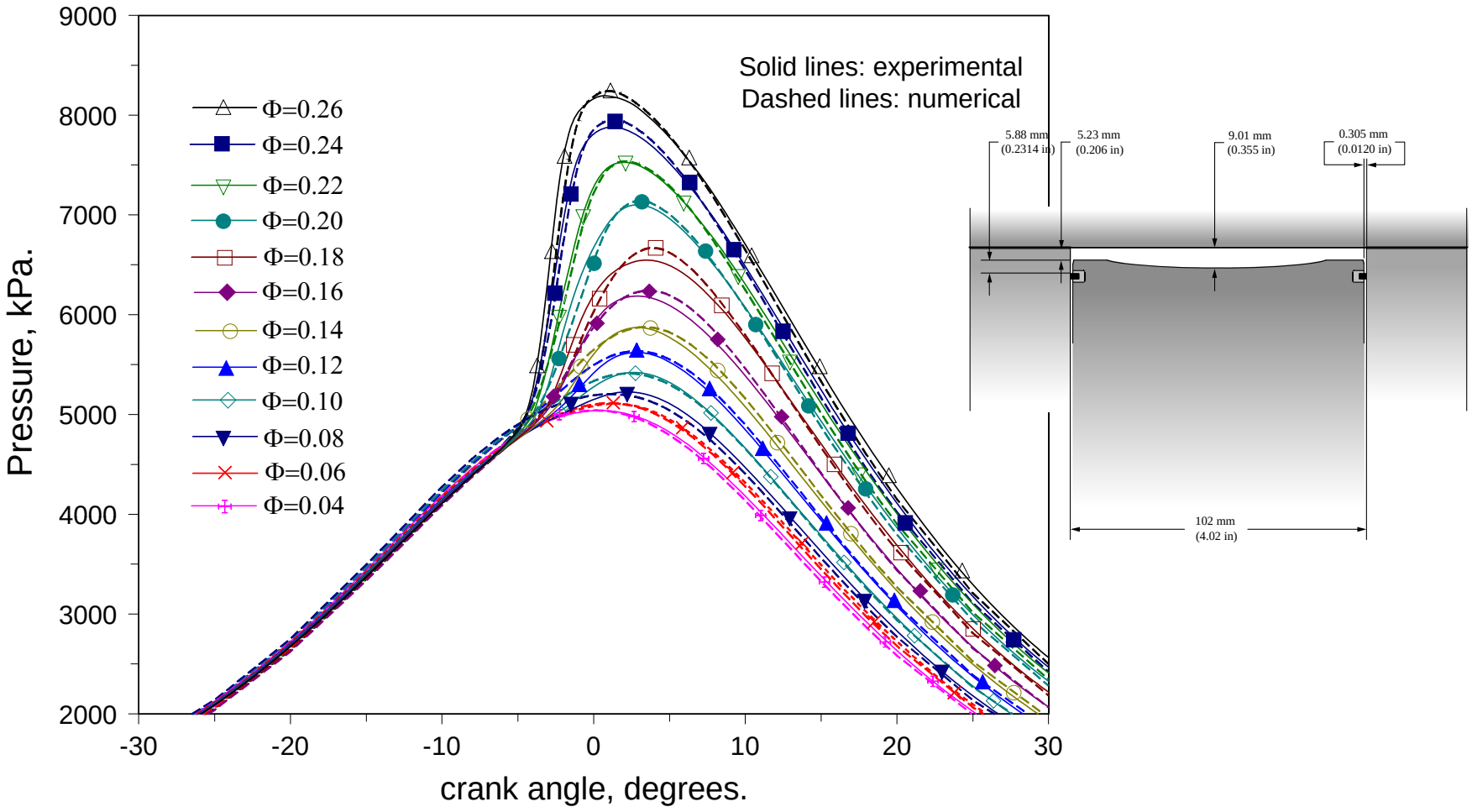
- **Our chemical kinetic model matches ORNL spark-ignited pressure traces**



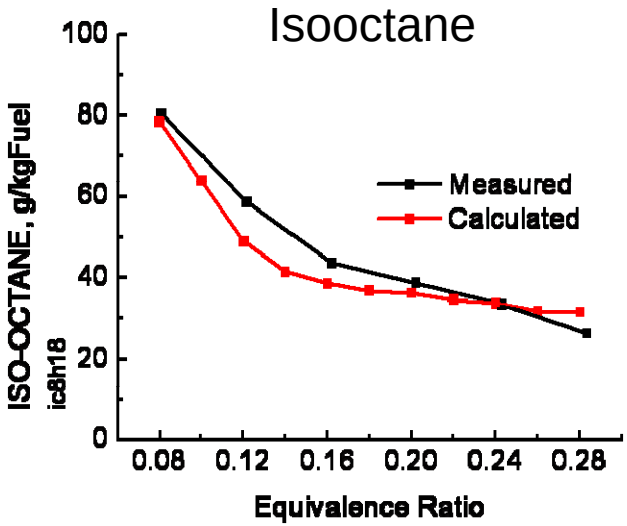
- **We are validating KIVA4Z against Sandia data**

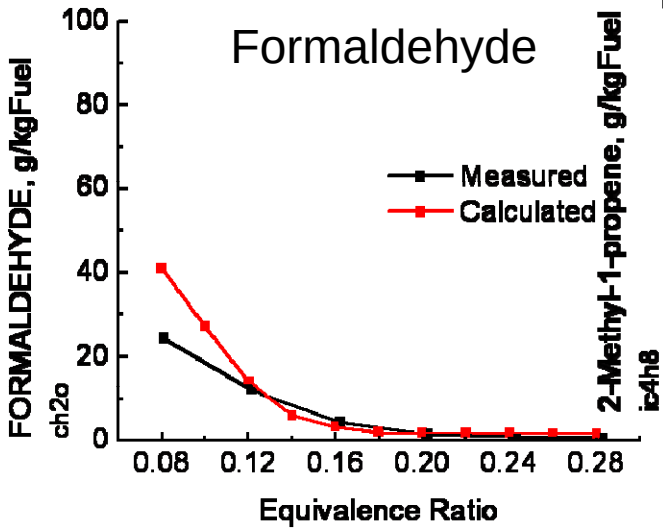


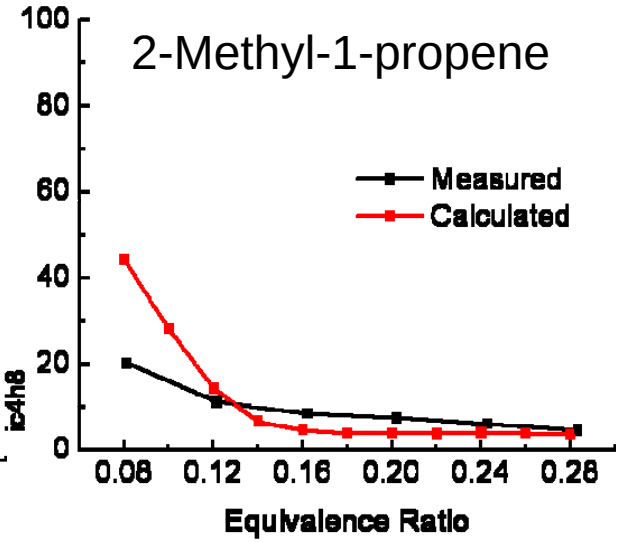
In the last few years we have been able to demonstrate high fidelity modeling tools for homogeneous (HCCI) combustion

