Lawrence Livermore National Laboratory

High Fidelity Modeling of Premixed Charge Compression Ignition Engines

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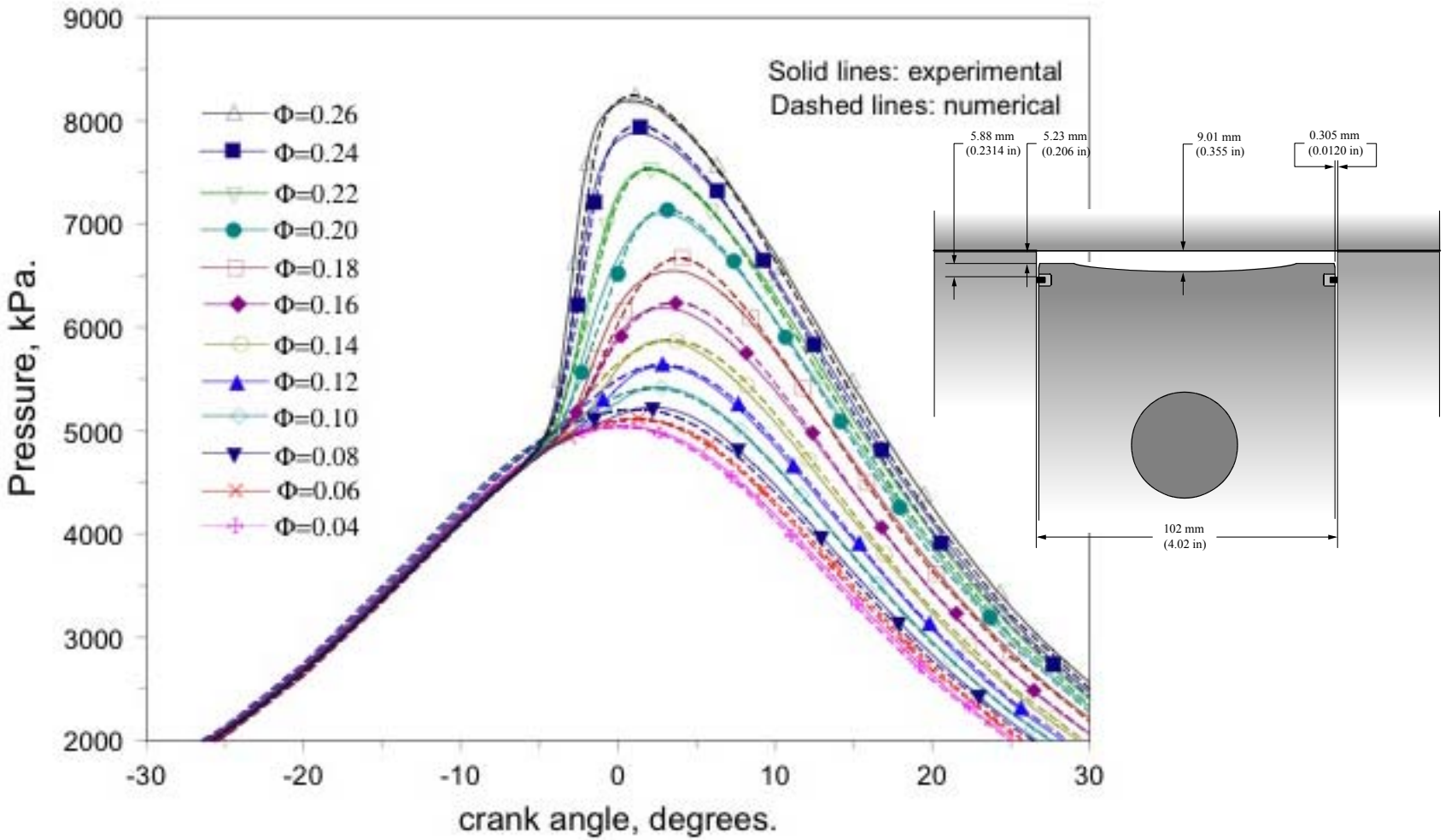
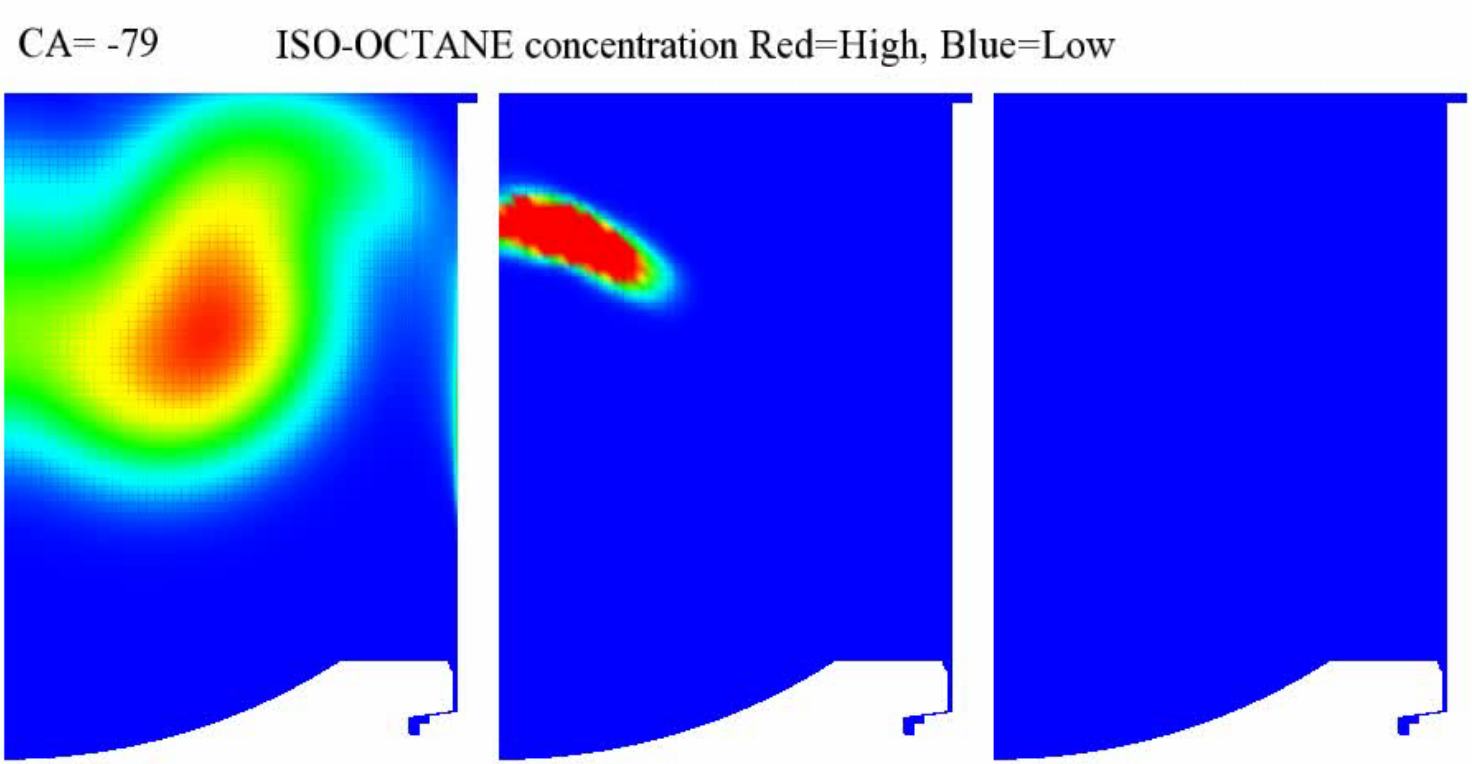
Our multi-zone models have enabled fast, high fidelity analysis of homogeneous (HCCI) combustion

