Modeling of high efficiency clean combustion engines

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Project ID #
ace_12_aceves

Overview

Timeline

- Start date: October 2005
- End date: September 2012
- Percent complete: 60%

Budget

- Total project funding
  - DOE share: $4M
- FY09 Funding: $1M
- FY08 Funding: $1M

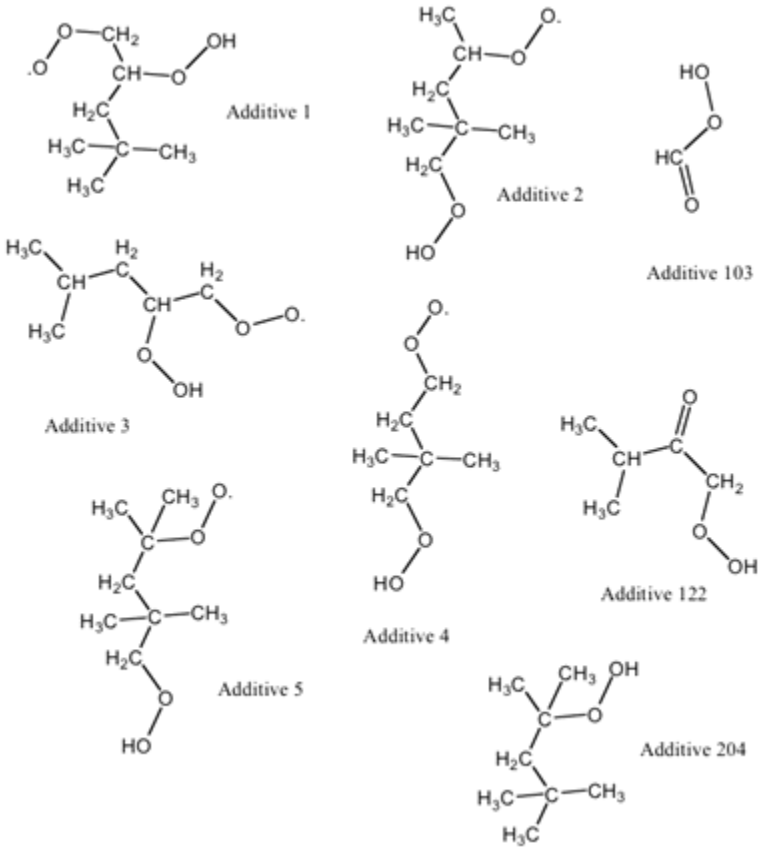
Barriers

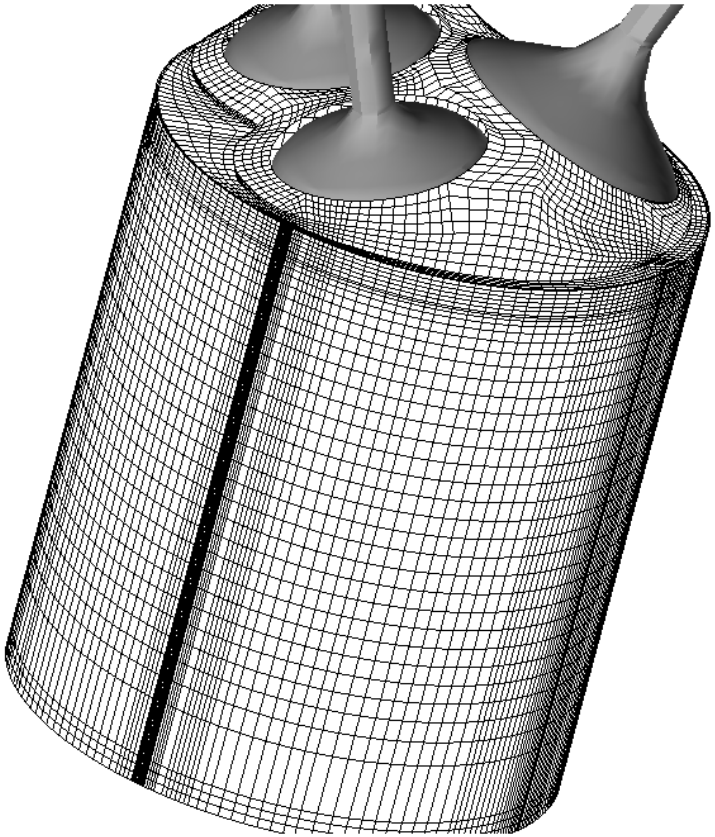
- Inadequate understanding of the fundamentals of LTC
- Inadequate understanding of the fundamentals of mixed mode operation

Partners

- Sandia Livermore
- Oak Ridge
- Los Alamos
- International
- UC Berkeley
- University of Wisconsin
- University of Michigan
- Chalmers University
- FACE working group
- SAE

Objective: Enhance understanding of clean and efficient engine operation through detailed numerical modeling

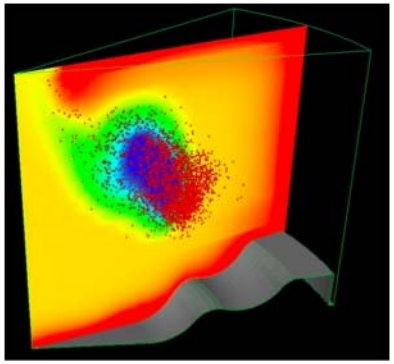


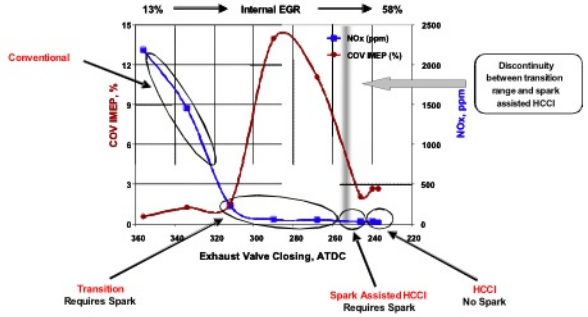


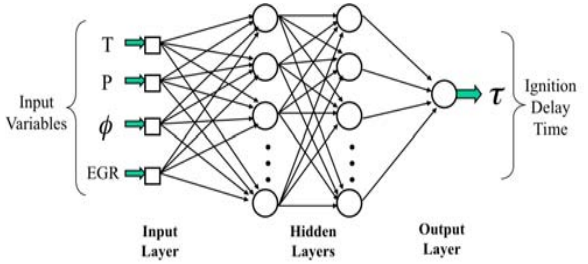
Chemical kinetics

Fluid mechanics

Milestones: We have developed and experimentally validated detailed engine modeling tools

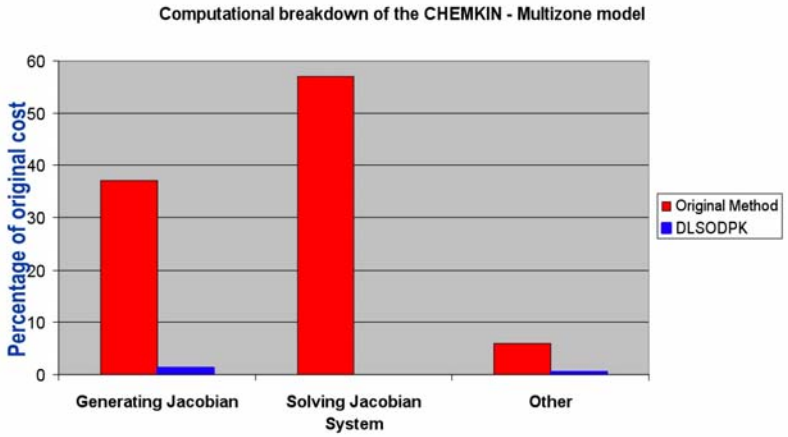




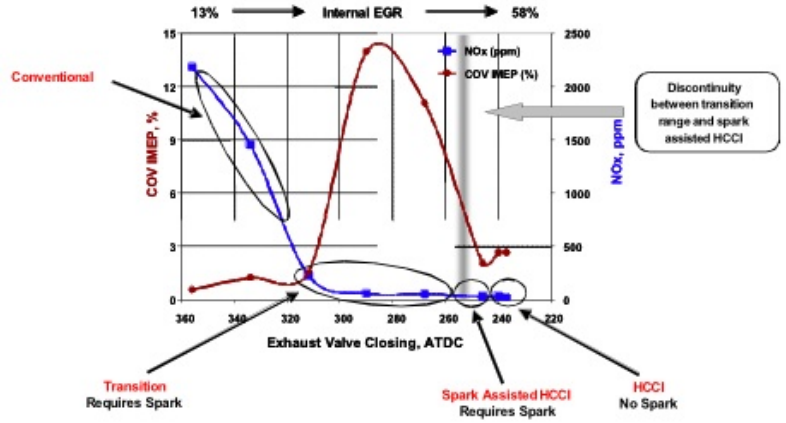


- ***Demonstrated accurate prediction of partially stratified combustion*** **(January 2009)**
- ***Developed improved surrogate chemical kinetic model for gasoline*** **(January 2009)**
- ***Analyzed SI-HCCI transition in ORNL experiment (March 2009)***
- ***Calculated PCCI combustion with an artificial neural network-based chemical kinetic model (March 2009)***

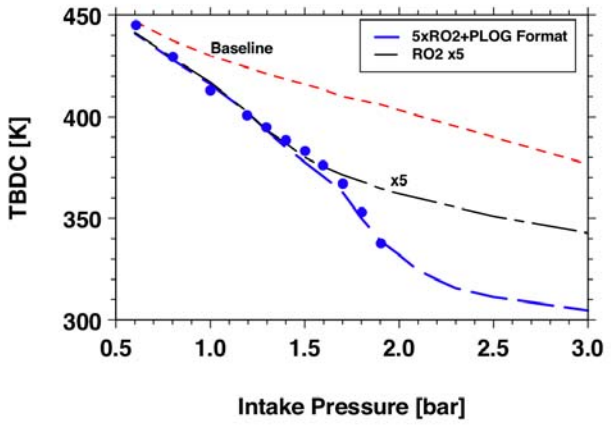
Approach: collaborate with industry, academia and national labs in the development of analysis tools leading to clean, efficient engines