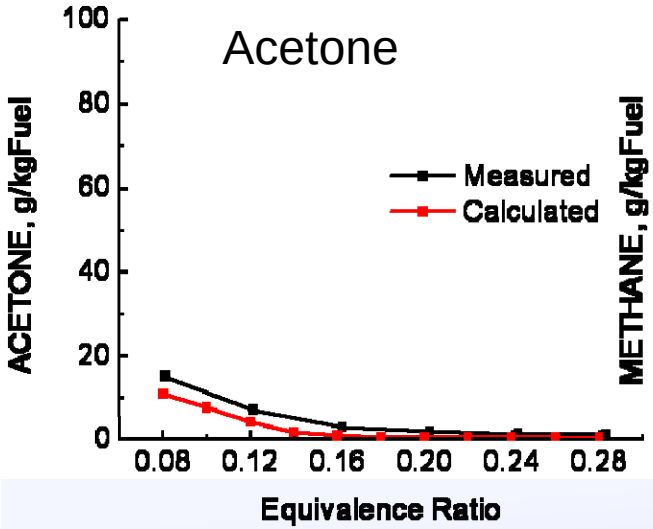


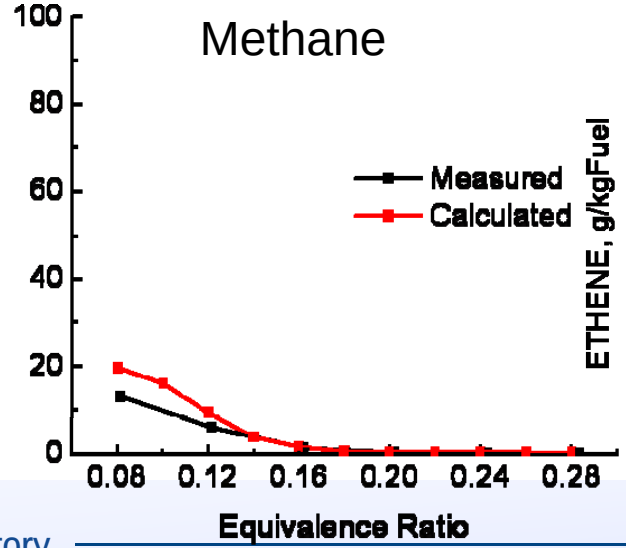
We have demonstrated *unprecedented* modeling fidelity accurately predicting exhaust composition of 50 species

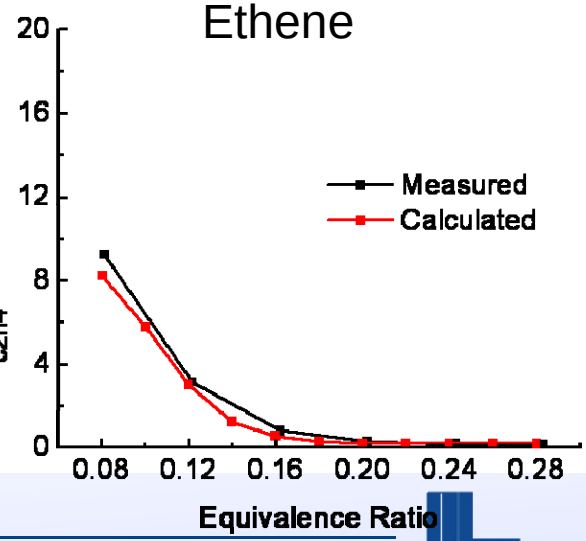




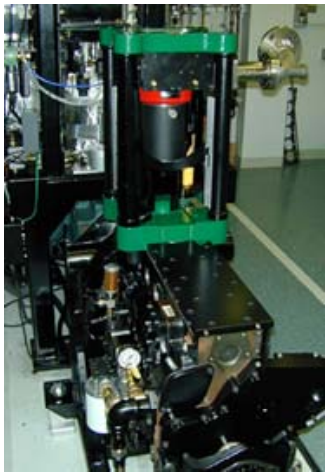






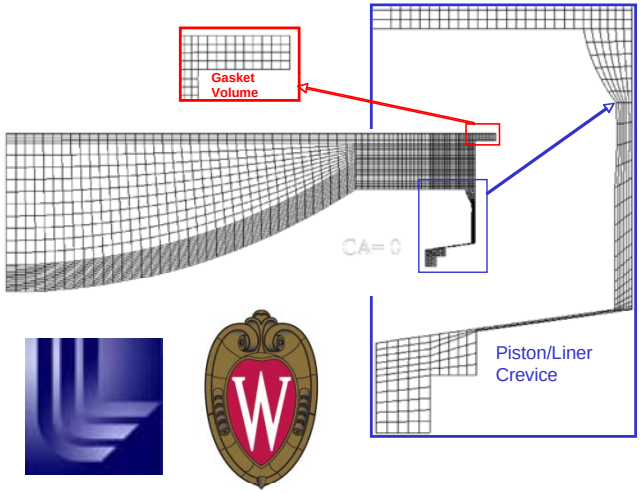


Accurate prediction of specific exhaust components possible due to synergies in collaborators' unique capabilities

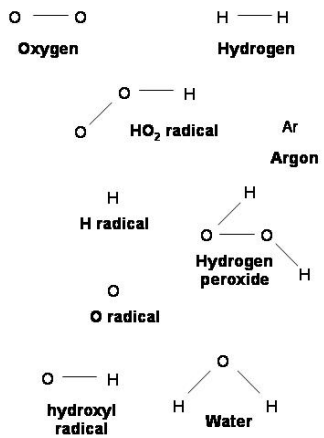


High quality HCCI engine experiments (Sandia)

Analytical chemistry for detailed exhaust speciation



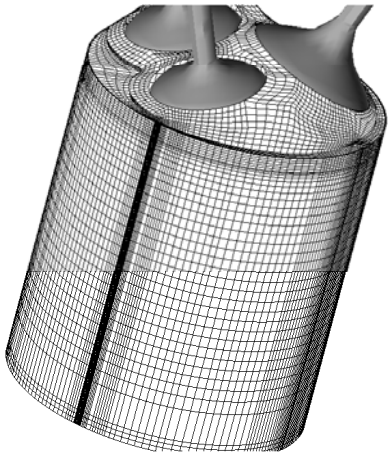
High fidelity engine analysis



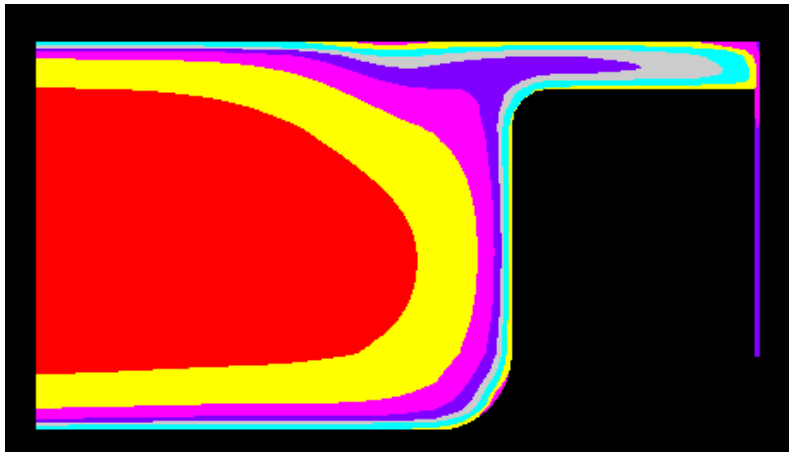
Extensively validated chemical kinetic models