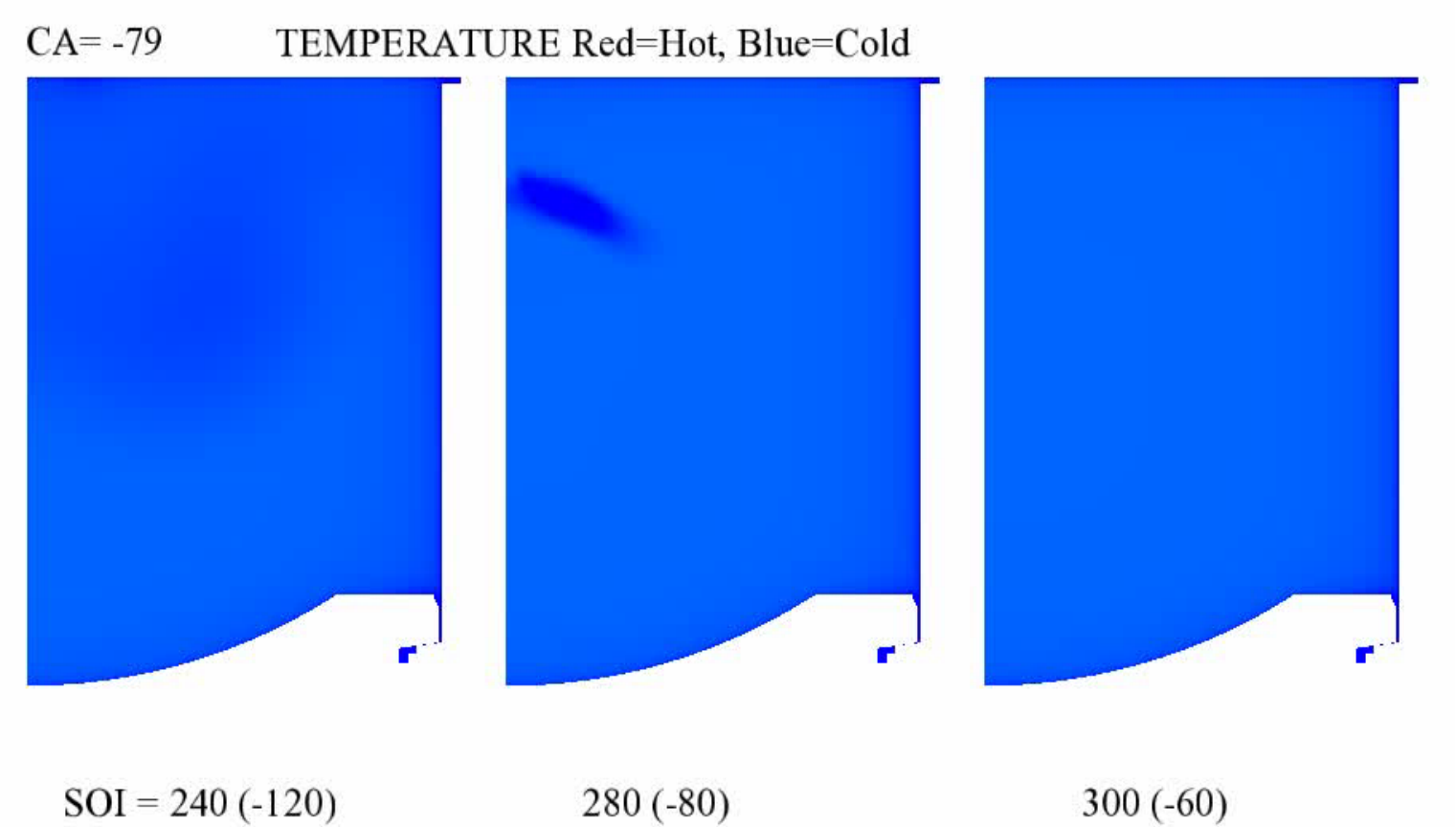


Unprecedented level of agreement obtained between experimental (Sandia) and numerical (LLNL) results

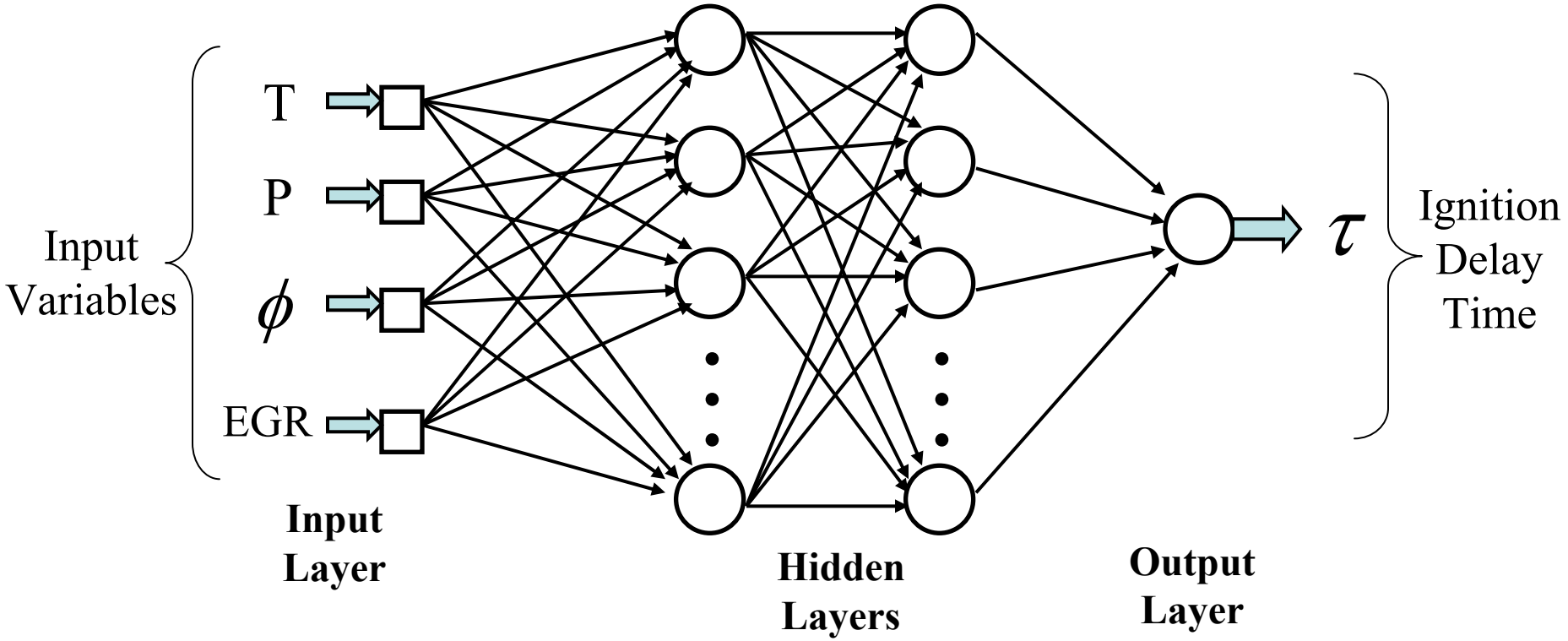
We are now modeling Sandia PCCI experiments with KIVA3V-MZ-MPI



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



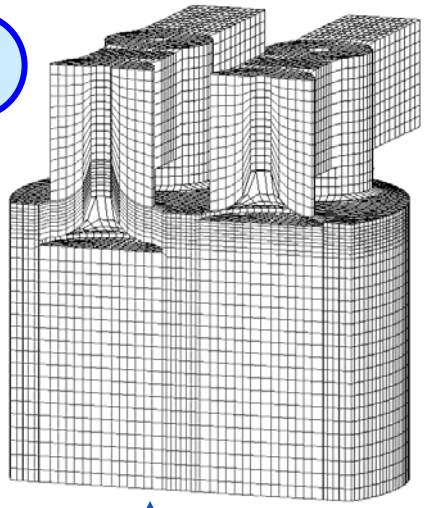
We have incorporated neural network chemical kinetics into KIVA3V for fast analysis of HCCI combustion and emissions (KIVA3V-ANN)



Ignition Condition: $$I(t) = \int_{t(0)}^{t_k} \frac{1}{\tau} dt = 1$$

The ignition integral criterion determines ignited cells and a two step chemical kinetic mechanism analyzes combustion

1



2

Calculate Ignition Integral in Each Cell

$$I(t) = \int_{t(0)}^{t_k} \frac{1}{\tau} dt$$

3

Is Ignition Criterion met?