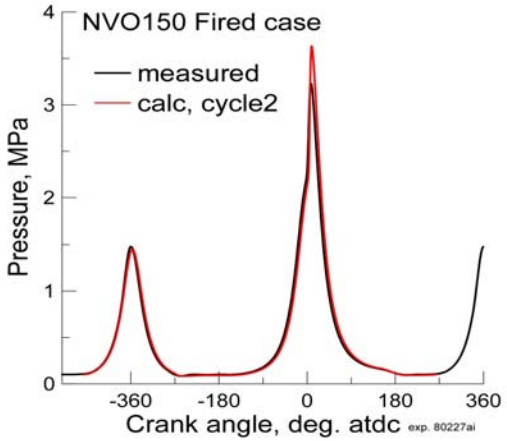
Improved Chemkin multizone numerics



Analysis of HCCI-SI transition



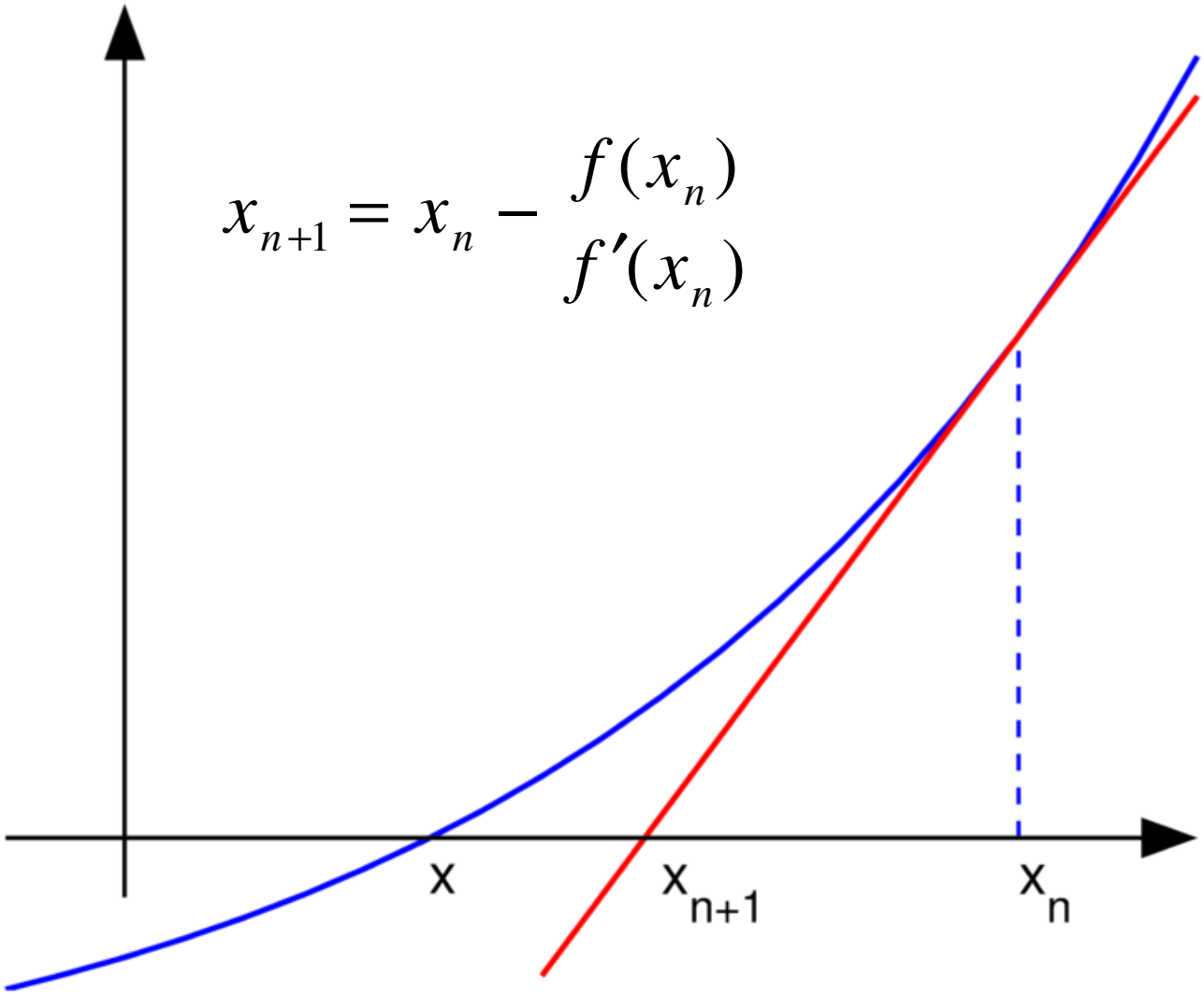
Gasoline surrogate mechanism



PCCI modeling

Accomplishments: The Newton-Raphson method efficiently solves nonlinear equations

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$



When solving a system of differential equations,

$$\frac{\hat{y}_i - y_i}{\Delta t} = f_i(\hat{y}_1, \ldots, \hat{y}_N) \qquad \text{where } y_i = y_i(t) \text{ and } \hat{y}_i = y_i(t + \Delta t)$$

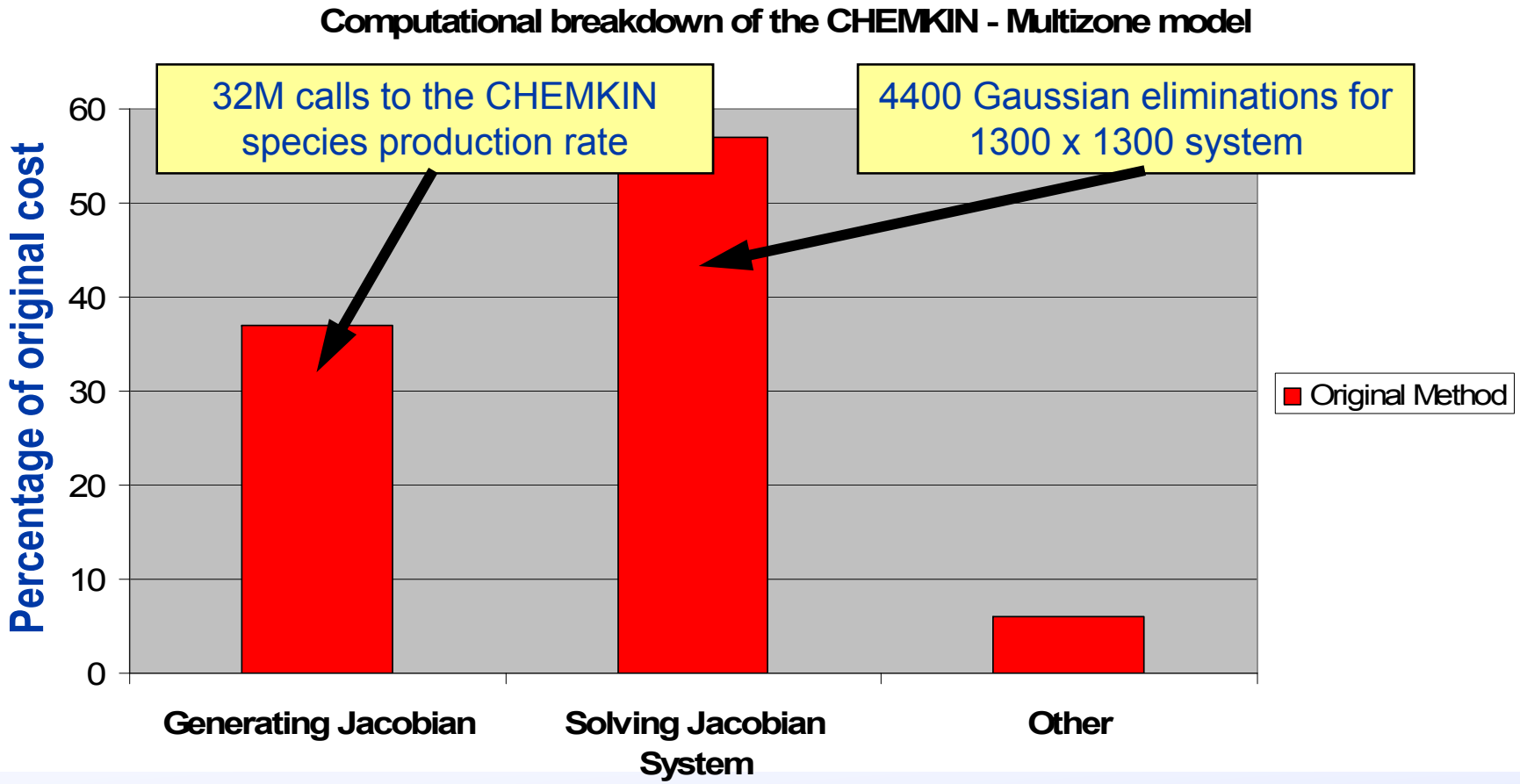
the Jacobian matrix $J = \frac{\partial f_i}{\partial y_j}$ plays the role of the derivative

$$\left(I - \Delta t \frac{\partial f_i}{\partial y_j}\right)(\hat{y}_j^{k+1} - \hat{y}_j^k) = -\hat{y}_i^k + y_i + \Delta t f_i(\hat{y}_1^k, \ldots, \hat{y}_N^k)$$

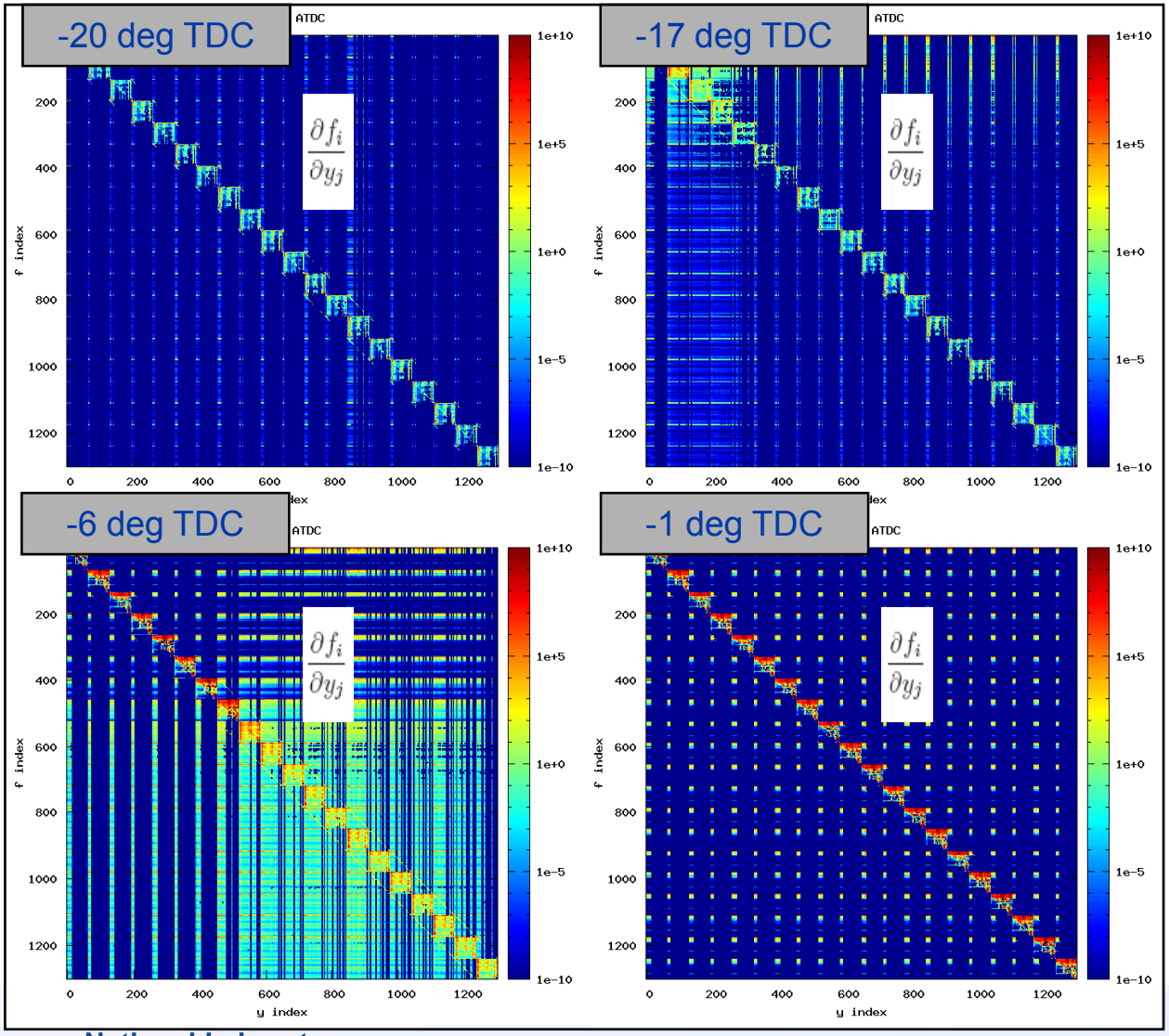
$$\frac{\partial f_i}{\partial y_j} = \begin{pmatrix} \frac{\partial f_1}{\partial y_1} & \cdots & \frac{\partial f_1}{\partial y_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_N}{\partial y_1} & \cdots & \frac{\partial f_N}{\partial y_N} \end{pmatrix}$$

Processing the Jacobian is the most computationally expensive part of CHEMKIN-Multizone

- 94% of the total computational cost is spent generating the Jacobian and solving the associated linear system.