Speciation experiments are optimum for model validation & mechanism tuning

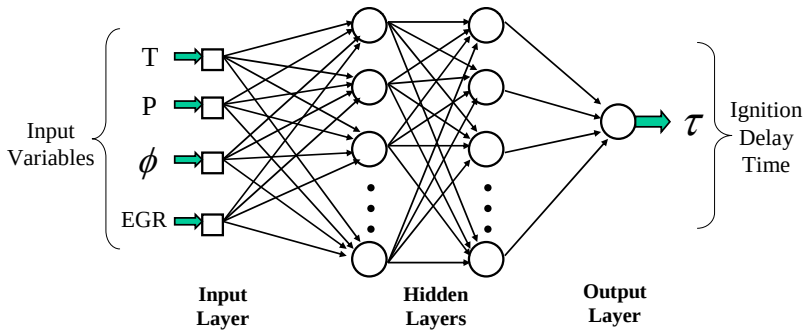
We are now conducting an all-out effort on partially stratified combustion



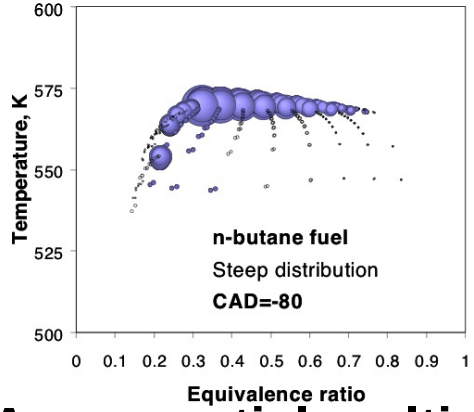
1. KIVA3V with CHEMKIN calculations in every cell: *months* in 100 processor computer. For benchmarking only



