Numerical Modeling of HCCI Combustion

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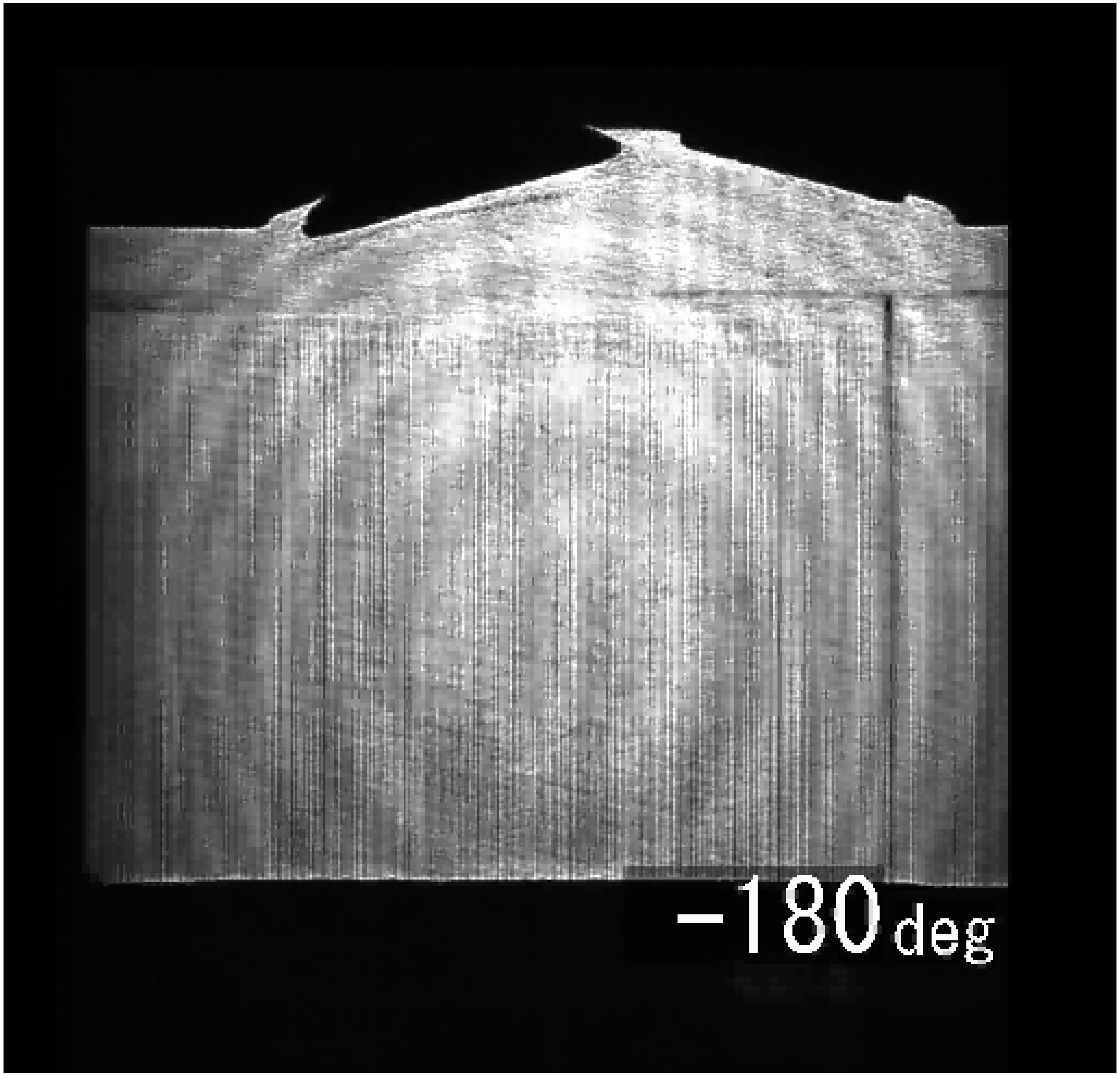
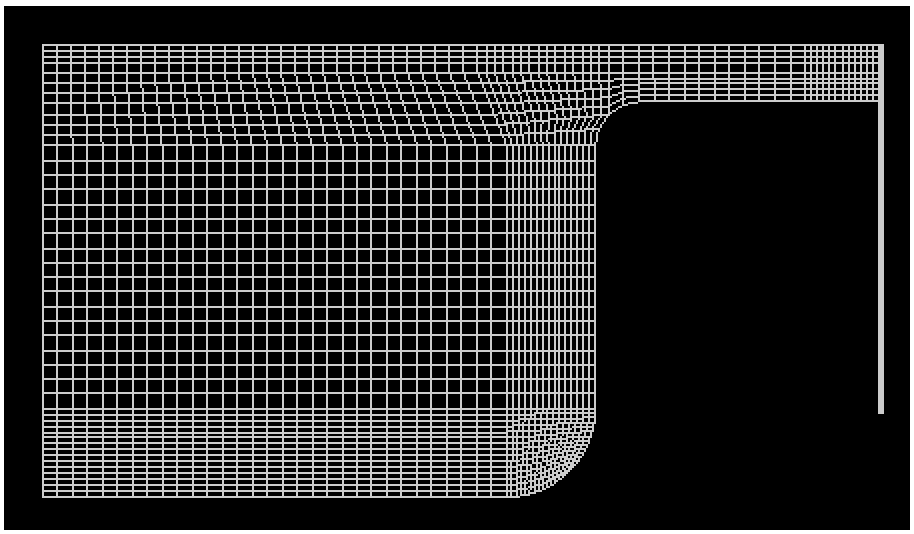
Homogeneous charge compression ignition (HCCI) combustion is an autoignition process controlled by chemical kinetics