Chemkin multizone produces a block-diagonal Jacobian
Can we take advantage for reduced computational time?

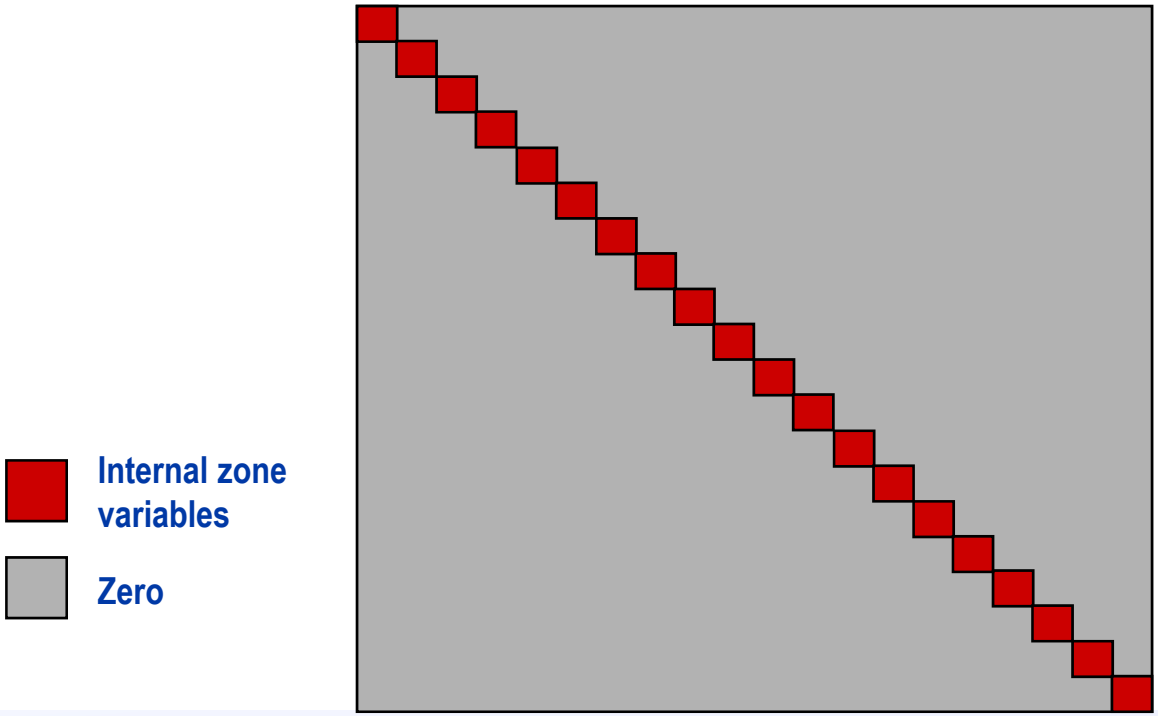


New procedure: use LLNL's ODE integrator with an iterative matrix solver (DLSODPK)

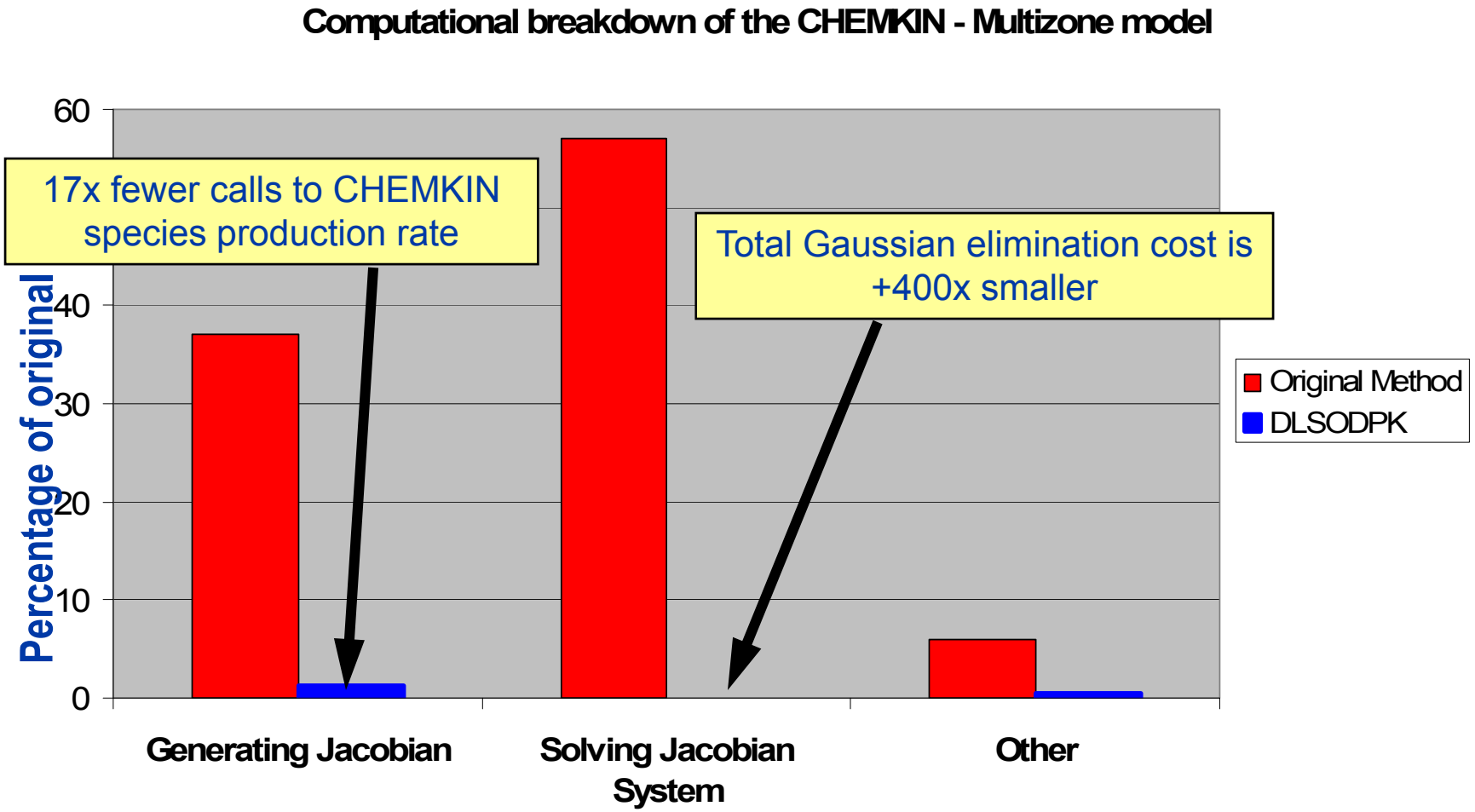
- Use LLNL's iterative solver DLSODPK along with a preconditioner matrix P

$$P^{-1}Ax = P^{-1}b$$

- Here P is the Jacobian of a simplified CHEMKIN-multizone model that yields a block diagonal matrix (neglecting interaction between zones)



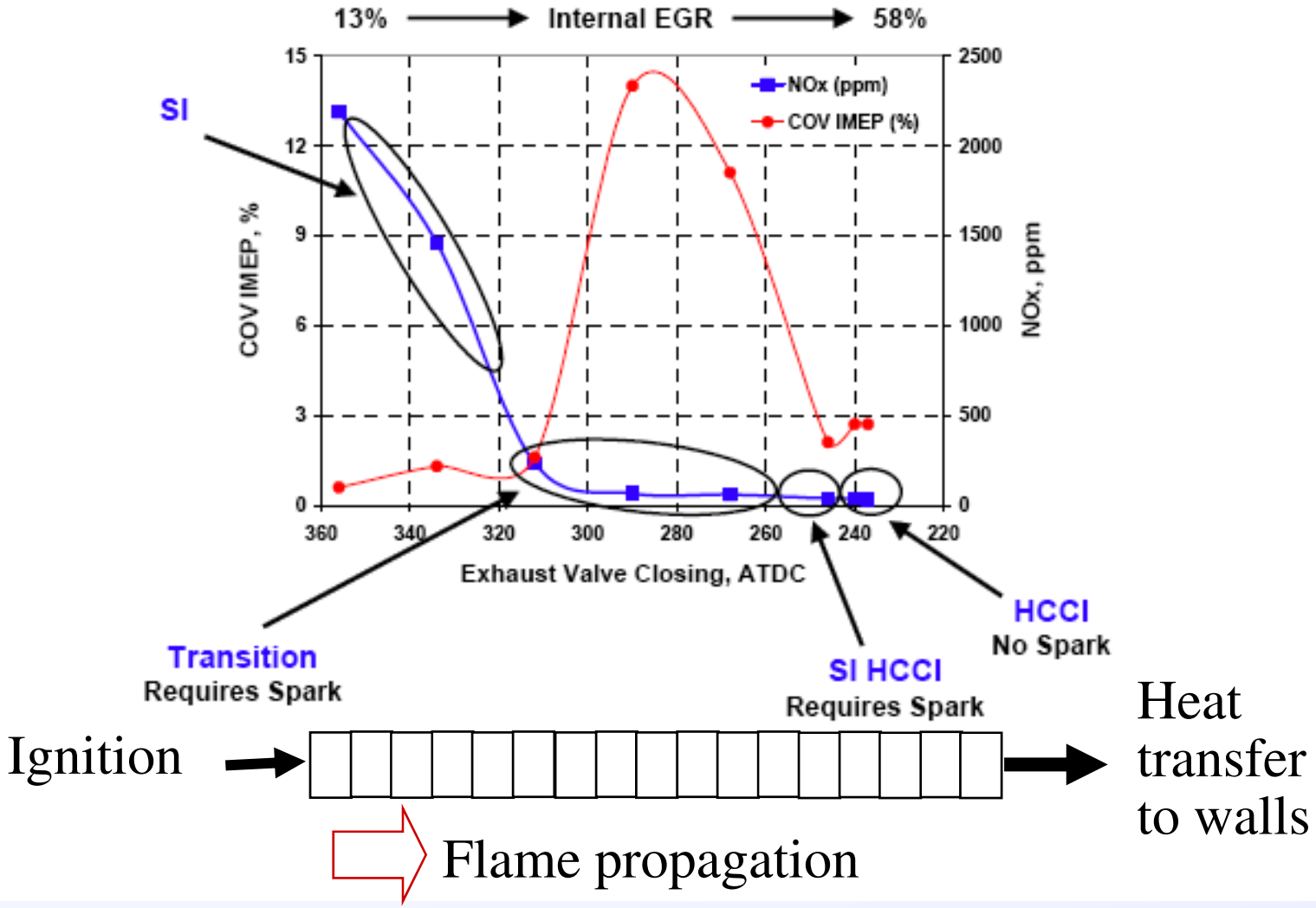
The new DLSODPK scheme accelerates computations enabling detailed multizone kinetics on desktop PCs