2. KIVA multi-zone (KIVA3V-MZ-MPI, Kiva4-MZ): *1 week* in 100 processor machine

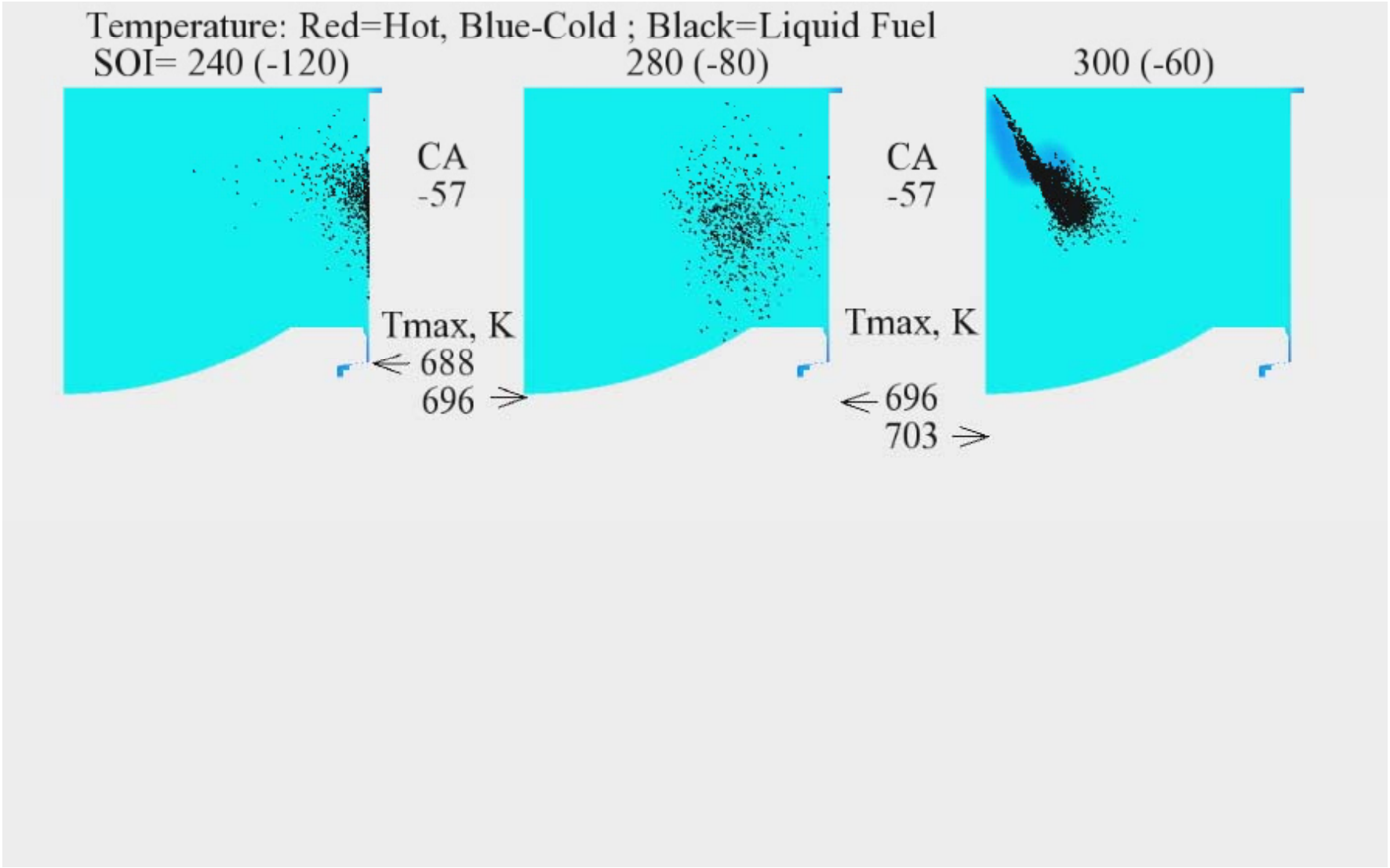


3. KIVA artificial neural network (KIVA-ANN): *4 hours* in single processor computer



4. KIVA-sequential multi-zone cloud model: *1 day* in single processor computer

We are now modeling Sandia PCCI experiments with KIVA3V-MZ-MPI



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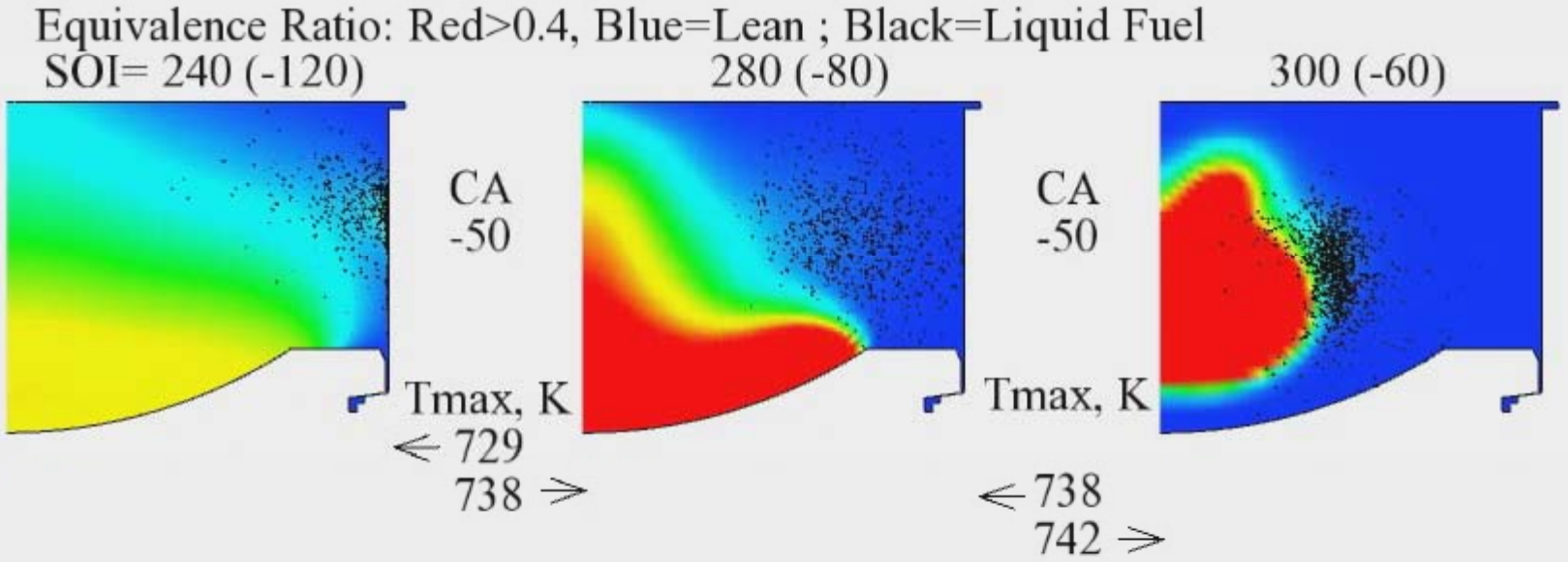
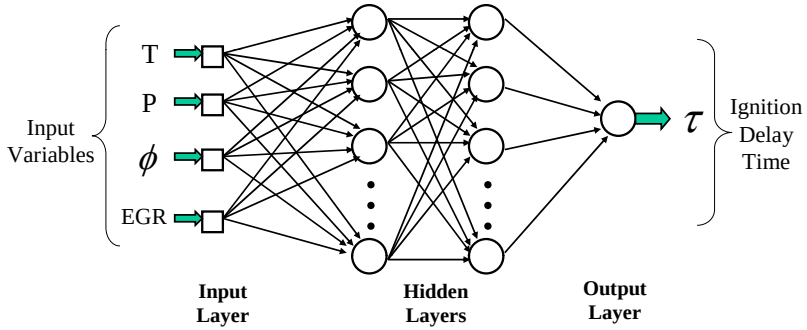
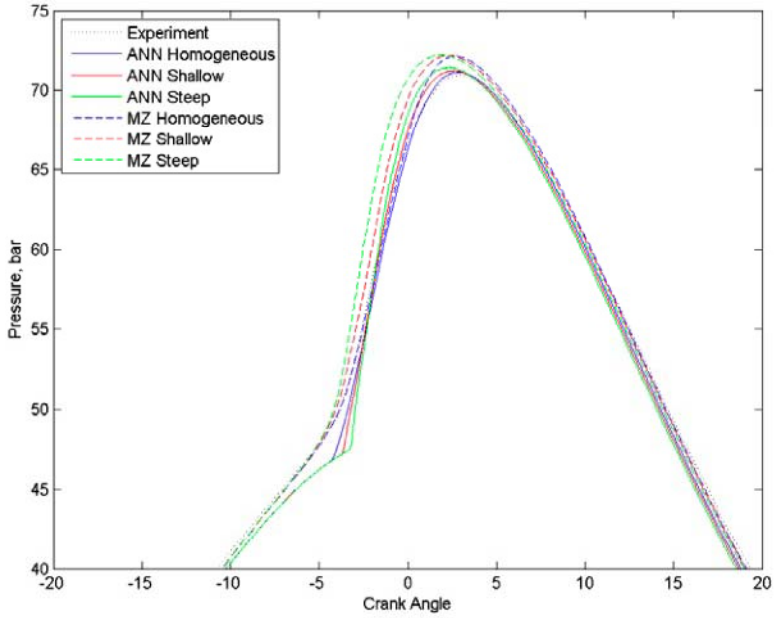
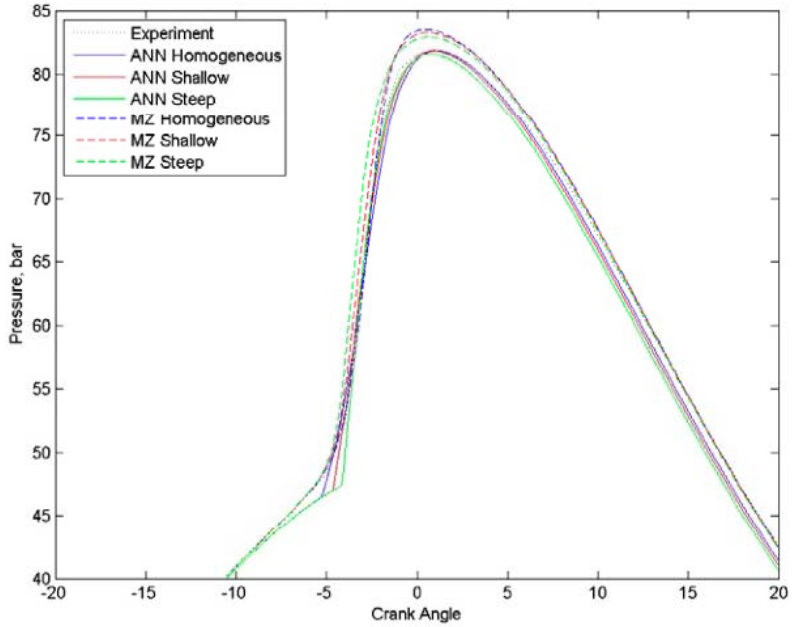


Our artificial neural network model (KIVA-ANN) can predict partially stratified PCCI combustion with 1000 times less computational effort