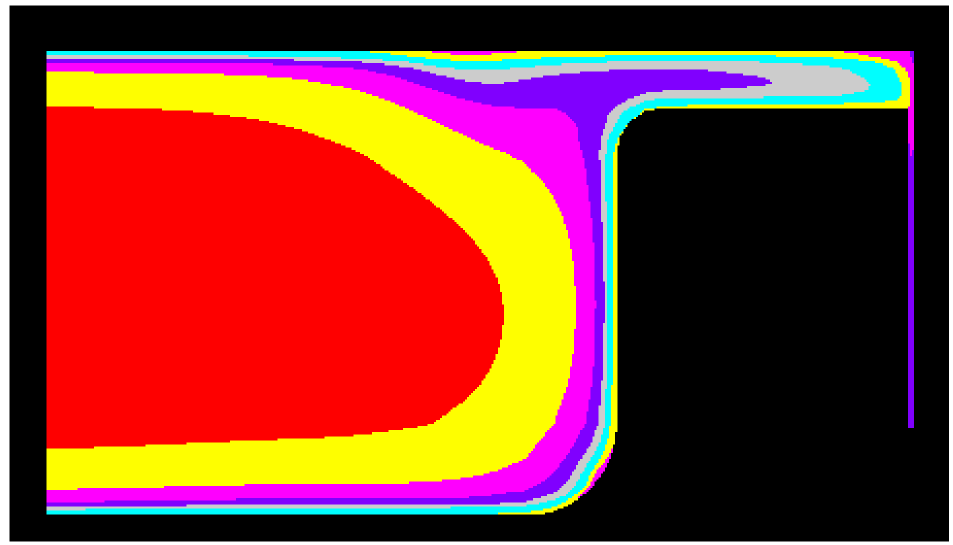
Courtesy of
Professor Yuuji
Ikeda, Kyoto
University

The physics of HCCI combustion can be well captured with a sequential fluid mechanics-chemical kinetics model

High resolution CFD simulation (10^5-10^6 cells)