60x speedup for 20 zones; 6 minutes (6 hours) with 63 species

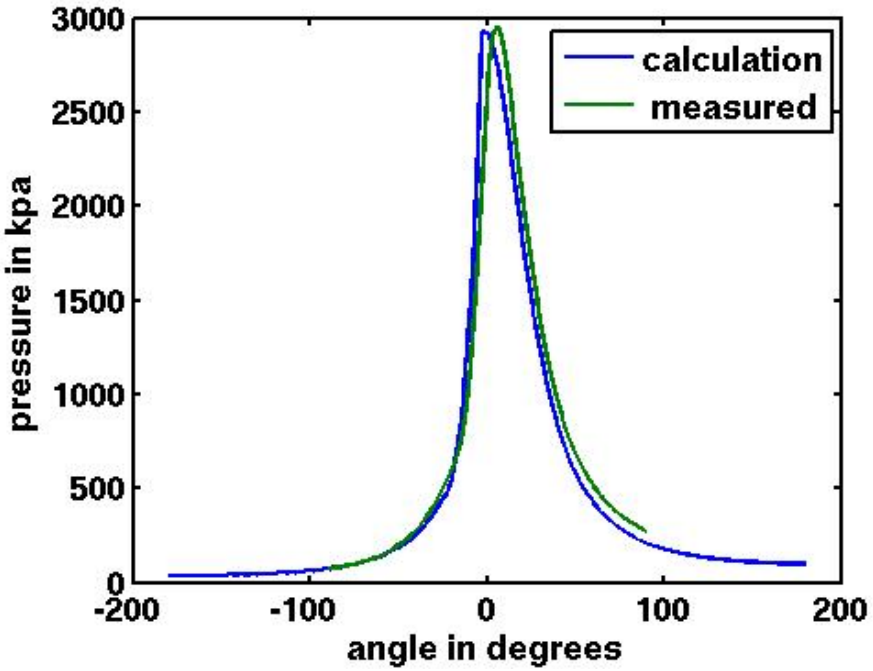
250x speedup for 40 zones; 24 minutes (100 hours) 63 species

We are analyzing ORNL results for stability and emissions during SI-HCCI transition due to increased residual gas fraction

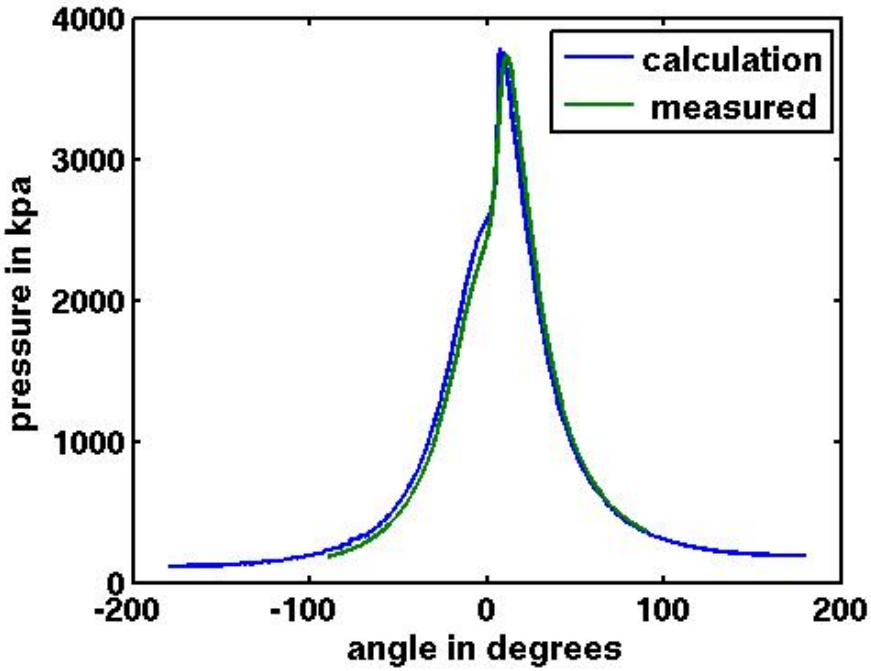


1-dimensional chemical kinetic model accurately matches pressure traces for motored, SI and HCCI cases

- Spark-ignited



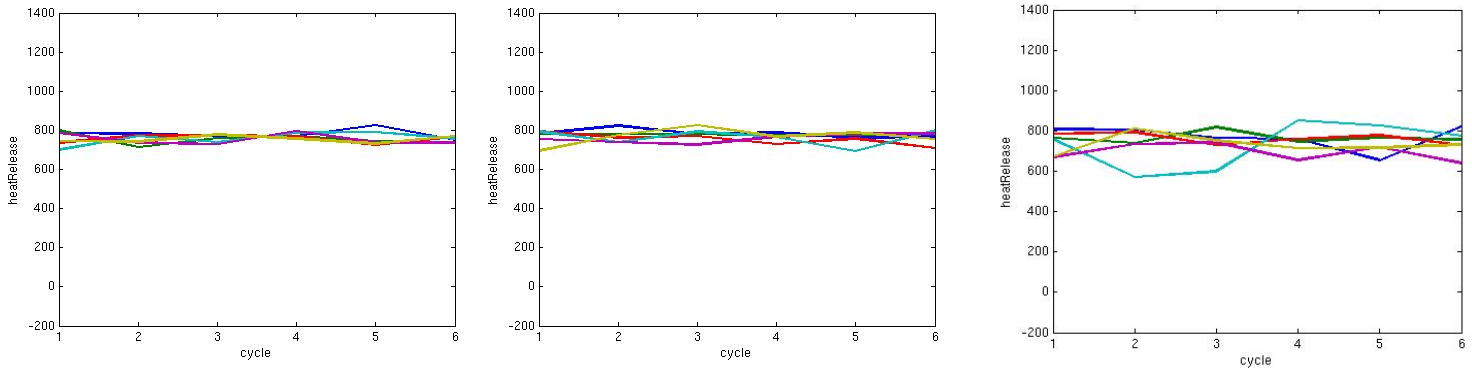
- HCCI (EGR=74.7%)



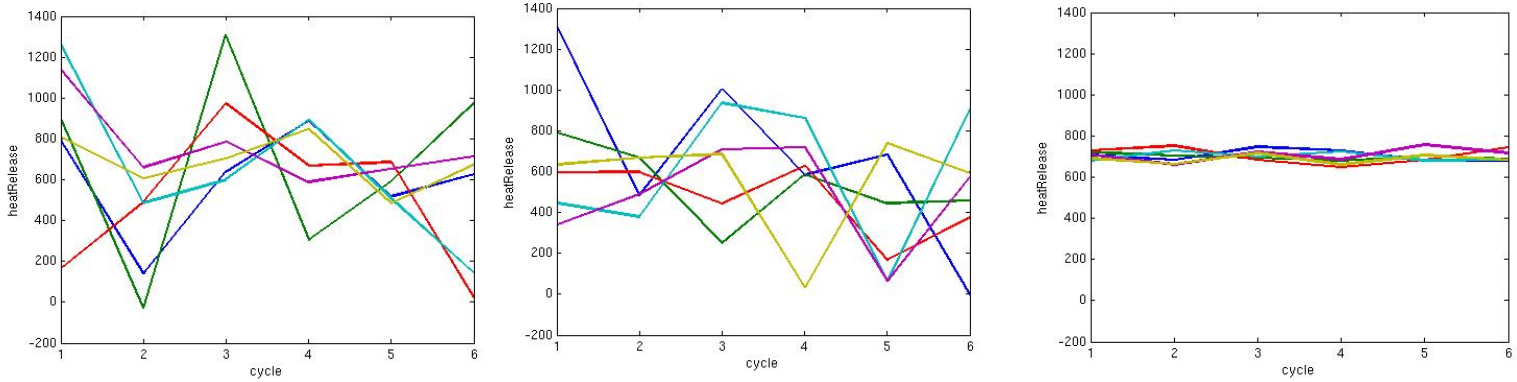
ORNL Test data for SI to HCCI transition: heat release patterns vary with residual gas fraction

Spark-ignited (EGR~10%)

Increasing EGR



Increasing EGR

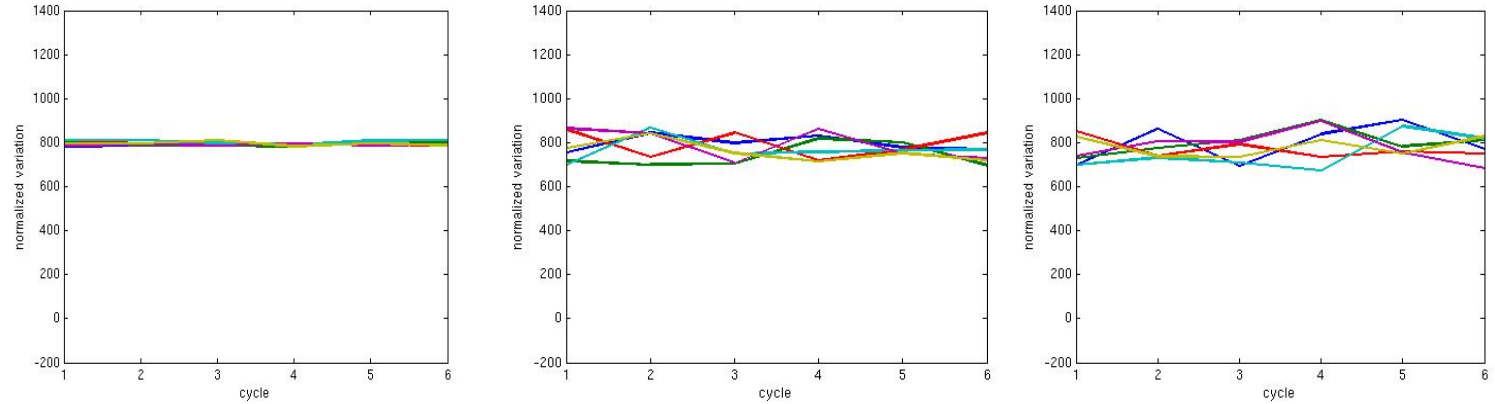


HCCI (EGR~60%)

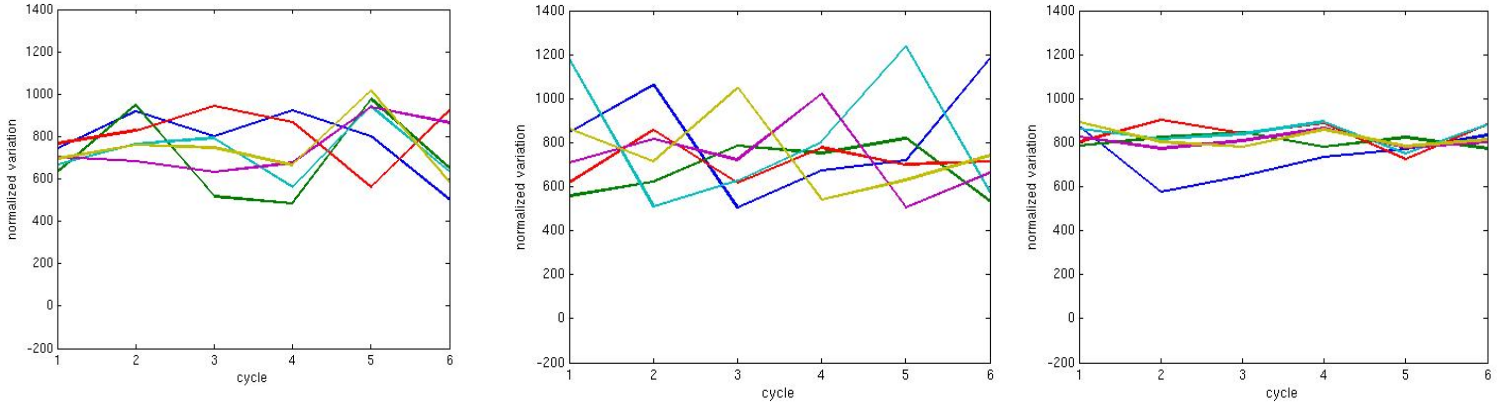
LLNL Simulation results for SI to HCCI transition: heat release patterns vary with residual gas fraction

Spark-ignited (EGR~10%)