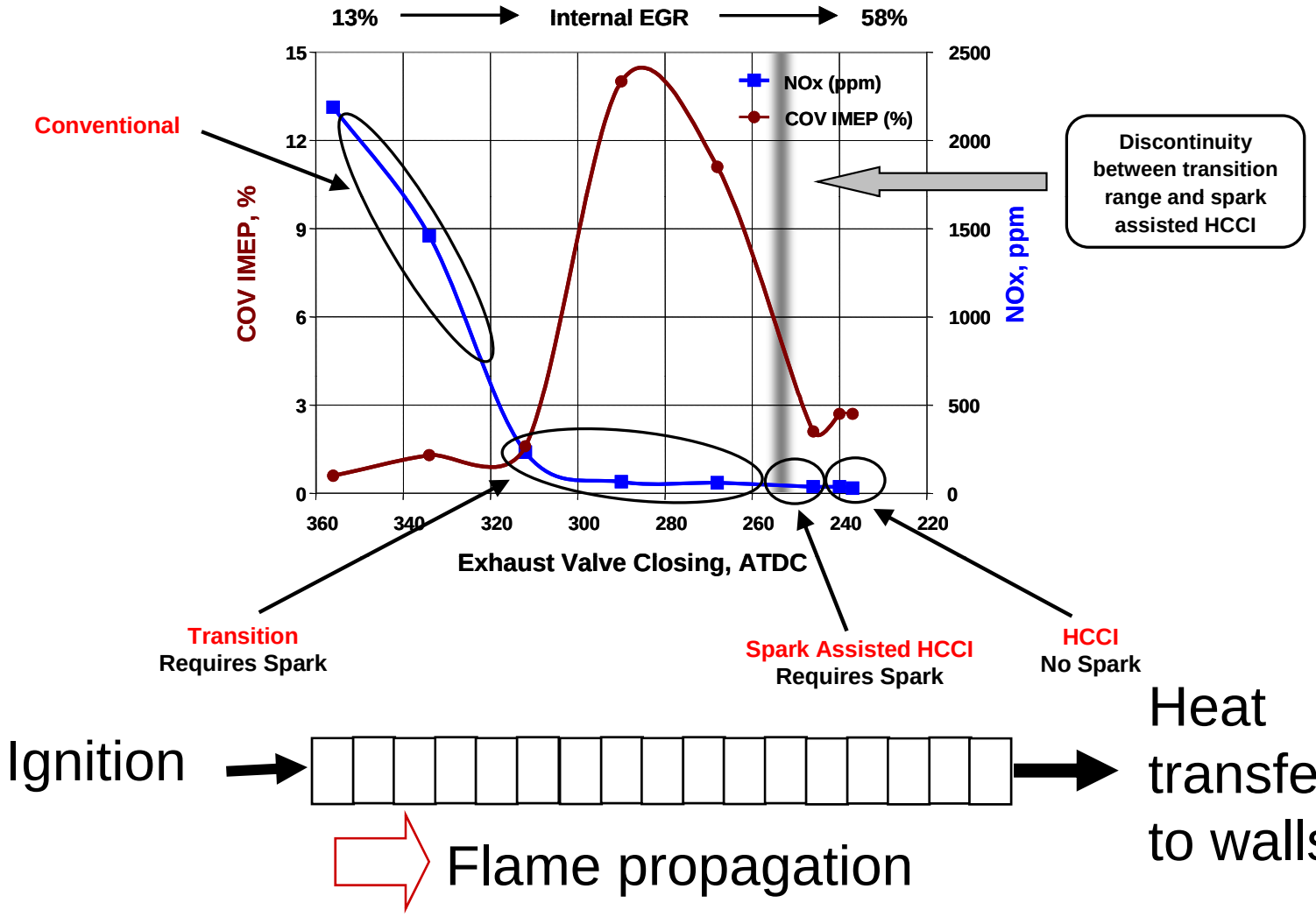




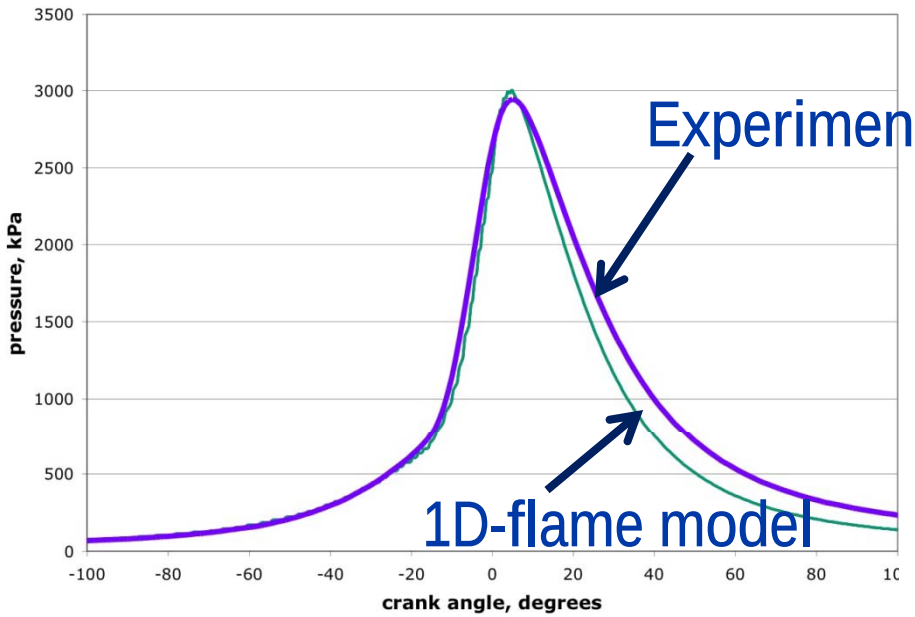


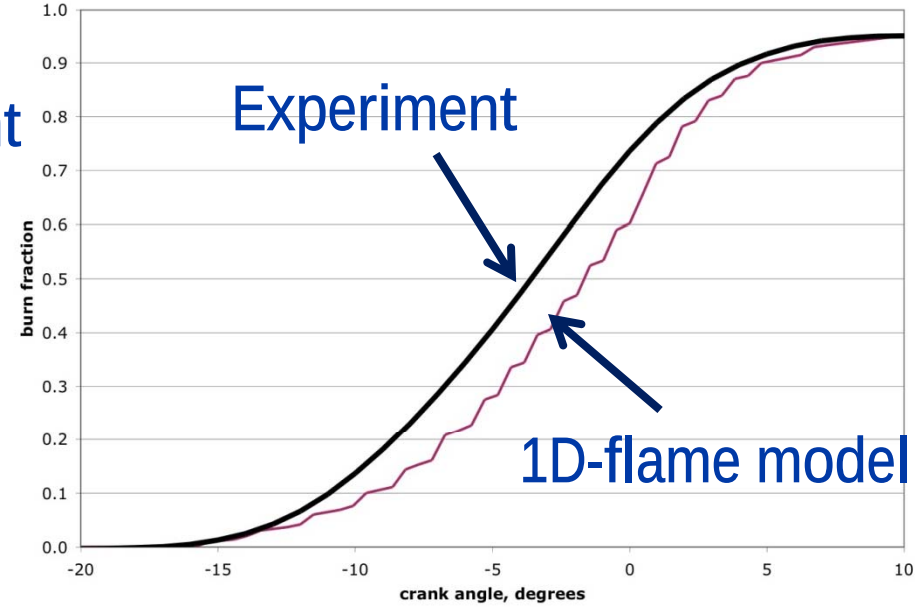
KIVA-ANN predictions of the effect of stratification on PCCI combustion agree well with KIVA3V-MZ-MPI