Yes

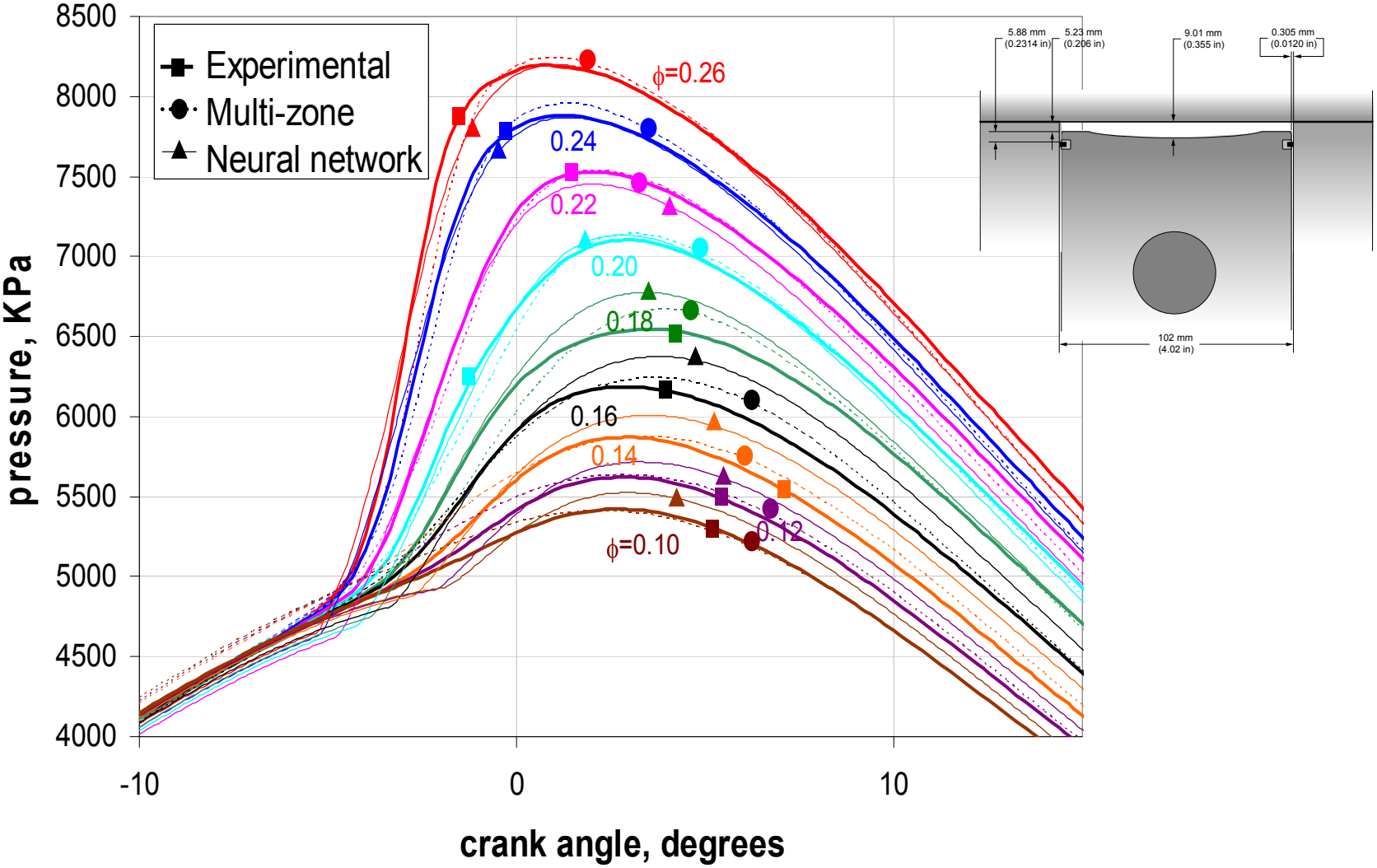
No

Turn on global fuel conversion mechanism

$$C_8H_{18} + 8.5O_2 \rightarrow 8CO + 9H_2O$$
$$CO + \tfrac{1}{2}O_2 \rightarrow CO_2$$

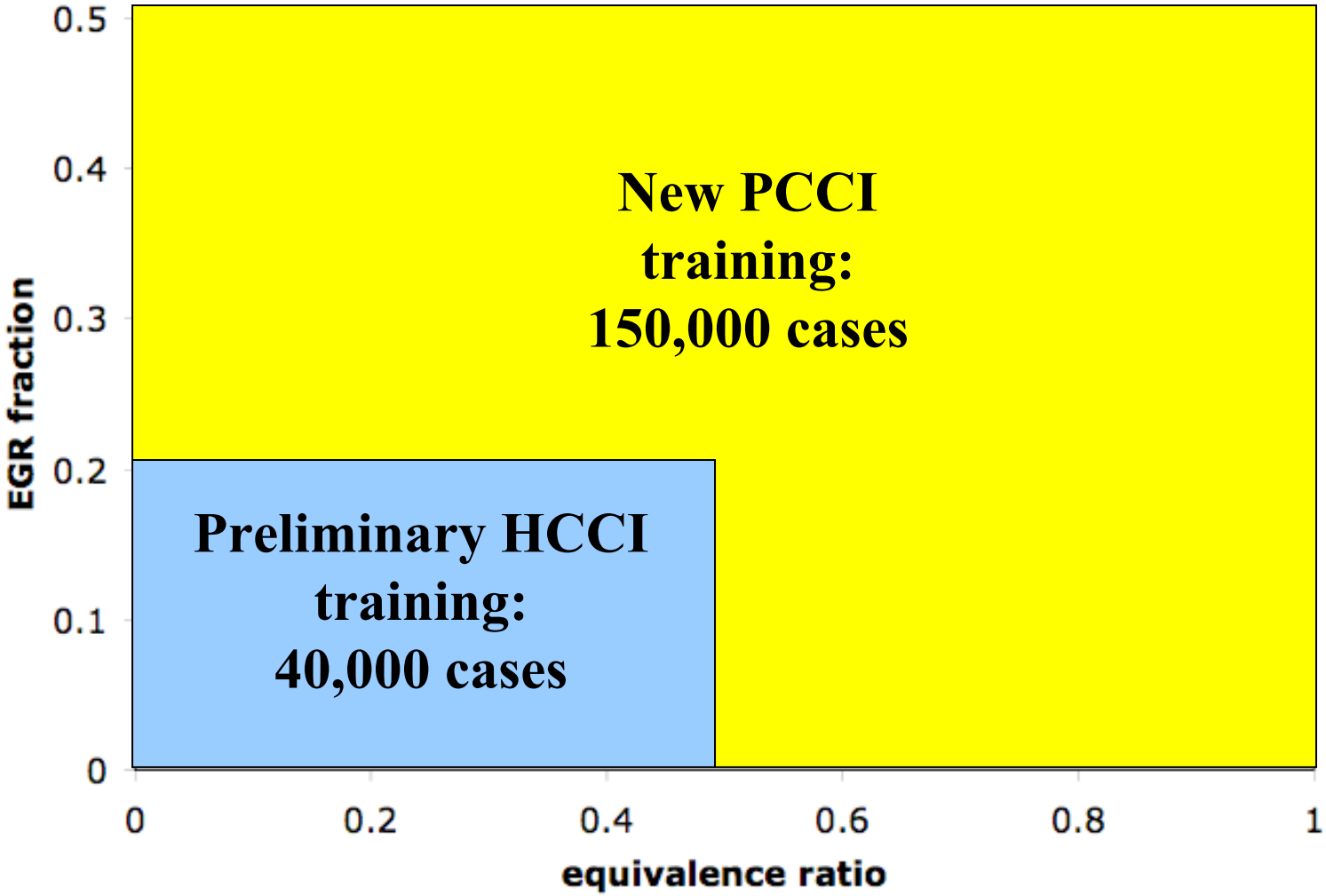
4

Our artificial neural network engine combustion code (KIVA-ANN) permits ultra fast and accurate modeling of iso-octane HCCI/PCCI

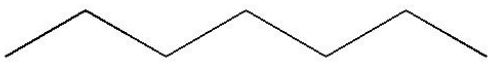


KIVA-ANN is almost as accurate as detailed kinetic models while considerably reducing computational cost (4 hours for 50,000 element mesh)

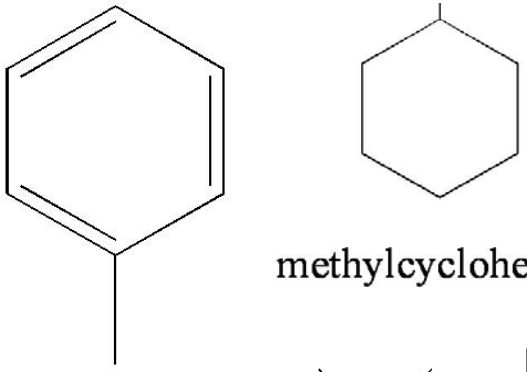
Our ANN has been trained over a broad range of ϕ-EGR enabling fast and accurate analysis of partially stratified combustion