Increasing EGR

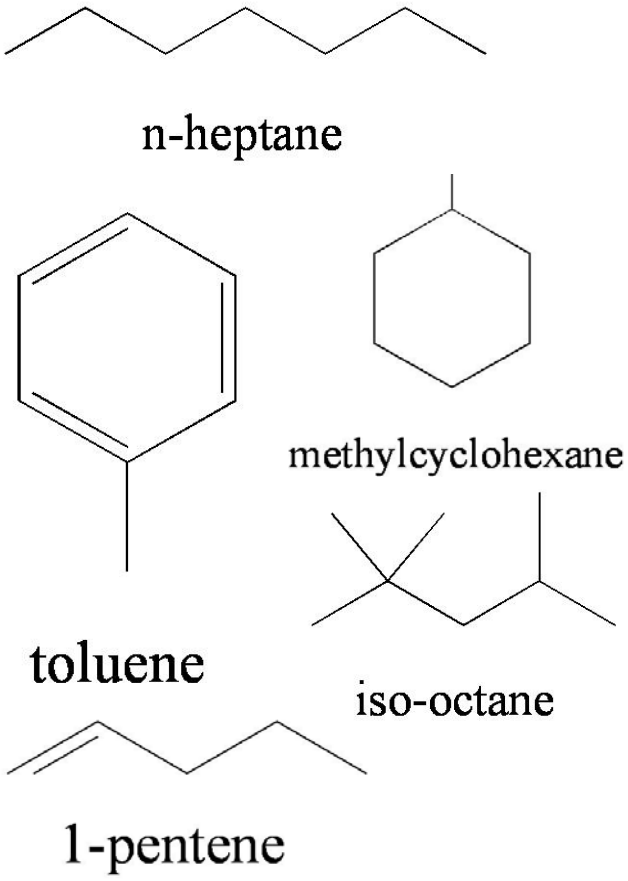


Increasing EGR



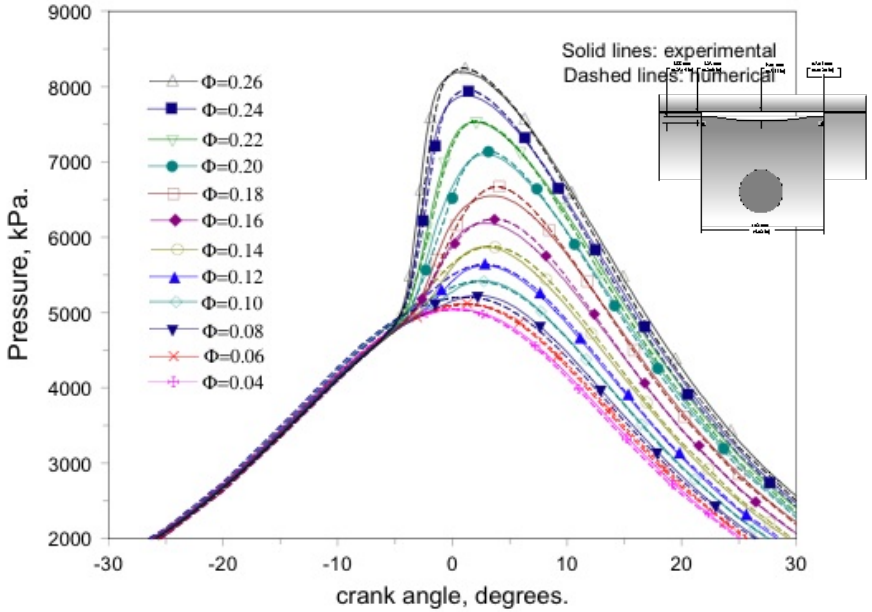
HCCI (EGR~60%)

HCCI is more than a promising engine operating regime. HCCI is also an excellent platform for developing & testing high fidelity chemical kinetic models



testing

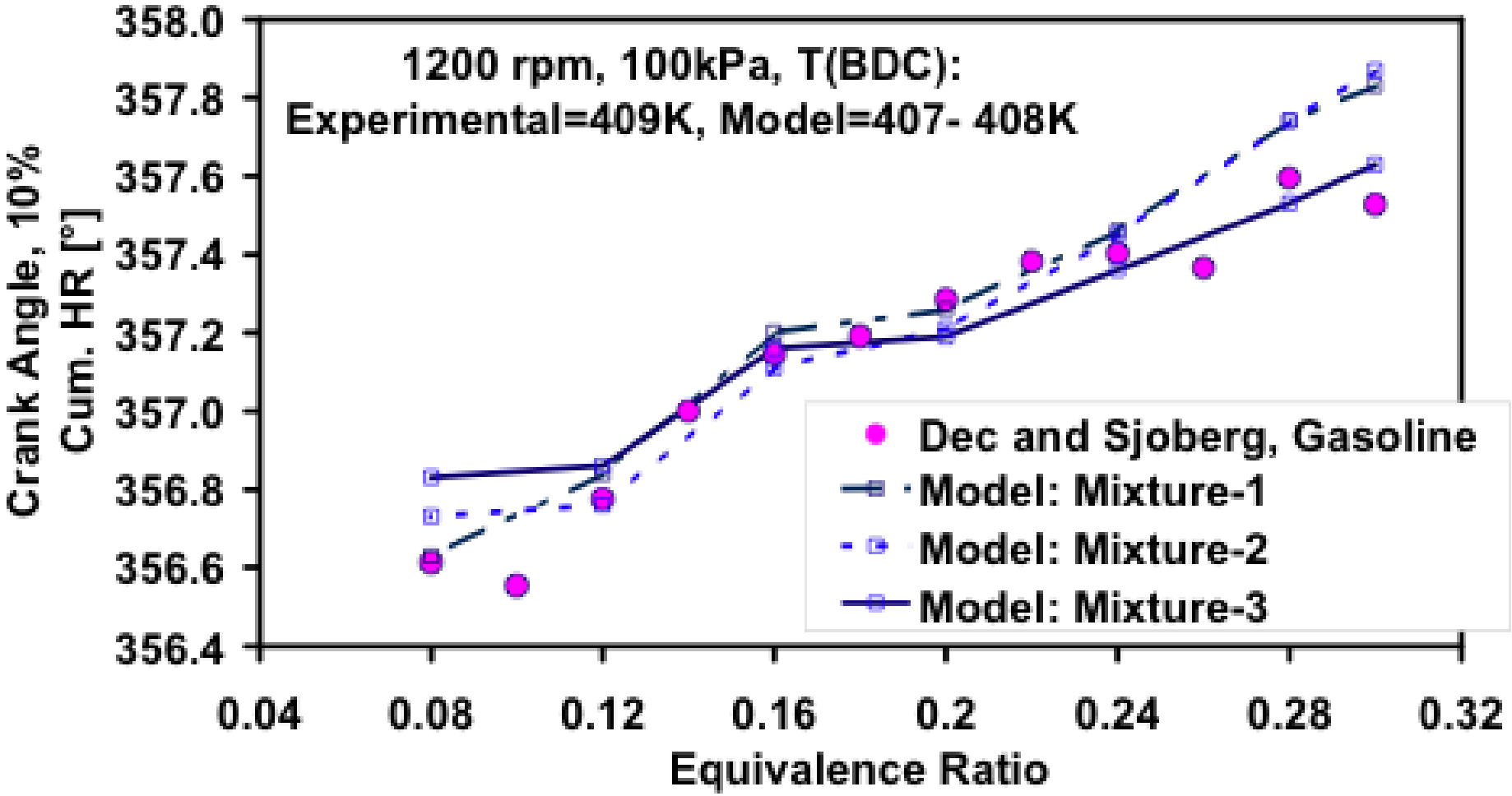
tuning



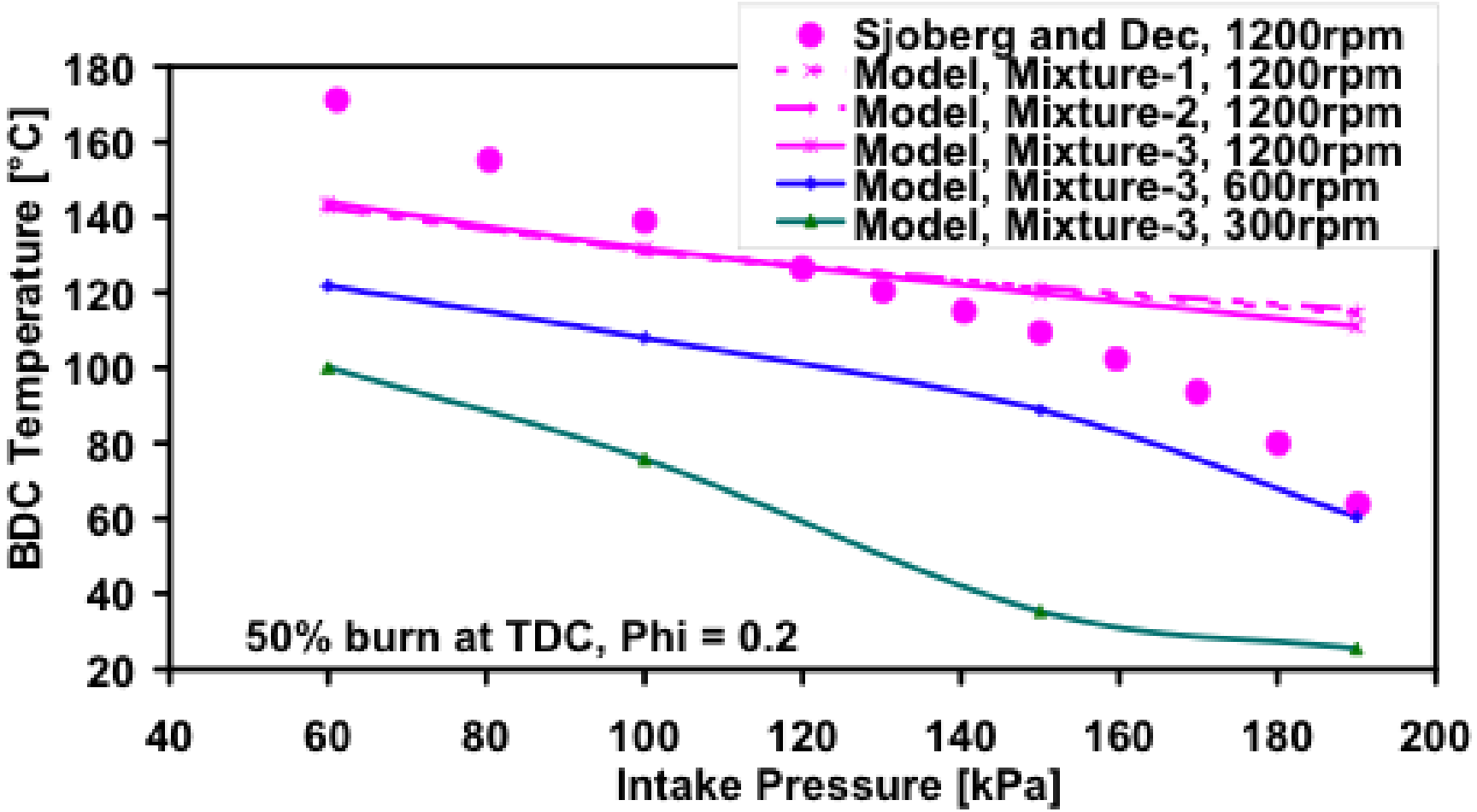
Detailed kinetics of gasoline surrogates