We are analyzing ORNL gasoline SI-HCCI transition experiments with a 1-D flame propagation/autoignition code



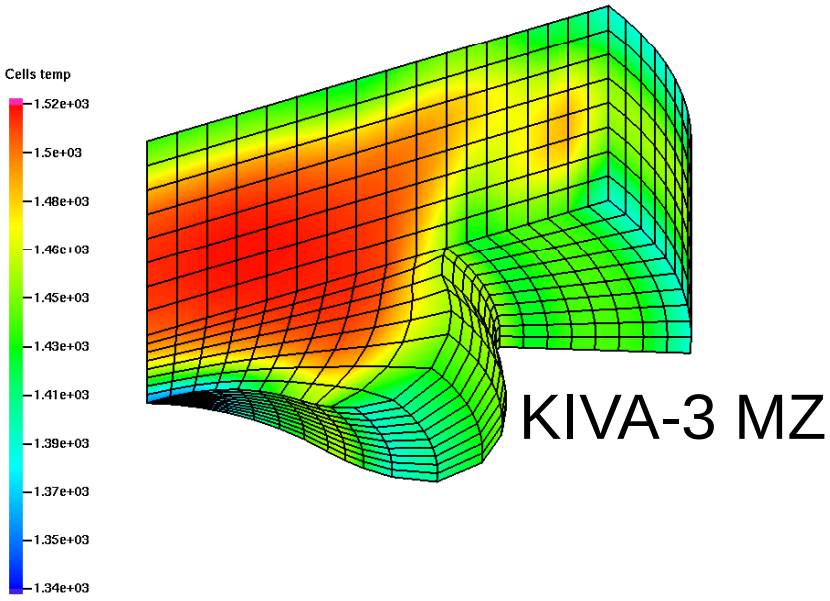
Our 1-dimensional kinetics-based flame propagation model has been able to predict pressure and burn fraction as a function of crank angle



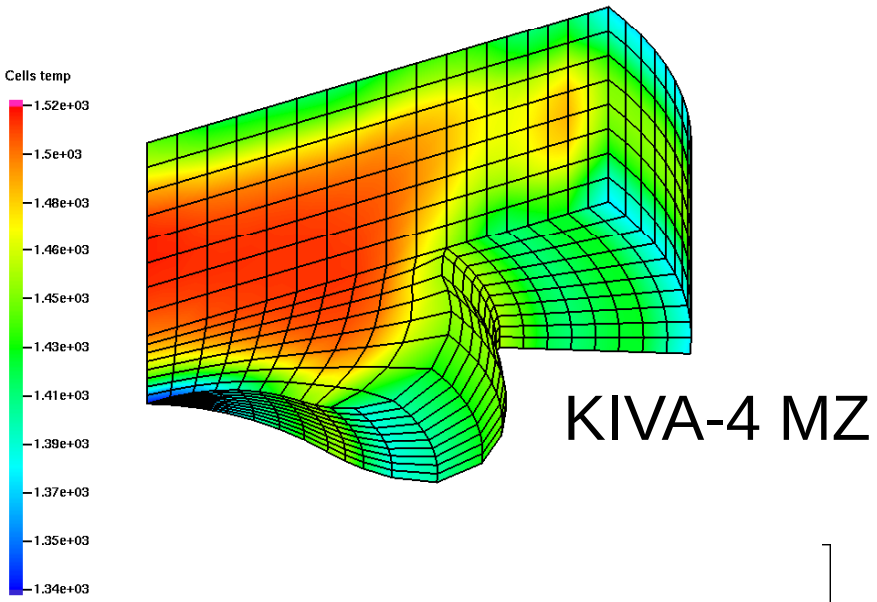


In progress are simulations of sequentially running multiple cycles to determine combustion stability

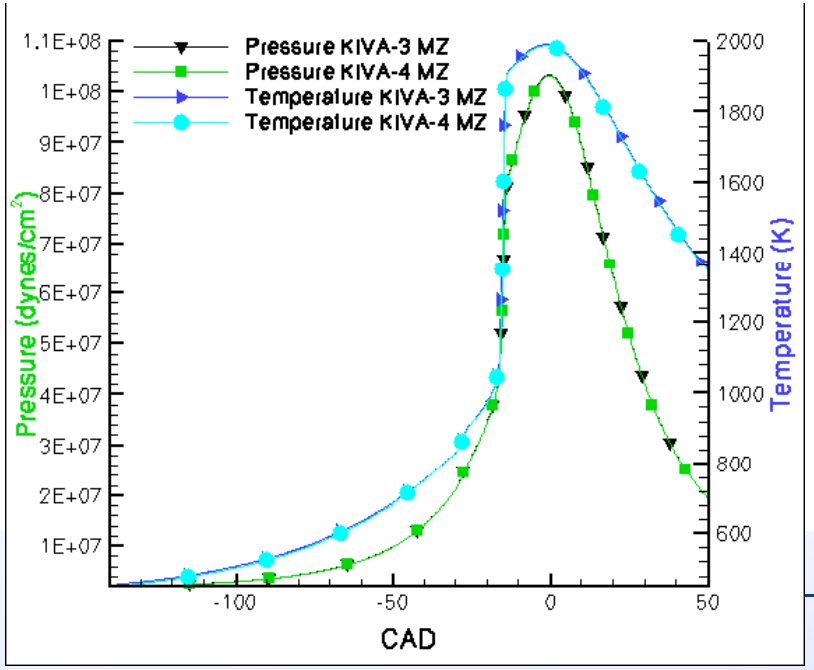
We have been working with David Torres at LANL to integrate our multizone model into KIVA4 (KIVA4-MZ)