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

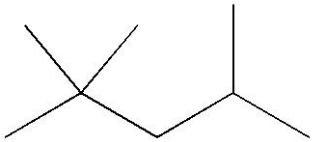


n-heptane

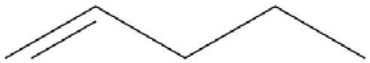


methylcyclohexane

toluene



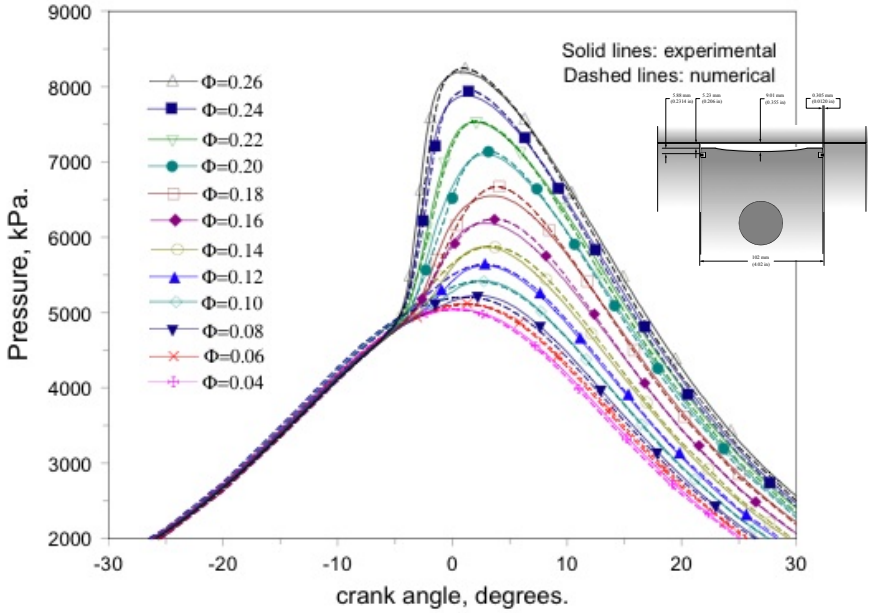
iso-octane



1-pentene

testing

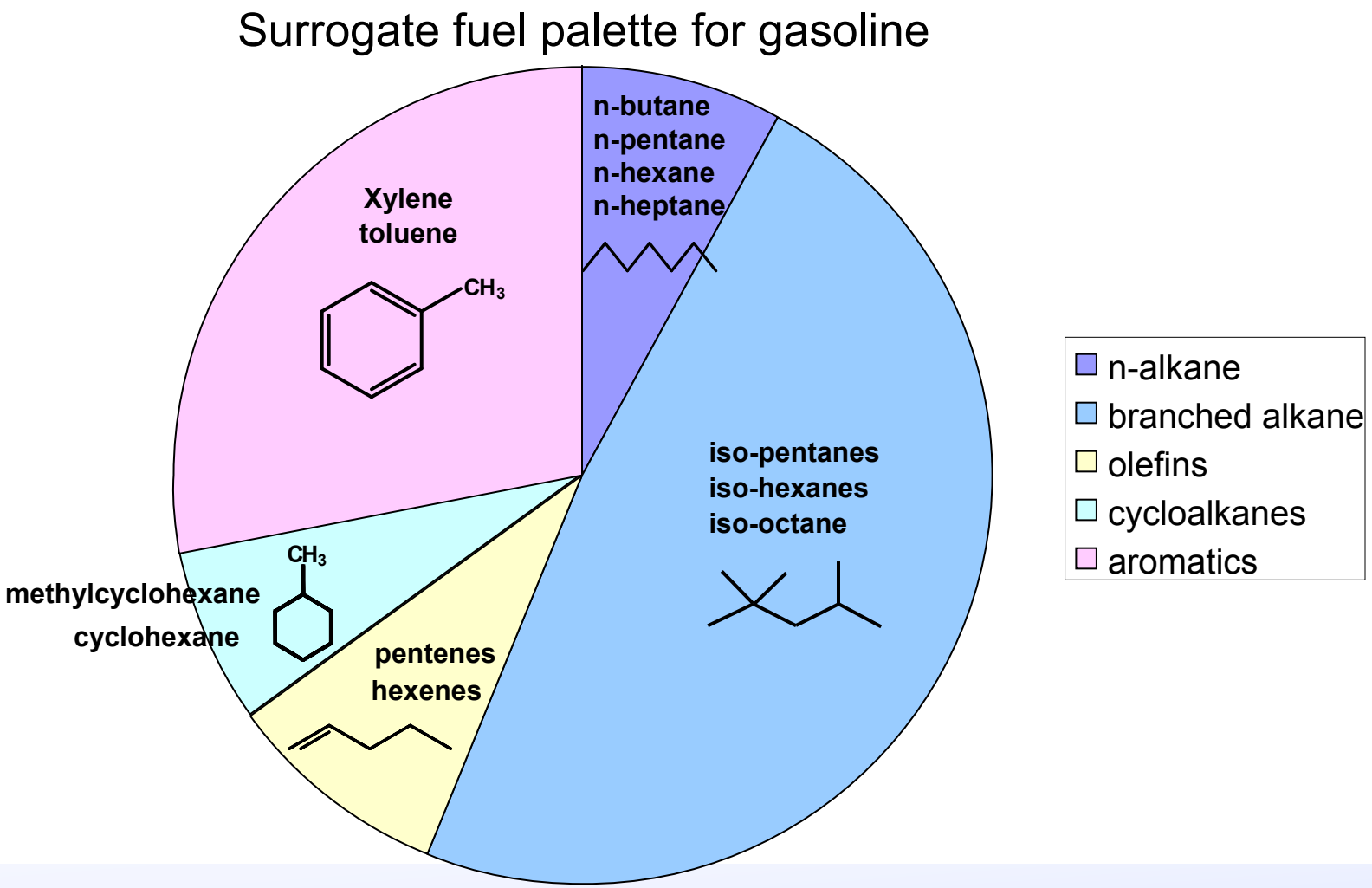
tuning



Detailed kinetics of gasoline surrogates

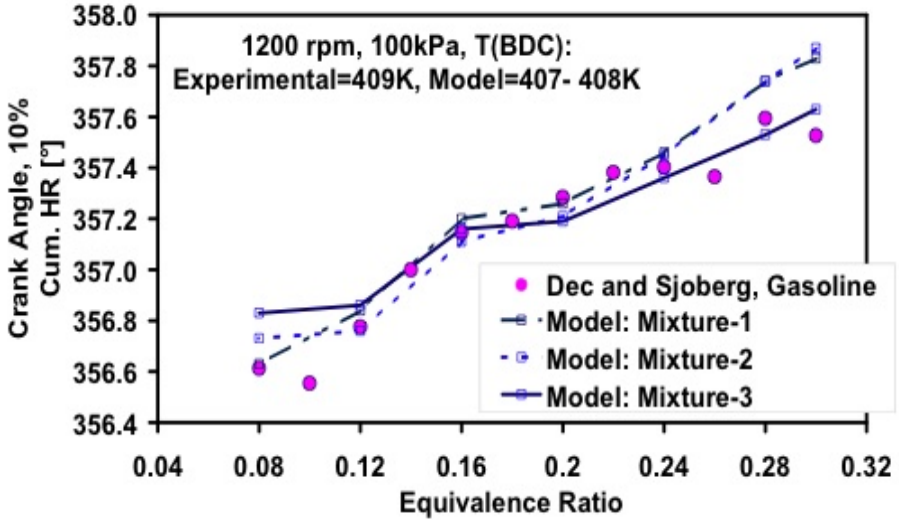
High fidelity engine models

We develop & refine surrogate gasoline chemical kinetic models by producing detailed mechanisms for all the major chemical classes

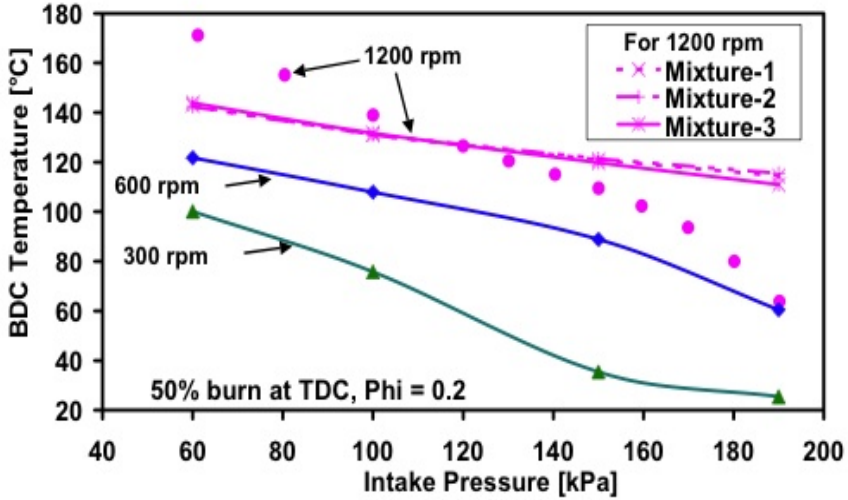


We have proposed and tested three gasoline surrogate mechanisms

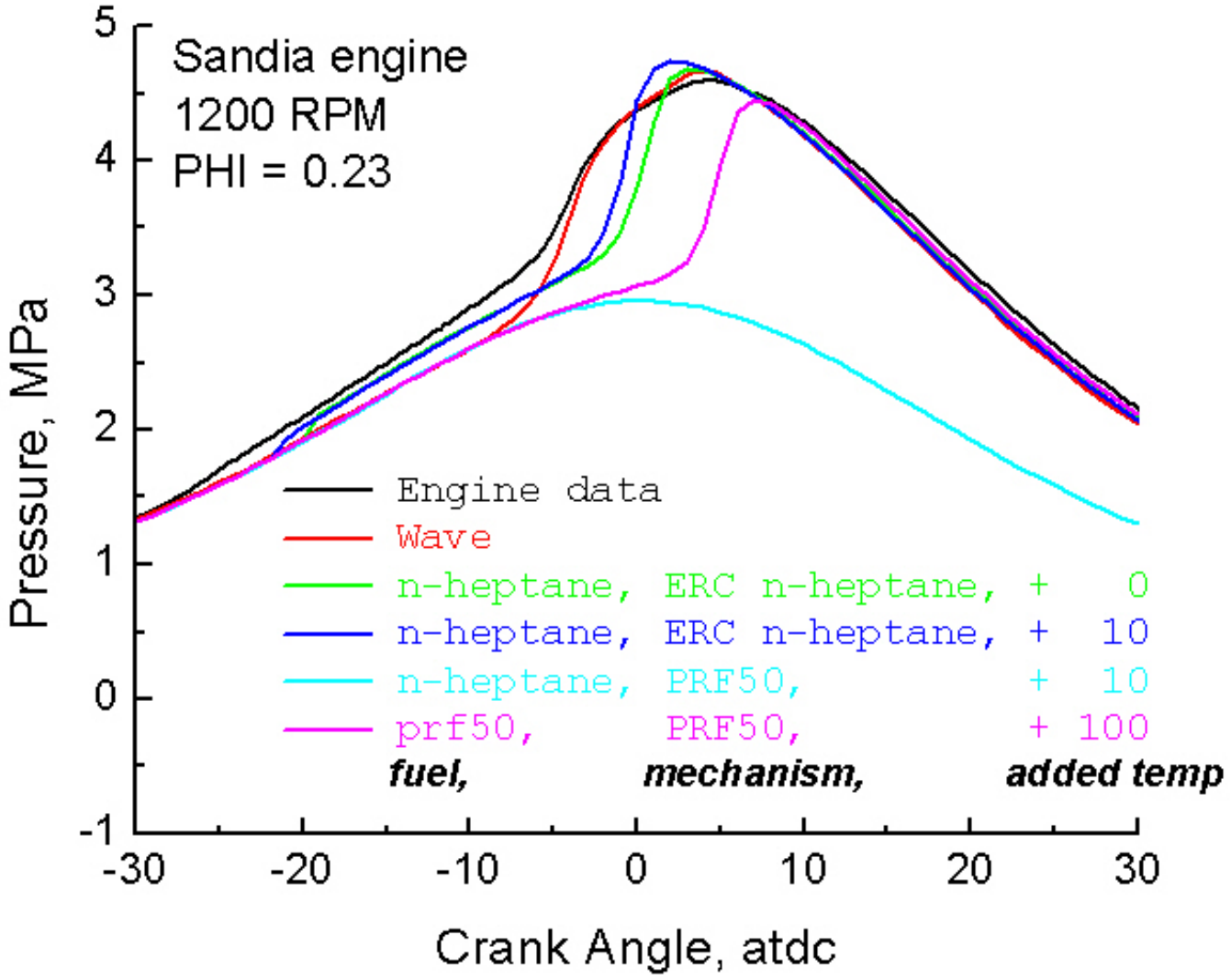
% Molar Composition	Mixture 1	Mixture 2	Mixture 3
iso-Octane	60	40	40
n-Heptane	8	10	20
Toluene	20	10	10
Methyl cyclohexane	8	40	30
1-Pentene	4	0	0
RON (linear)	92.9	82.2	74.5
MON (linear)	90.6	80.0	72.7
RON (blend)	96.3	92.9	82.5
MON (blend)	92.9	84.9	76.3