High fidelity engine models

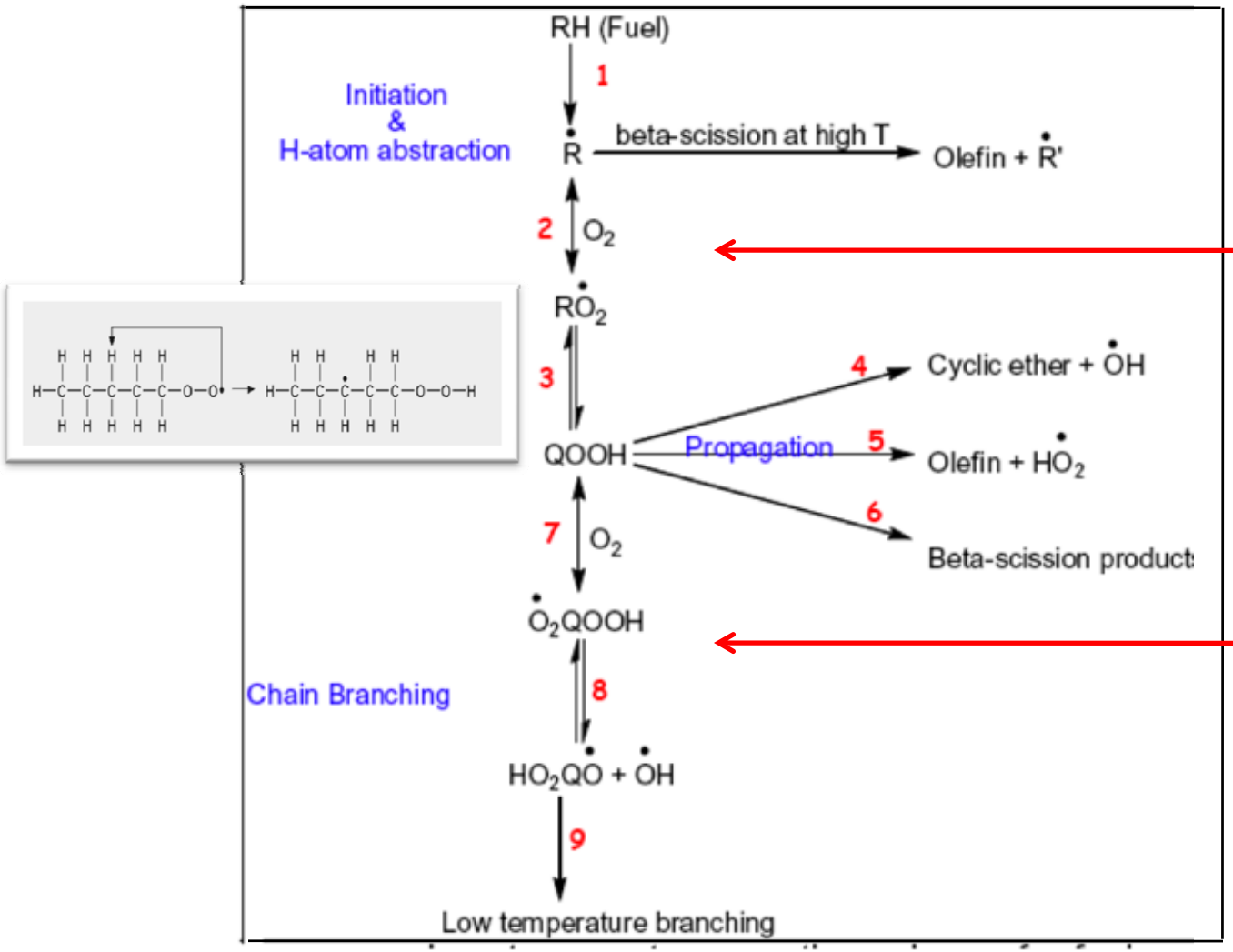
Gasoline surrogate model accurately predicts ignition time as a function of equivalence ratio



But it does not properly replicate ignition time as a function of intake pressure



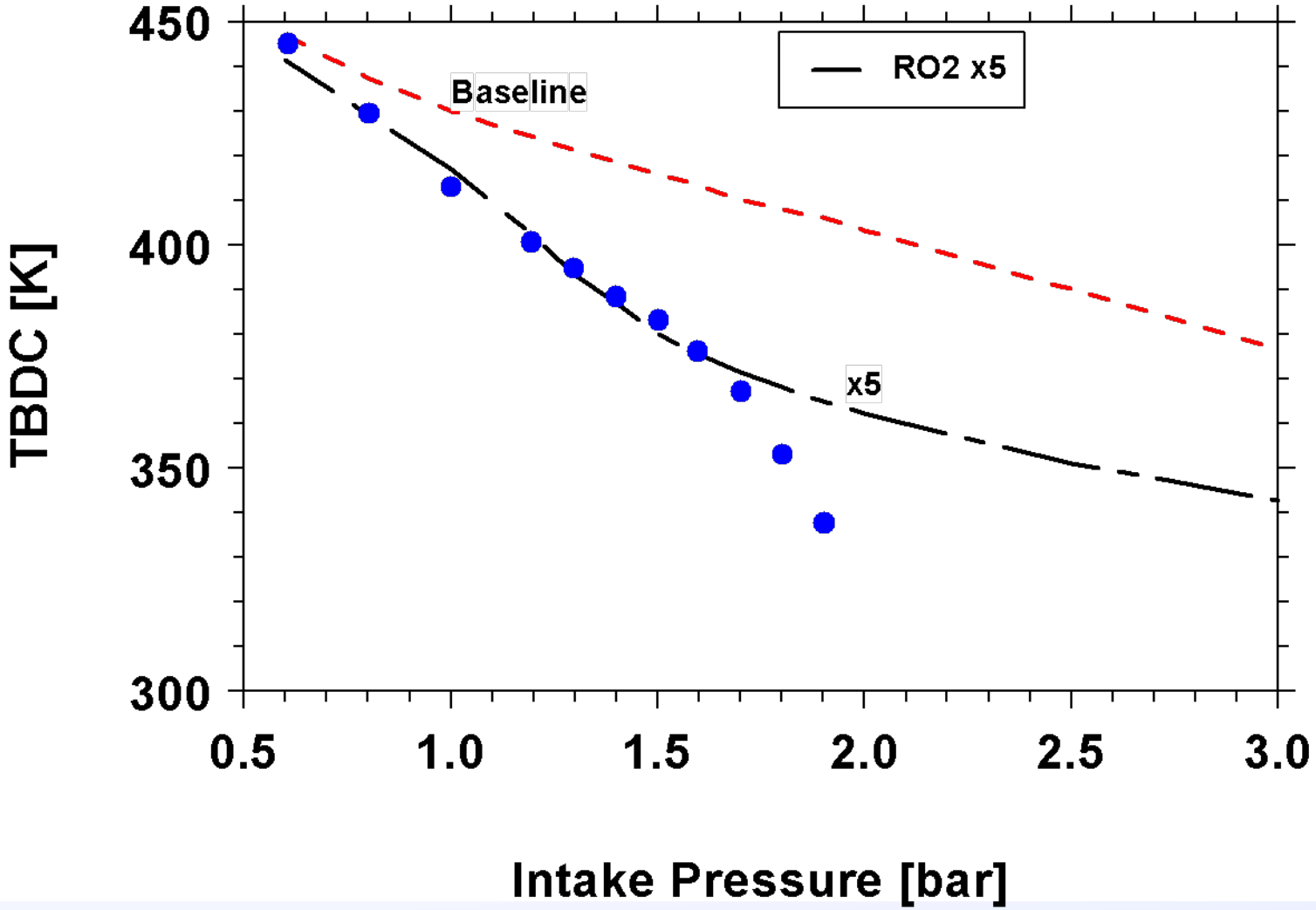
Analysis of pressure sensitivity of low temperature reaction steps may offer guidance toward improving quality of agreement



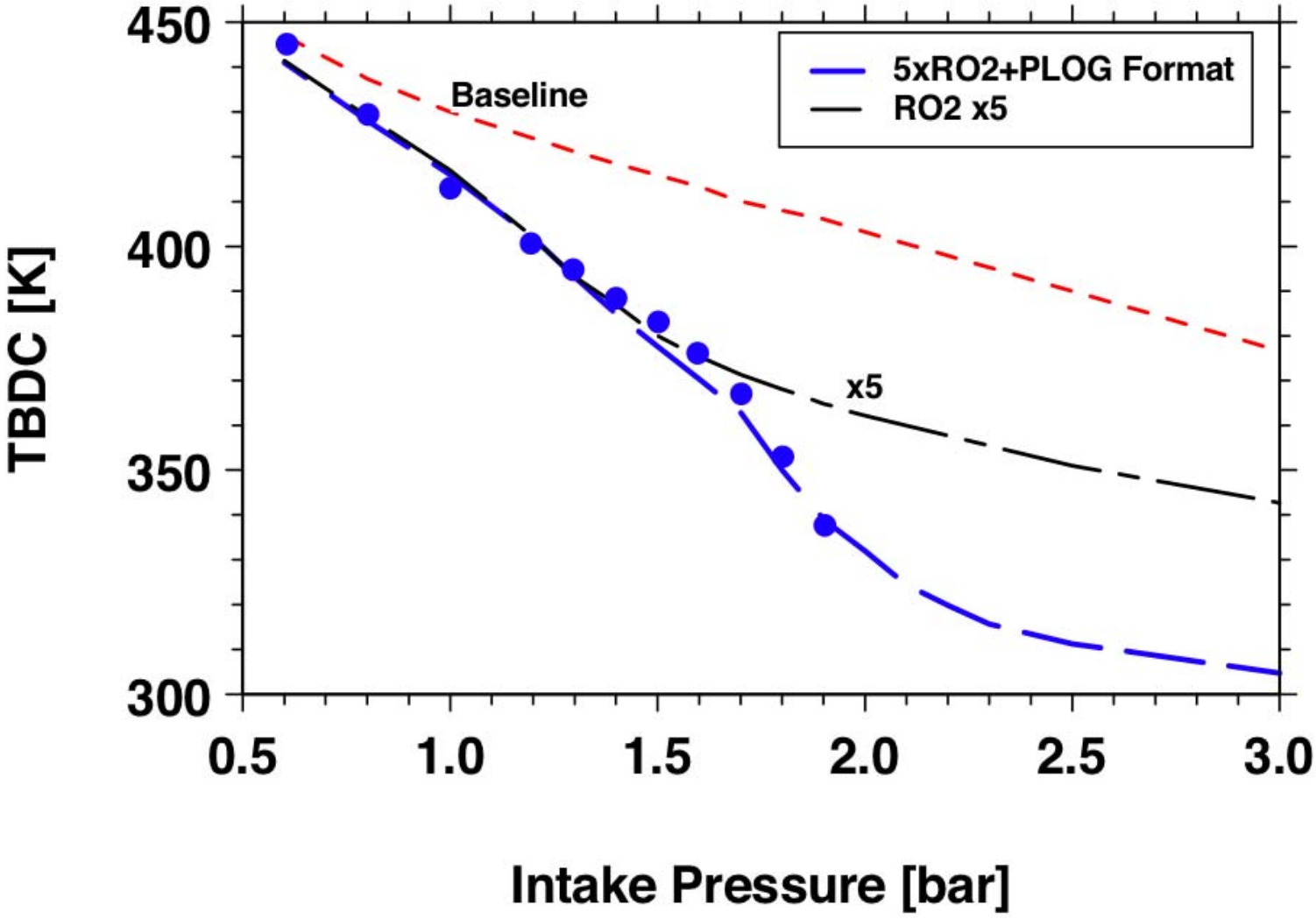
Radical recombination
$R + O_2 \rightarrow RO_2$