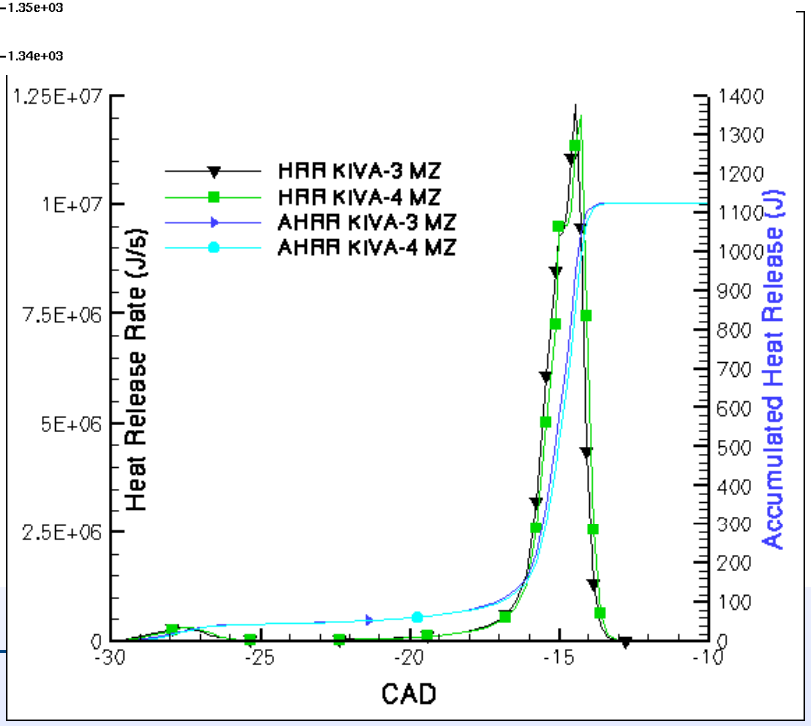


KIVA-3 MZ



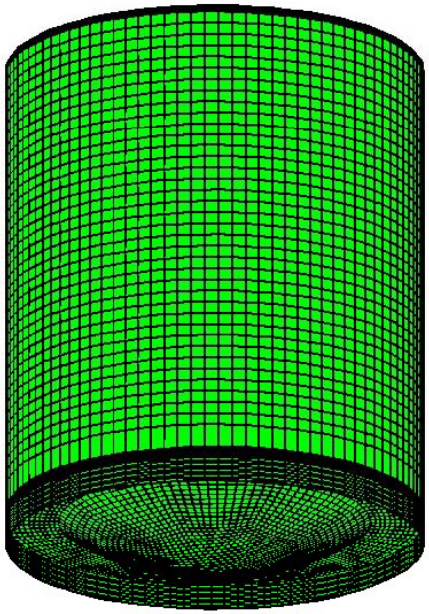
KIVA-4 MZ

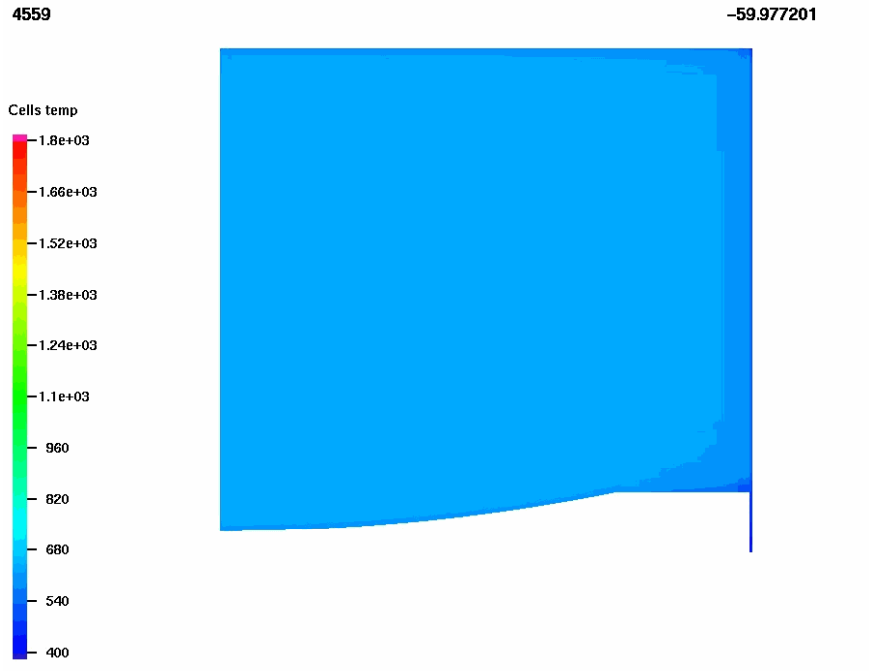




Kiva4MZ is significantly faster and more accurate because of unstructured grids and parallel computing

- Kiva4MZ enable analysis of ultra-high resolution grids (1 million to 10 million cells)





We are validating KIVA4MZ with Sandia HCCI Engine Experiments

Technical Publications during FY07-08

1. Analysis of Homogeneous Charge Compression Ignition (HCCI) Engines for Cogeneration Applications, Salvador M. Aceves, Joel Martinez-Frias, Gordon M. Reistad, Journal of Energy Resources Technology, Vol. 129, No. 4, pp. 332-337, 2007.
2. Gaseous Fuel Injection Modeling using a Gaseous Sphere Injection Methodology, Randy P. Hessel, Salvador M. Aceves, Daniel L. Flowers, SAE Paper 2006-01-3298, 2006.
3. Fast Prediction of HCCI Combustion with an Artificial Neural Network Linked to a Fluid Mechanics Code, Salvador M. Aceves, Daniel L. Flowers, J.Y. Chen, Aristotelis Babajimopoulos, SAE Paper 2006-01-3298, 2006.
4. A Simple HCCI Engine Model for Control, Nick Killingsworth, Salvador Aceves, Daniel Flowers, Miroslav Krstic, Proceedings of the IEEE International Conference on Control Applications, Munich, Germany, 2006.
5. A Comparison on the Effect of Combustion Chamber Surface Area and In-Cylinder Turbulence on the Evolution of Gas Temperature Distribution from IVC to SOC: A Numerical and Fundamental Study, Randy P. Hessel, Salvador M. Aceves, Daniel L. Flowers, SAE Paper 2006-01-0869.
6. Effect of Charge Non-uniformity on Heat Release and Emissions in PCCI Engine Combustion, Daniel L. Flowers, Salvador M. Aceves, Aristotelis Babajimopoulos, SAE Paper 2006-01-1363, 2006.
7. Overview of Modeling Techniques and their application to HCCI/CAI Engines, Salvador M. Aceves, Daniel L. Flowers, Robert W. Dibble, Aristotelis Babajimopoulos, in HCCI and CAI Engines for the Automotive Industry, Edited by Hua Zhao, CRC Press, Woodhead Publishing Limited, Chapter 18, pp. 456-474, 2007.
8. Improving Ethanol Life Cycle Energy Efficiency by Direct Utilization of Wet Ethanol in HCCI Engines, Joel Martinez-Frias, Salvador M. Aceves, Daniel L. Flowers, Paper IMECE2005-79432, Proceedings of the ASME International Mechanical Engineering Congress and Exhibition, 2005, Accepted for Publication, Journal of Energy Resources Technology.
9. Effect of Laser-induced Excitation of Oxygen on Ignition in HCCI Engines Analyzed by Numerical Simulations, Daniel L. Flowers, Salvador M. Aceves and Robert W. Dibble, Combustion Theory and Modelling, Vol. 11, No. 3, pp. 455-468, 2007.
10. Extremum Seeking Tuning of an Experimental HCCI Engine Combustion Timing Controller, Nick Killingsworth, Dan Flowers, Salvador Aceves, Miroslav Krstic, Proceedings of the American Control Conference, New York, NY, July 2007.
11. In Pursuit of New Engine Dynamics, Daniel Flowers, Nick Killingsworth and Robert Dibble, Mechanical Engineering, pp. 20-21, July 2007.
12. A Numerical Investigation into the Anomalous Slight NOx Increase when Burning Biodiesel: A New (Old) Theory, George A. Ban-Weiss, J.Y. Chen, Bruce A. Buchholz, Robert W. Dibble, Fuel Processing Technology, Vol. 88, pp. 659-667, 2007.
13. Pathline Analysis of Full-cycle Four-stroke HCCI Engine Combustion Using CFD and Multi-Zone Modeling, Randy P. Hessel, David E. Foster, Richard R. Steeper, Salvador M. Aceves, Daniel L. Flowers, SAE Paper 2008-01-0048.
14. Modeling Iso-octane HCCI using CFD with Multi-Zone Detailed Chemistry; Comparison to Detailed Speciation Data over a Range of Lean Equivalence Ratios, Randy P. Hessel, David E. Foster, Salvador M. Aceves, M. Lee Davisson, Francisco Espinosa-Loza, Daniel L. Flowers, William J. Pitz, John E. Dec, Magnus Sjöberg, Aristotelis Babajimopoulos, SAE Paper 2008-01-0047.