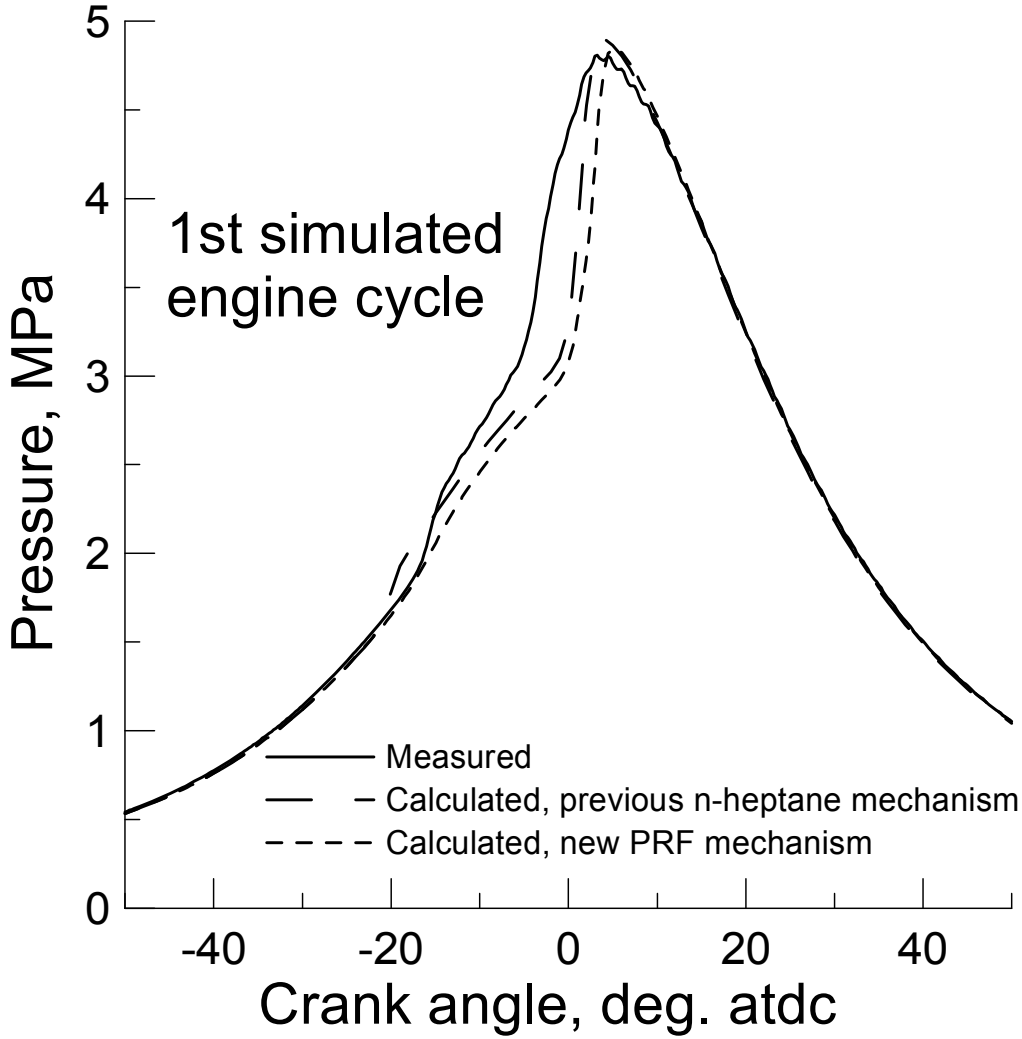
- **Mixture 1:** average gasoline composition
- **Mixture 2:** similar octane number as gasoline
- **Mixture 3:** enhanced reactivity



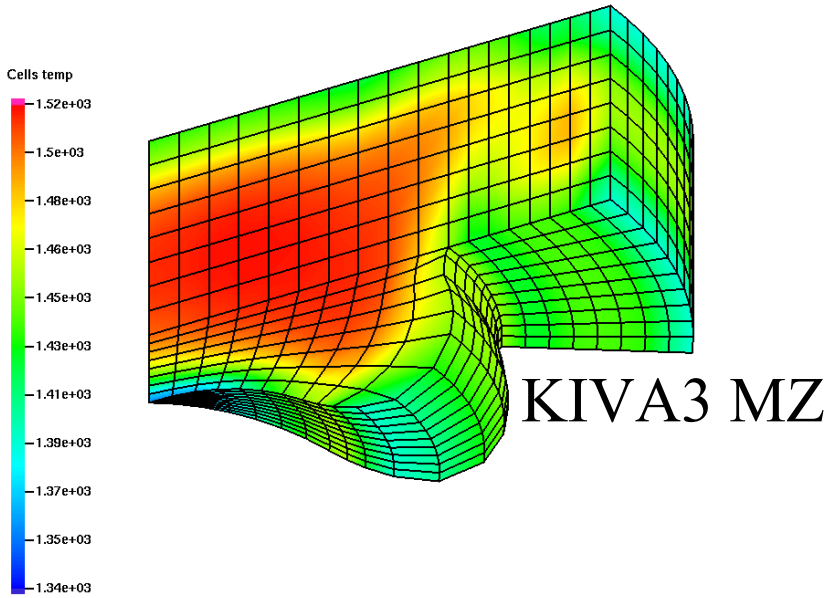
Today's detailed chemical kinetic models perform well for iso-octane but have limitations predicting low octane (n-heptane) fuel behavior



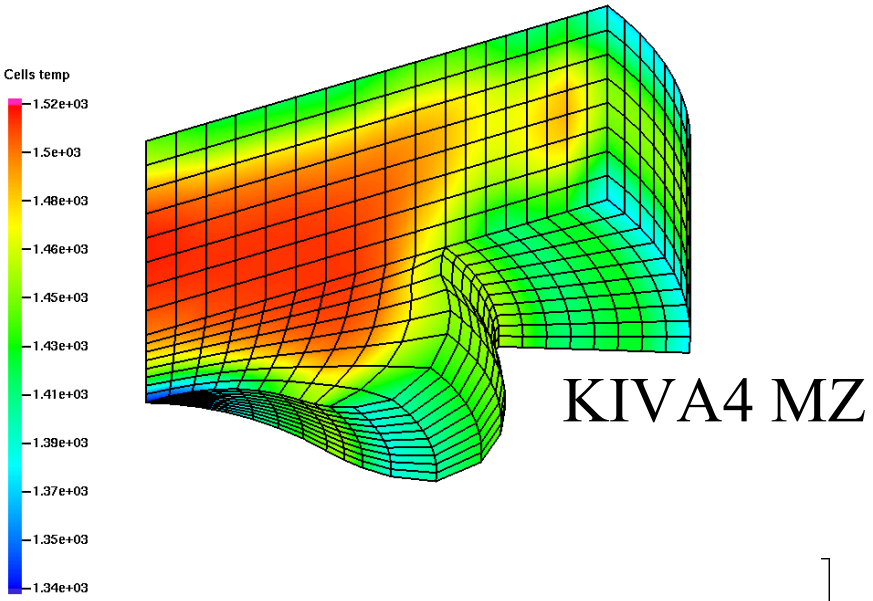
We have identified improved chemical kinetic models of n-heptane that can be further tuned with KIVA3V-MZ-MPI



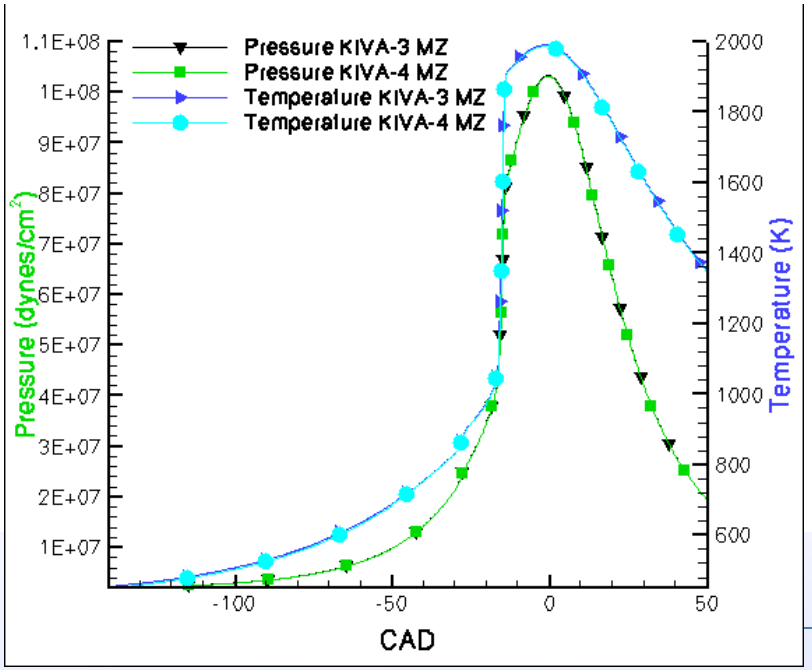
In collaboration with LANL, we have transitioned our multi-zone model to KIVA4