Chain branching
$O_2QOOH \rightarrow HO_2QO + OH$

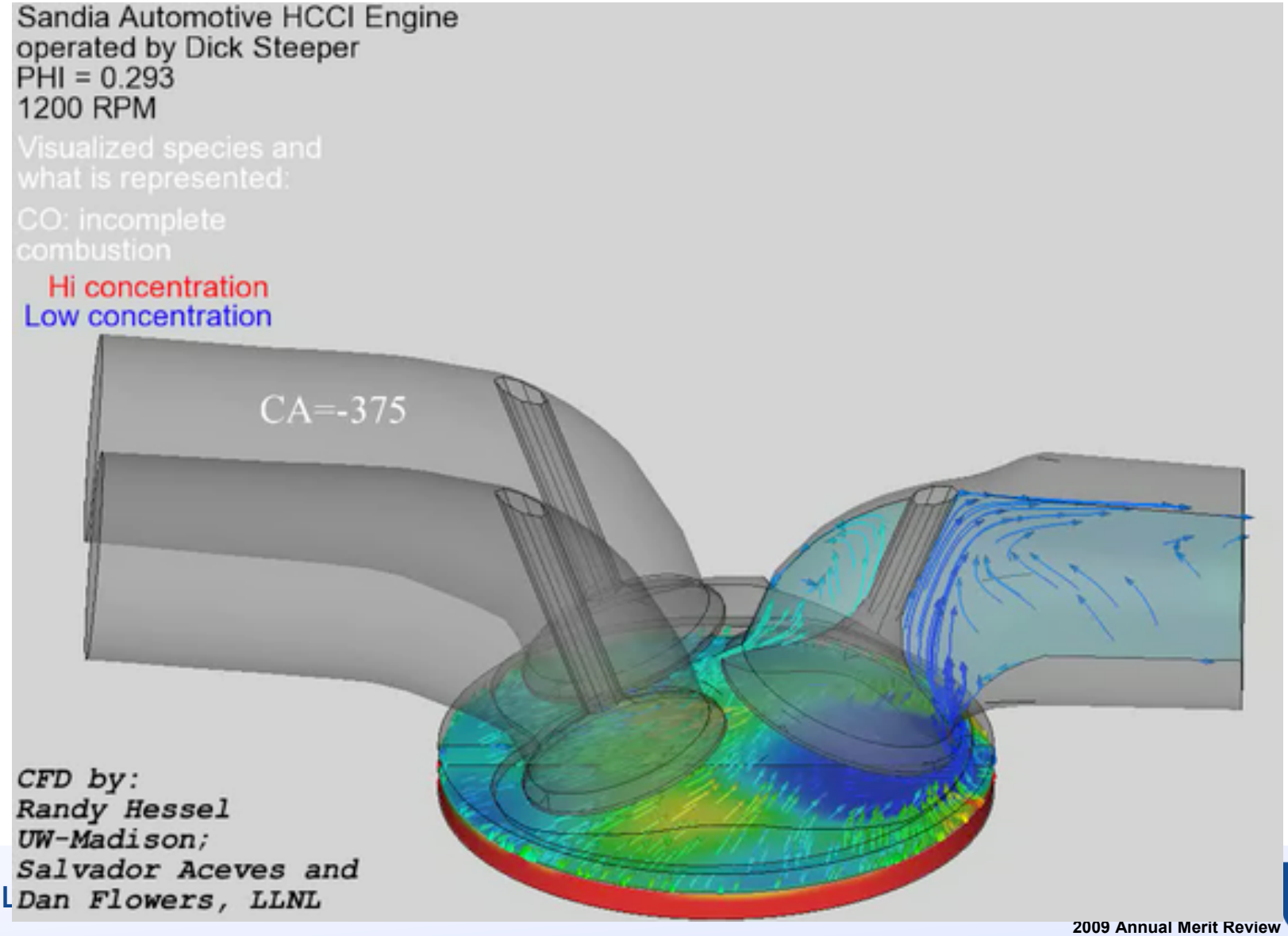
Increasing the reactivity of the radical recombination reaction $R + O_2 \rightarrow RO_2$ matches experimental results up to ~1.7 bar intake



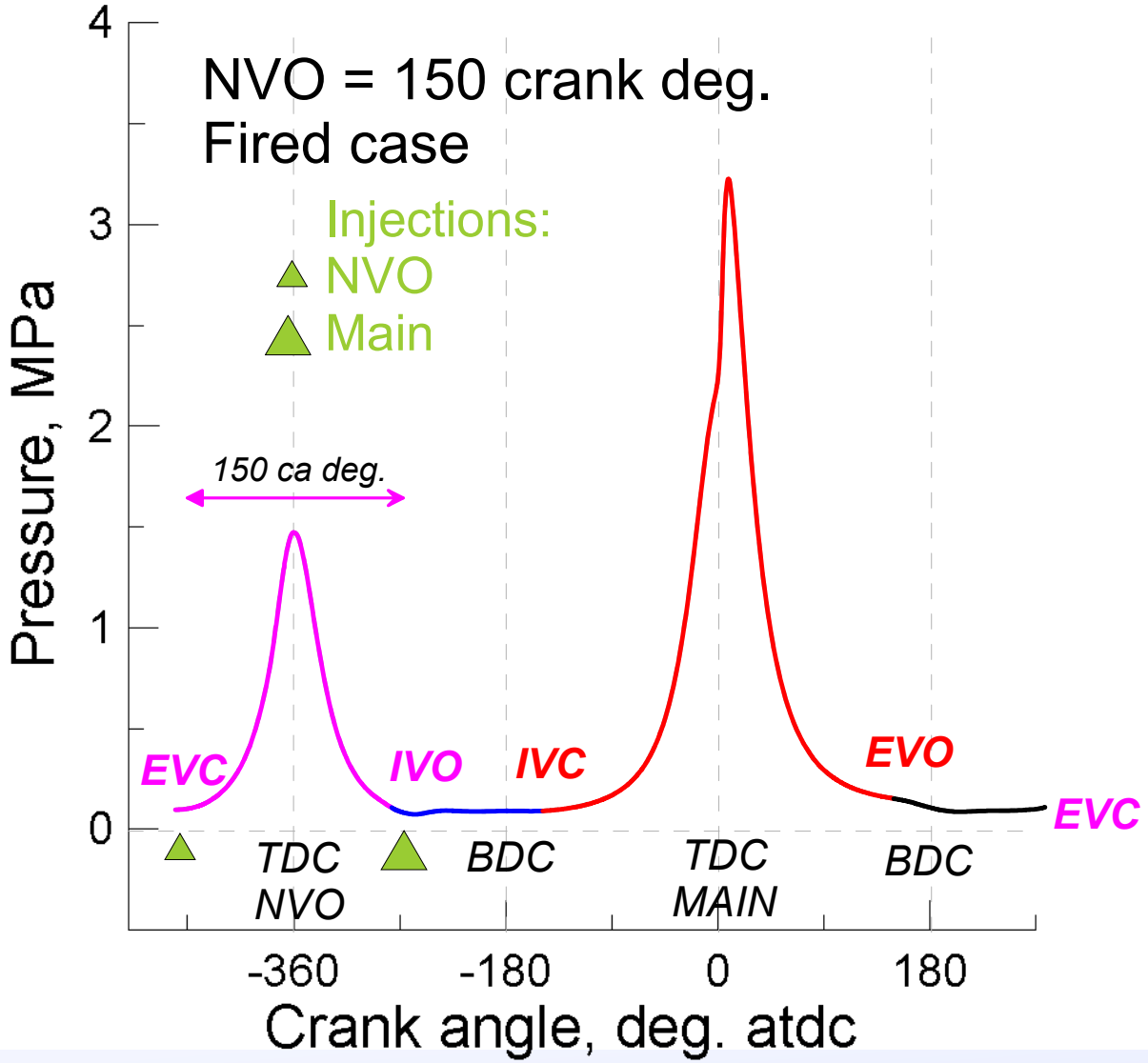
We obtain improved agreement by reducing activation energy of chain branching reactions as a function of pressure



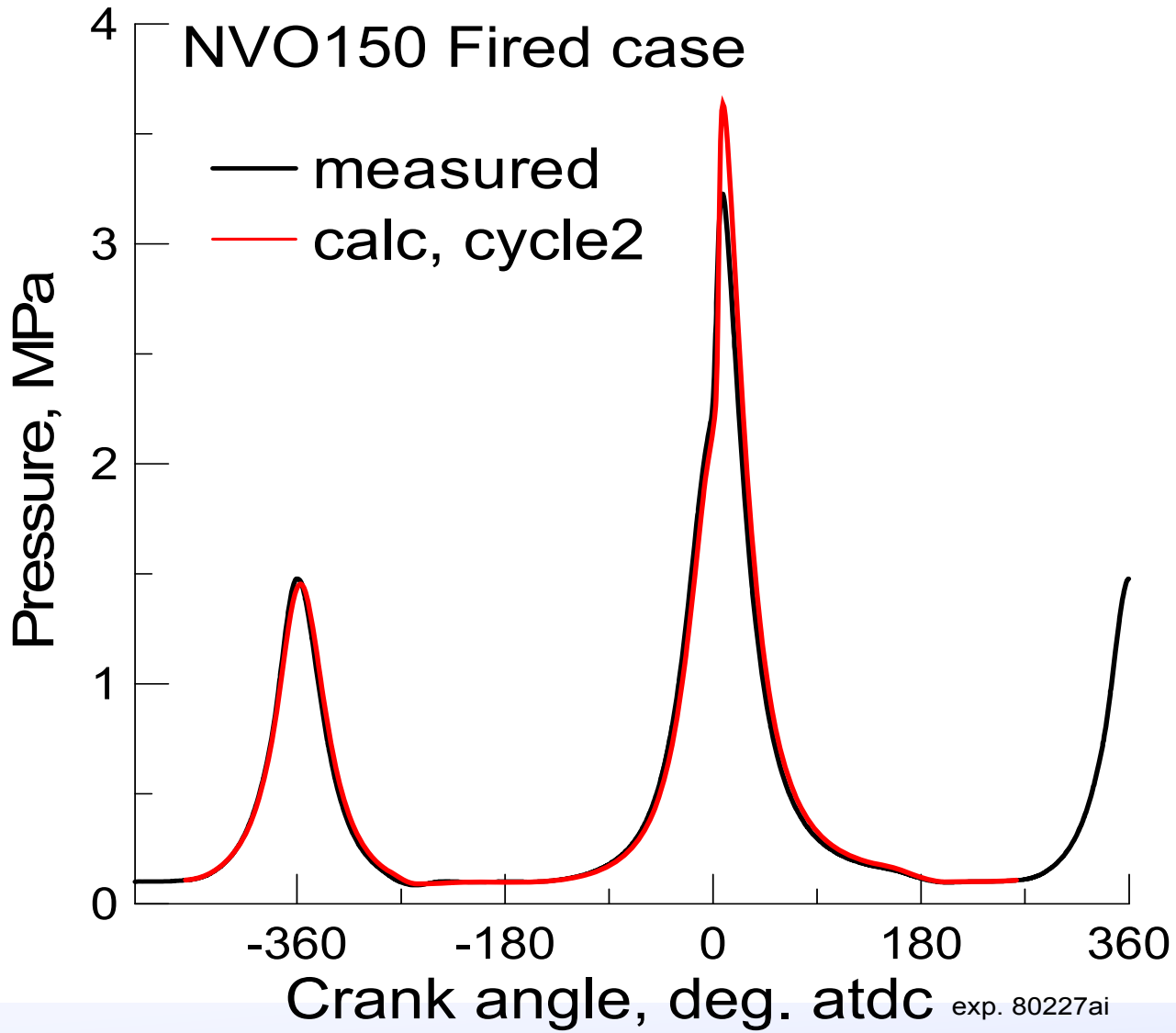
We are analyzing three consecutive cycles of the Sandia automotive PCCI engine (Steeper)



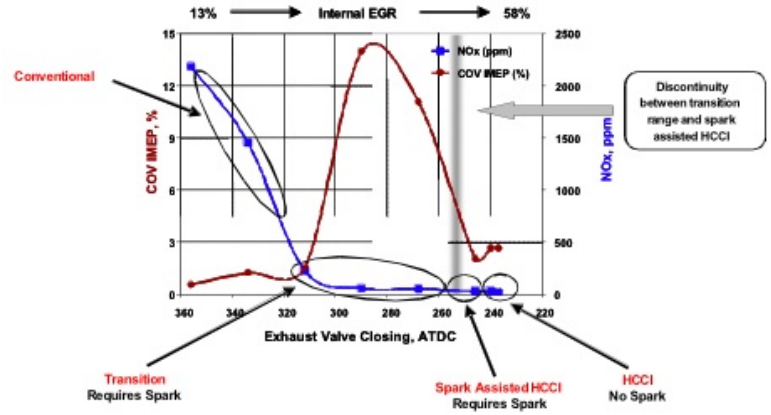
The Sandia engine runs in PCCI mode with dual injection: one injection during NVO and a main injection