Collaboration: We have long standing partnerships with industry, national labs, and academia

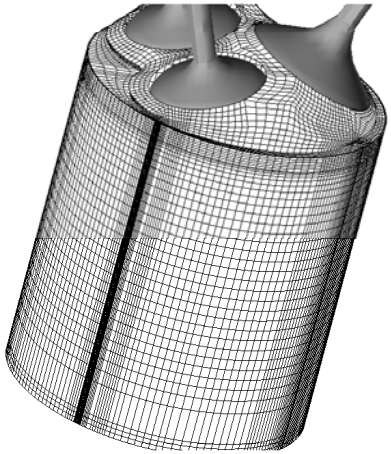
- Industry Partners:
  - ***Collaborative modeling and analysis of experiments***

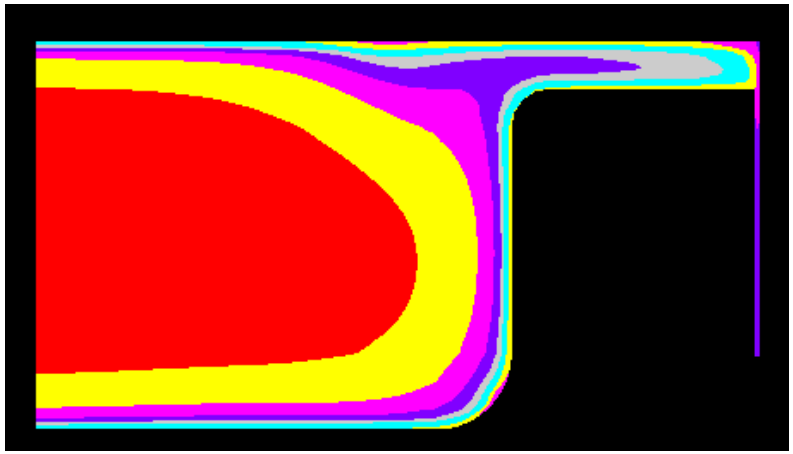
- National Labs and Universities:
  - ***Modeling tools, experiments, analysis***

Other collaborative activities

- Ongoing participation at MOU meetings with vehicle and engine manufacturers
- FACE working group
- HCCI symposium in Lund Sweden (2 invited presentation)
- Several collaborative publications involving National Laboratories and Universities in US and abroad:
  - Participation at SAE technical meetings and symposia
  - The Combustion Institute
  - International Journal of Engine Research
  - Combustion Theory and Modeling
  - Journal of Energy Resources Technologies
  - IEEE Control Systems Technology
  - 8 PhD and >15 MS through collaboration and direct support

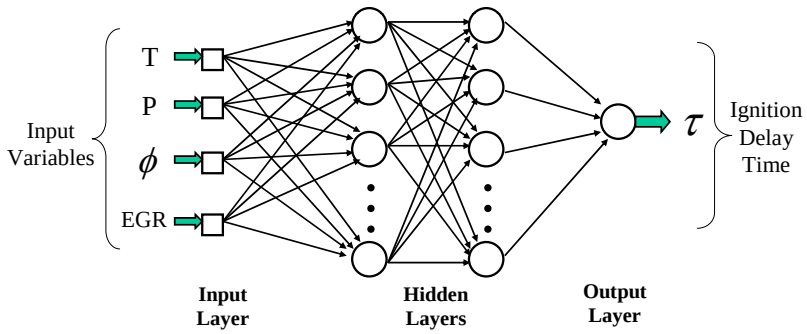
Future plans: We will complete validation of our PCCI codes by comparison with Sandia iso-octane results and exhaust speciation values

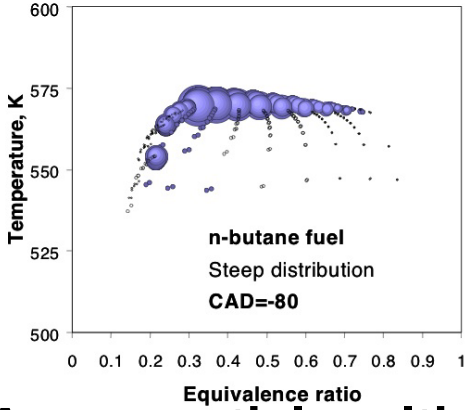




1. KIVA3V with CHEMKIN calculations in every cell: *months* in 100 processor computer. For benchmarking only

2. KIVA multi-zone (KIVA3V-MZ-MPI): *1 week* in 100 processor machine

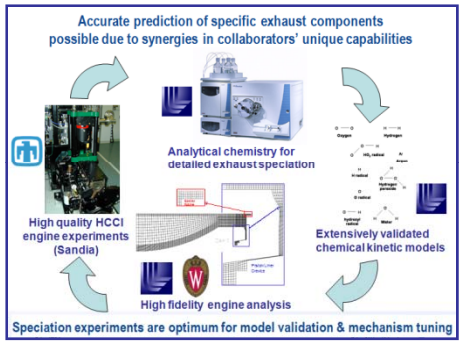


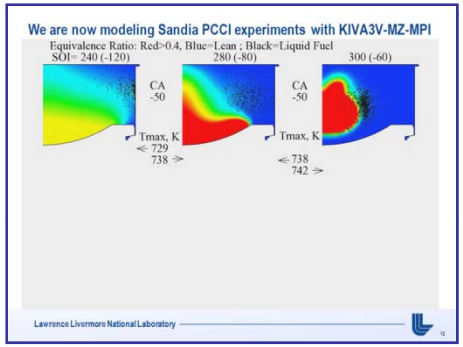


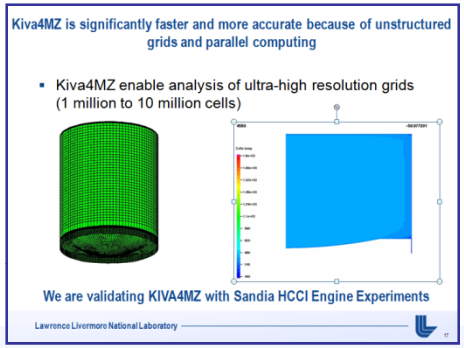
3. KIVA artificial neural network (KIVA-ANN): *4 hours* in single processor computer

4. KIVA-sequential multi-zone cloud model: *1 day* in single processor computer

Summary: We continue to develop high fidelity HCCI and PCCI analysis techniques with greatly improved computational efficiency







- Detailed exhaust species simulations demonstrate a powerful tool for validation and chemical mechanism development
- We are now conducting an all-out effort on partially stratified combustion
- Kiva4MZ is significantly faster and more accurate because of unstructured grids and parallel computing