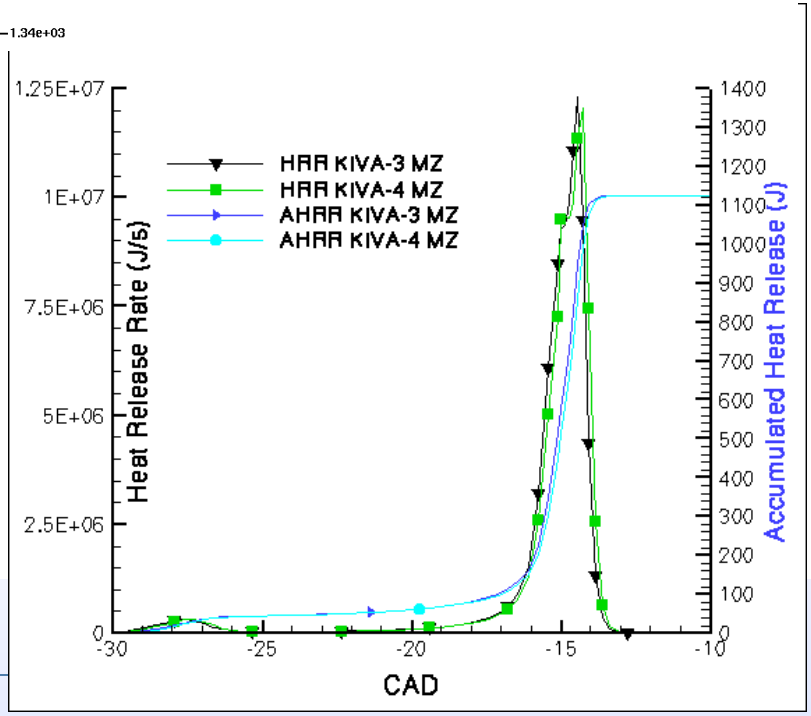


KIVA3 MZ

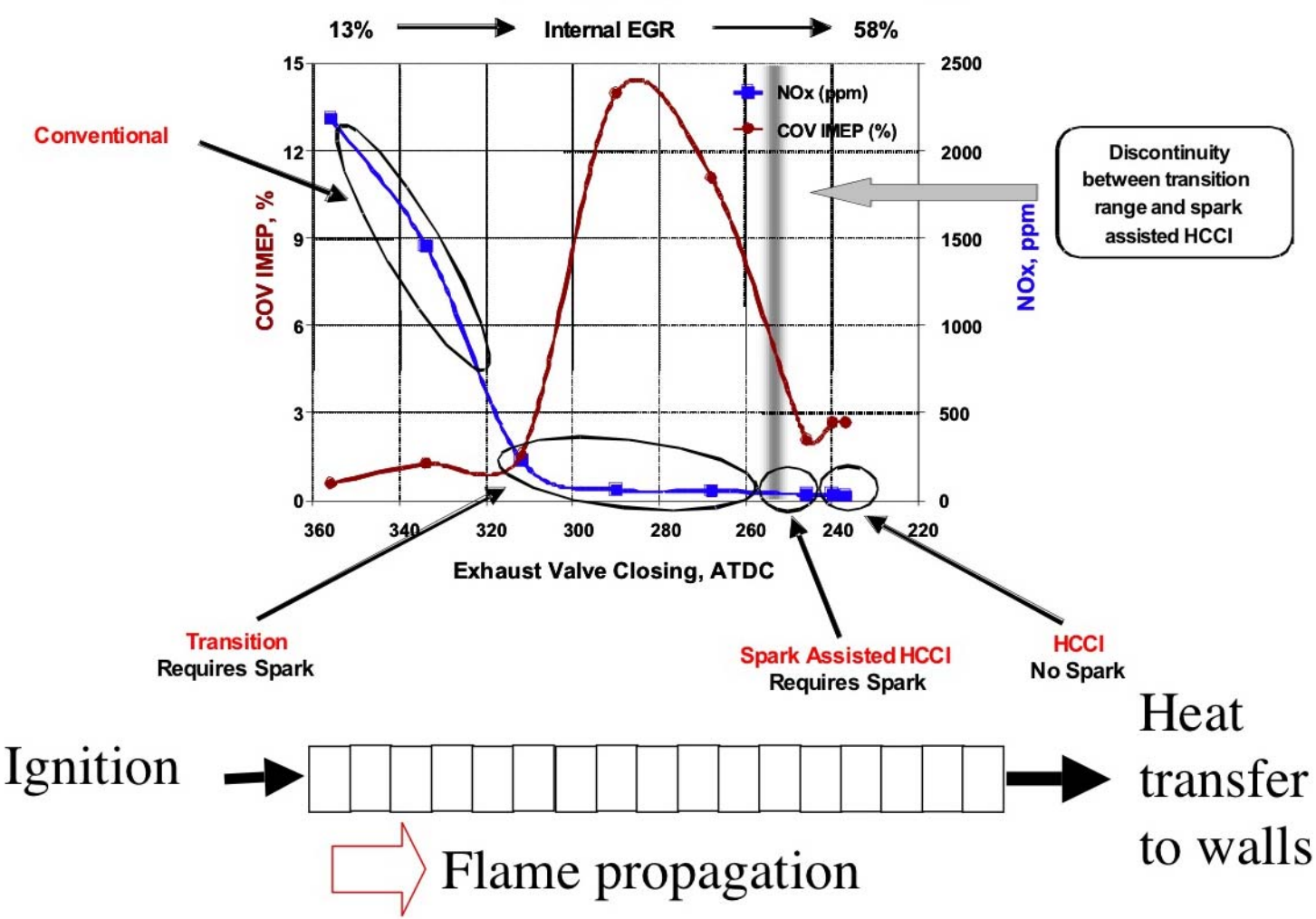


KIVA4 MZ

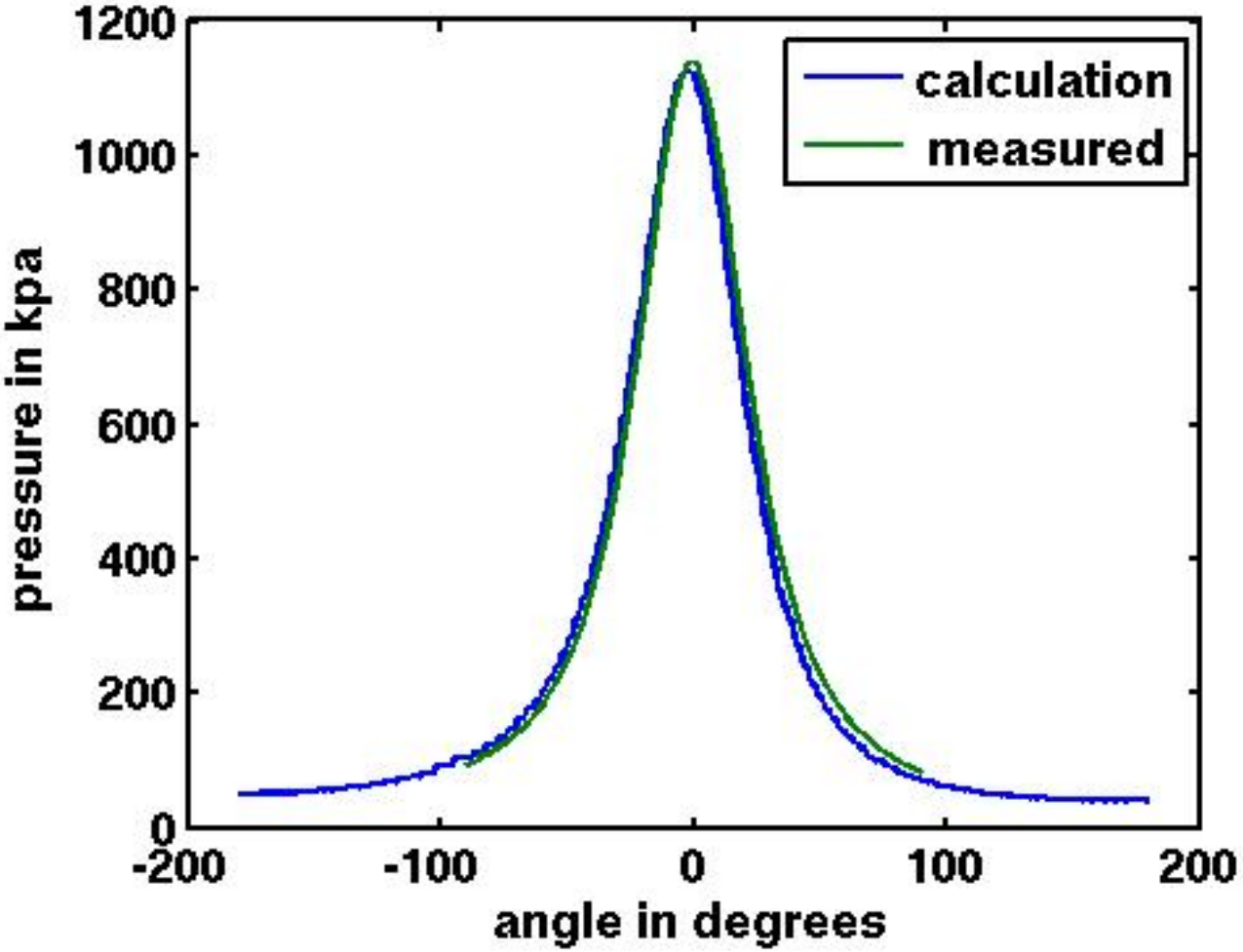




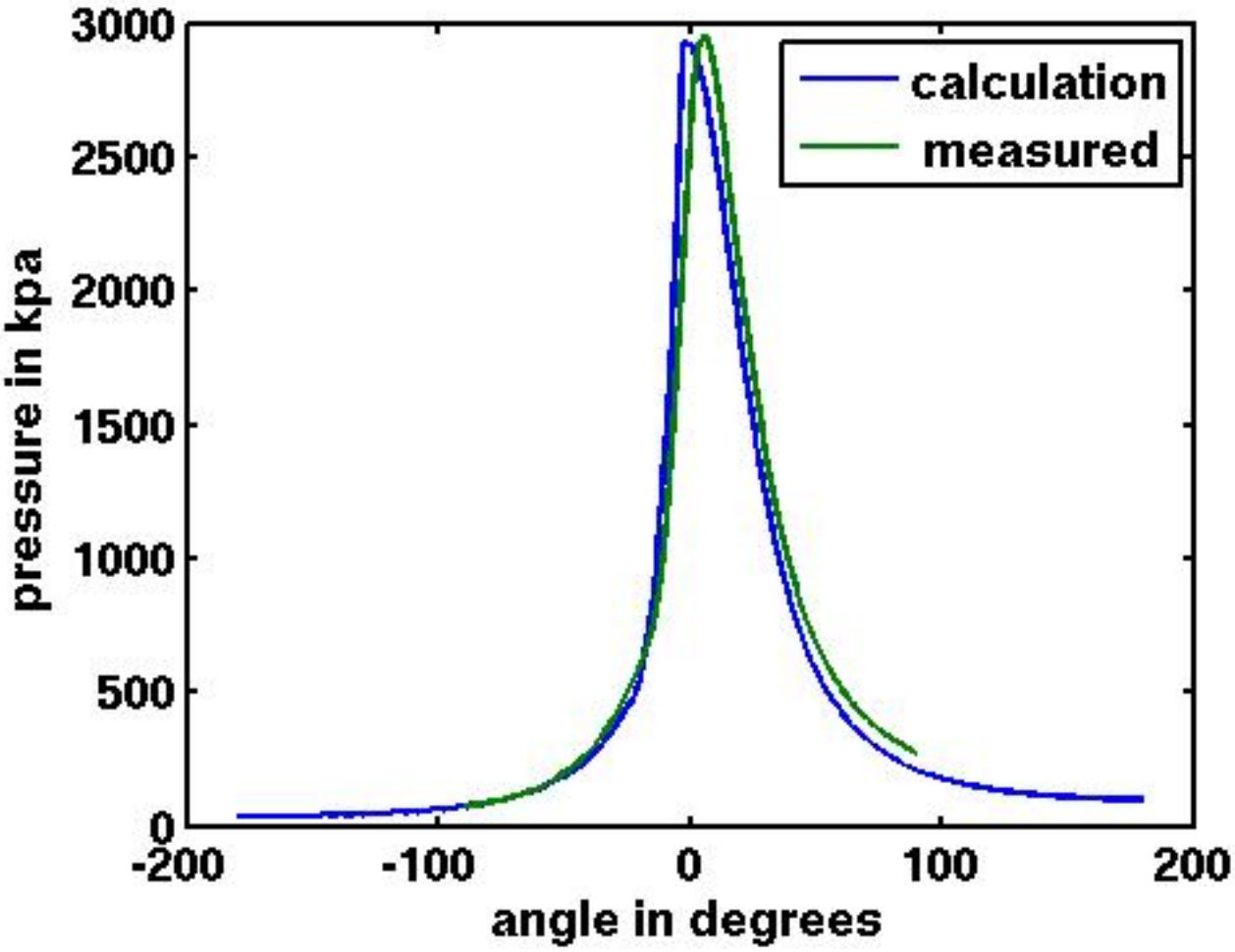