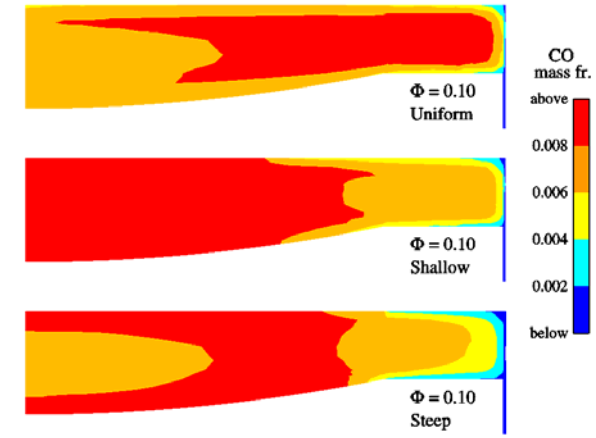
KIVA3V-MZ-MPI shows promise for accurately predicting direct injected PCCI



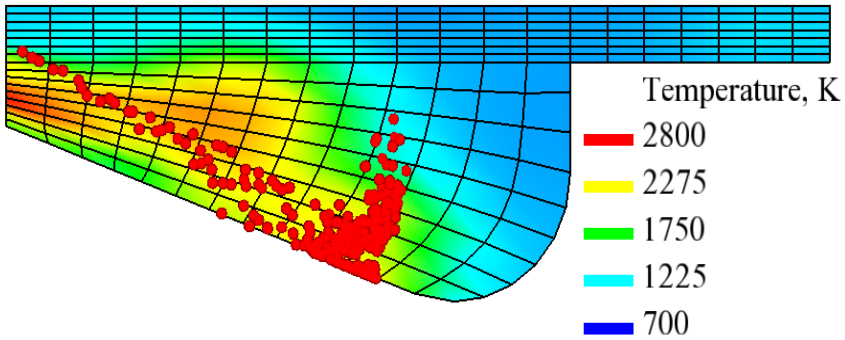
Future work: we are preparing our codes for public release



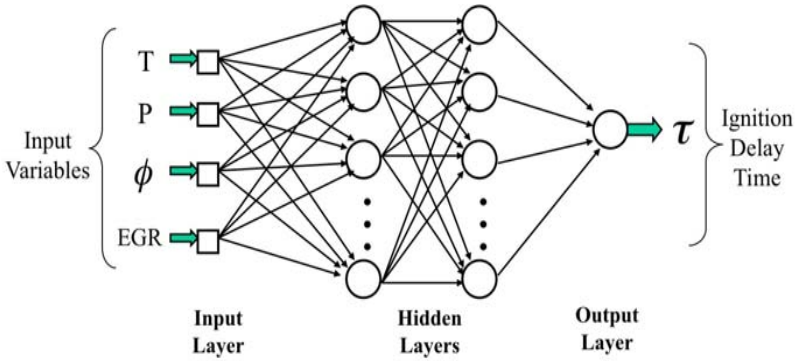
Chemkin multizone (1-D flame propagation & autoignition)



KIVA-sequential multizone (HCCI)

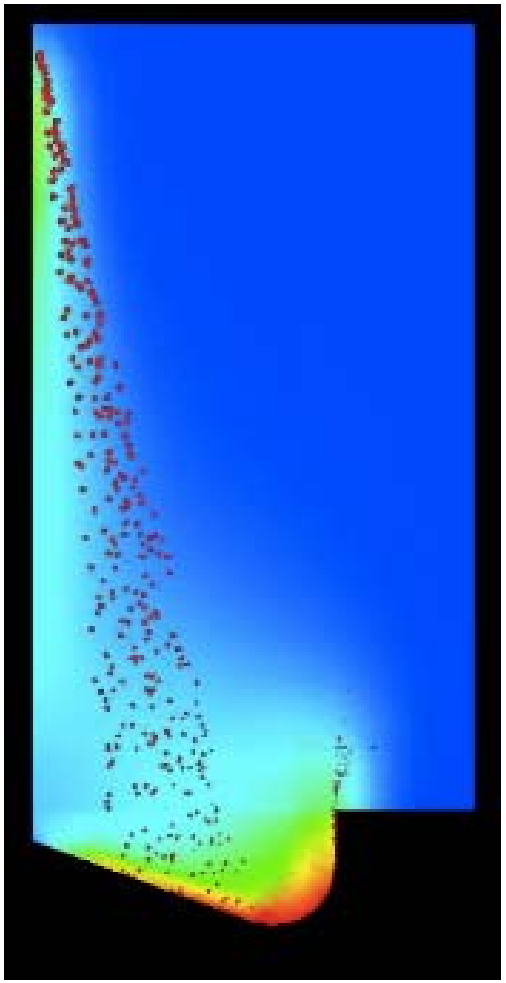


KIVA multizone (HCCI, PCCI)



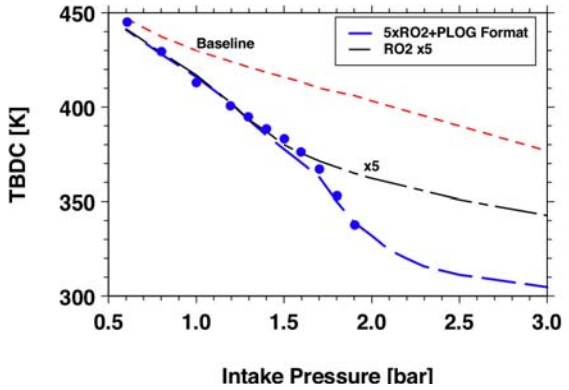
KIVA-artificial neural network (HCCI, PCCI)

Future work: extend applicability and computational efficiency of analysis tools

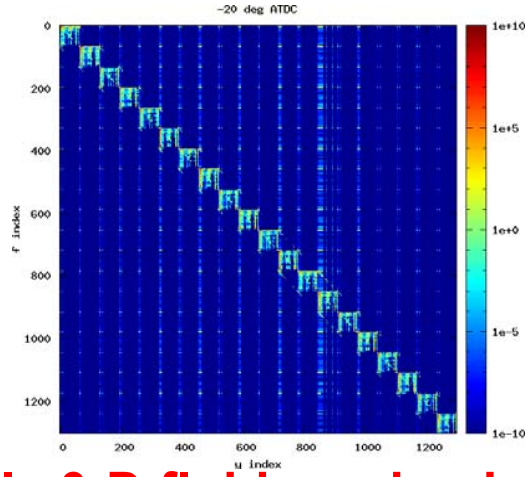


Full PCCI validation

KIVA-MZ, KIVA-ANN

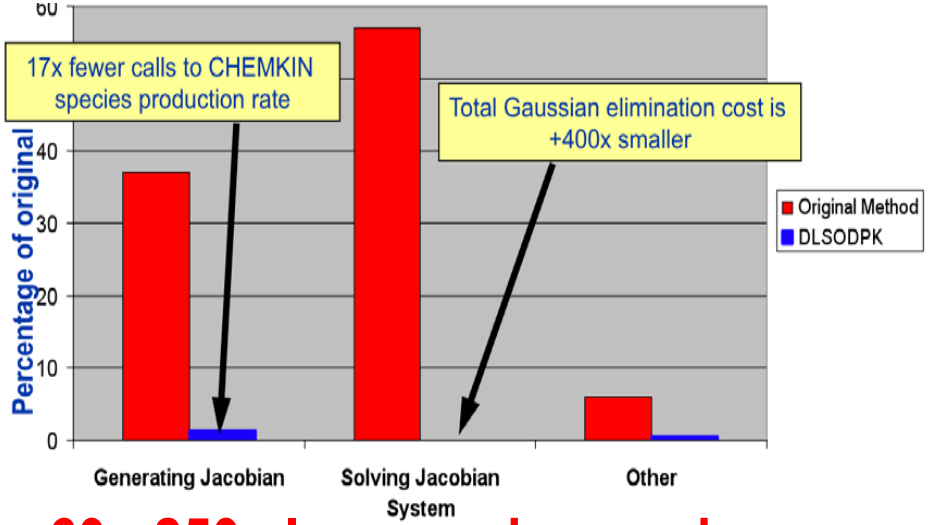


HCCI-based chemical kinetic mechanism testing and tuning

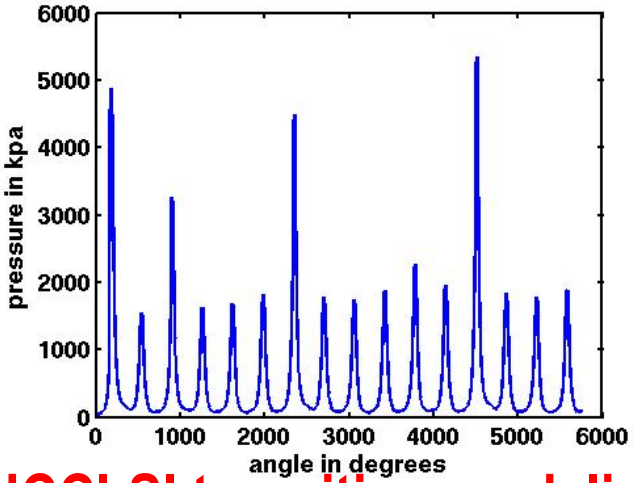


Enable 3-D fluid mechanics and detailed kinetics in today's desktop PCs

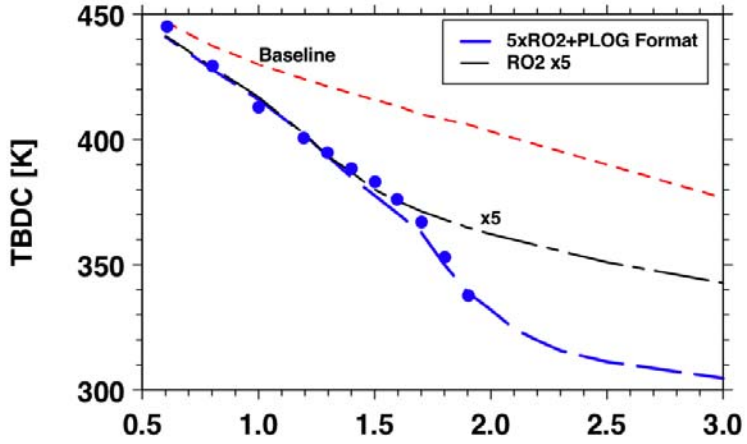
Summary: we are enhancing our analysis capabilities and improving computational performance



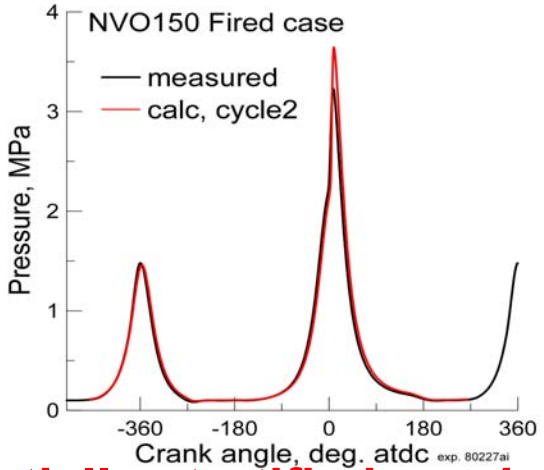
60x-250x Improved numerics



HCCI-SI transition modeling



Gasoline surrogate



Partially stratified combustion