We are analyzing gasoline SI-HCCI transition experiments with a 1-D flame propagation/autoignition code



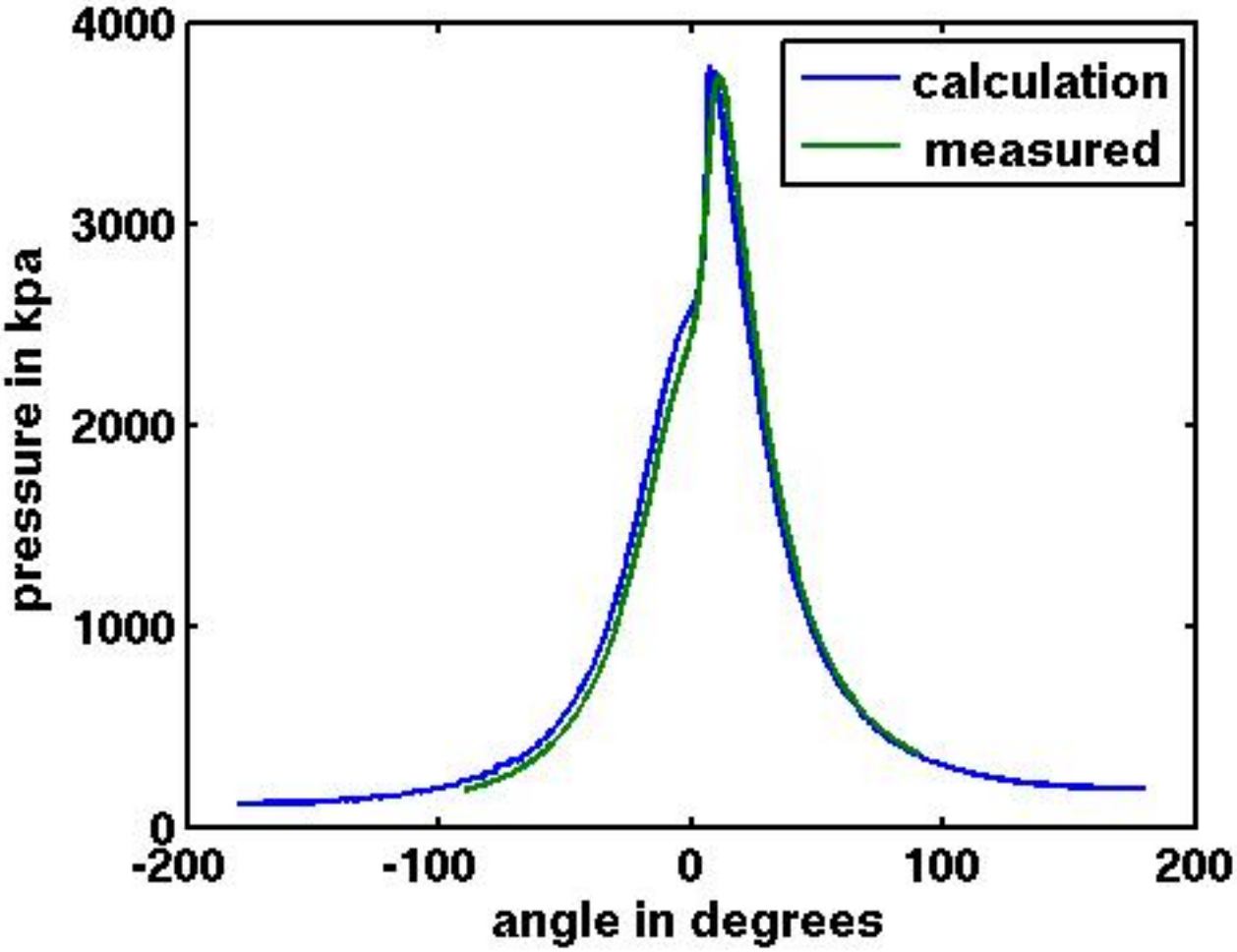
Our model accurately predicts ORNL motored pressure traces



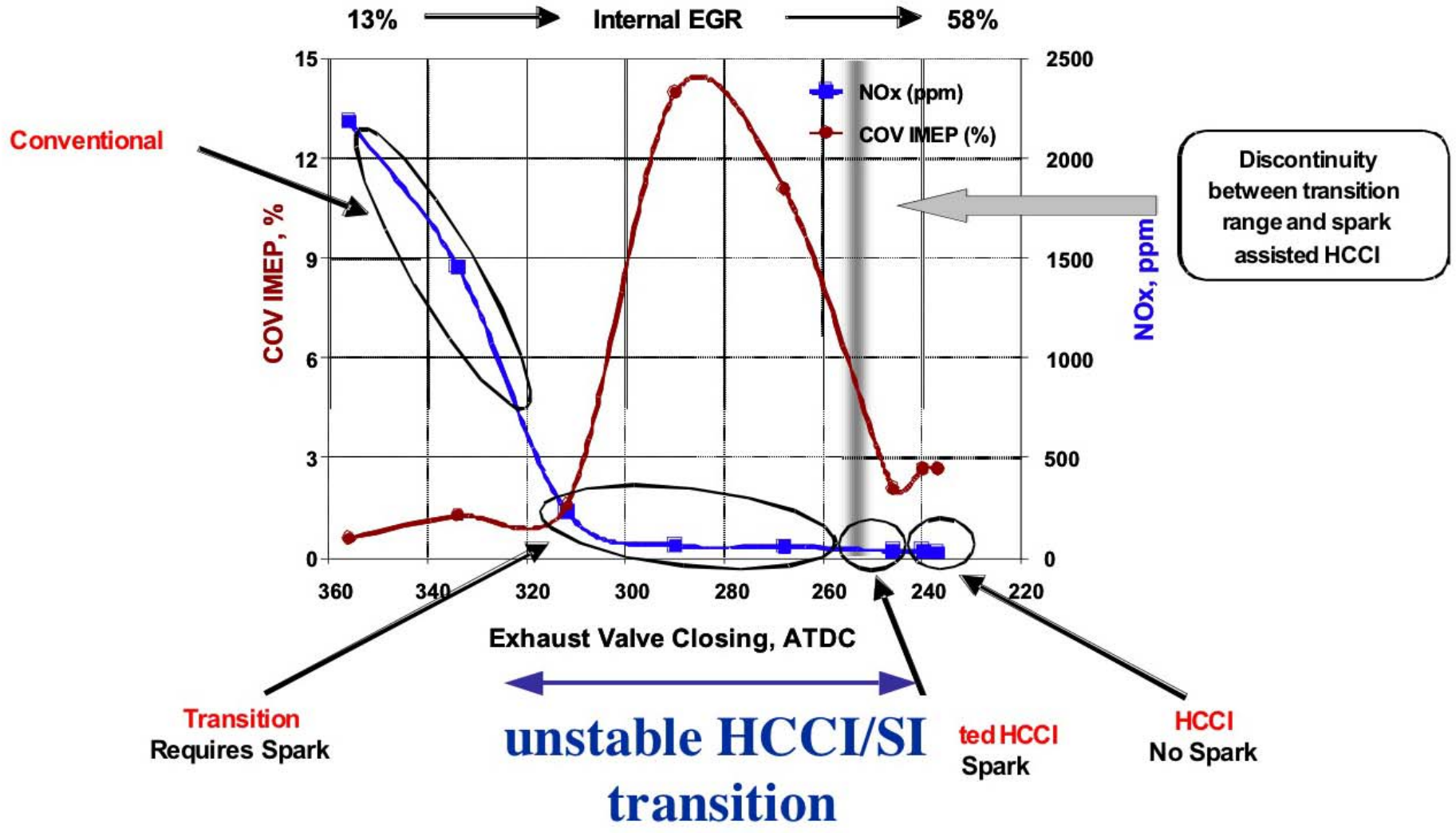
We can also make accurate predictions of ORNL SI engine results



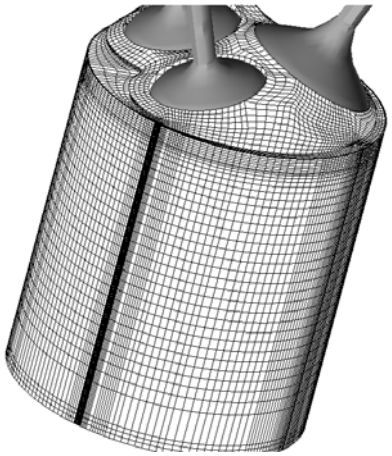
Our analysis results also match ORNL HCCI results.



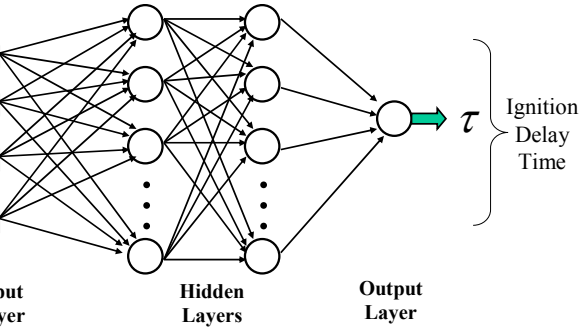
Next challenge: model consecutive cycles to evaluate unstable transition between HCCI and SI at intermediate EGR fractions



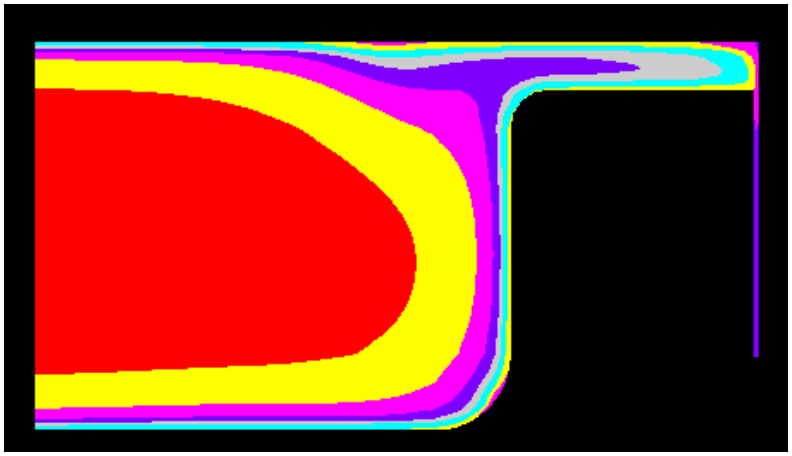
Future plans: We will complete validation of our PCCI codes by comparison with Sandia iso-octane results and exhaust speciation



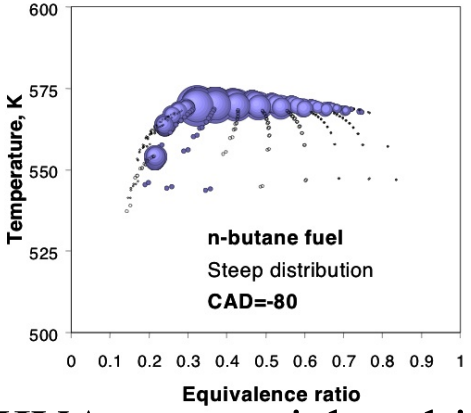
1. KIVA3V with CHEMKIN calculations in every cell: *months* in 100 processor computer. For benchmarking only



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

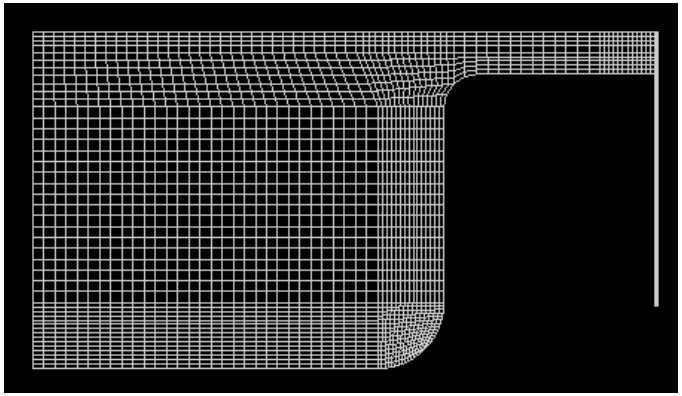


2. KIVA multi-zone (KIVA3V-MZ-MPI): *1 week* in 100 processor machine

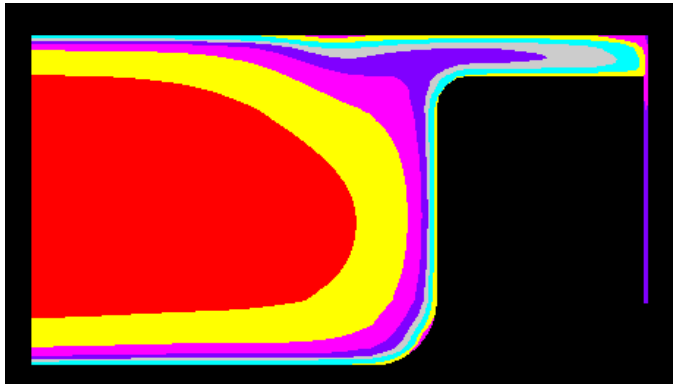


4. KIVA-sequential multi-zone cloud model: *1 day* in single processor computer

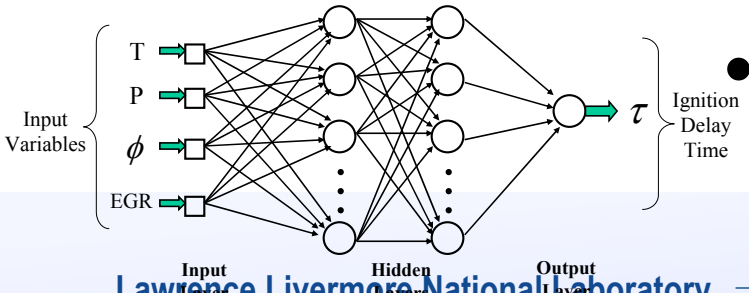
Summary: We continue to develop high fidelity HCCI and PCCI analysis techniques with greatly improved computational efficiency



- **Direct integration of KIVA and Chemkin**
  - **Years of computing time in single processor computer**



- **Multi-zone KIVA-Chemkin**
  - **Weeks of computing time in single processor computer**



- **KIVA-Artificial neural network**
  - **Hours of computing time in single processor computer**