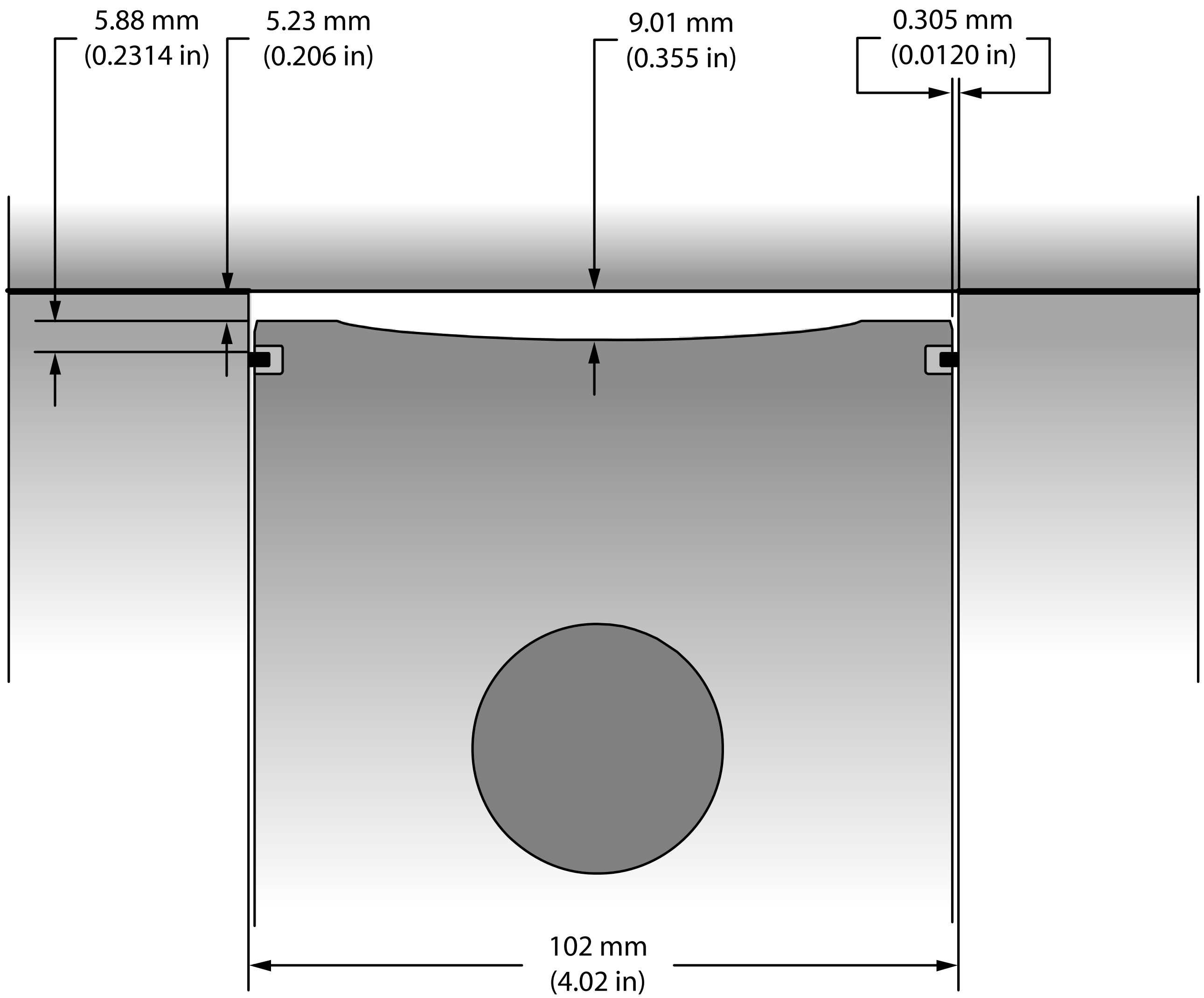
Lower resolution chemical kinetics discretization (10-100 zones)



Fluid mechanics sets the temperature distribution where autoignition occurs

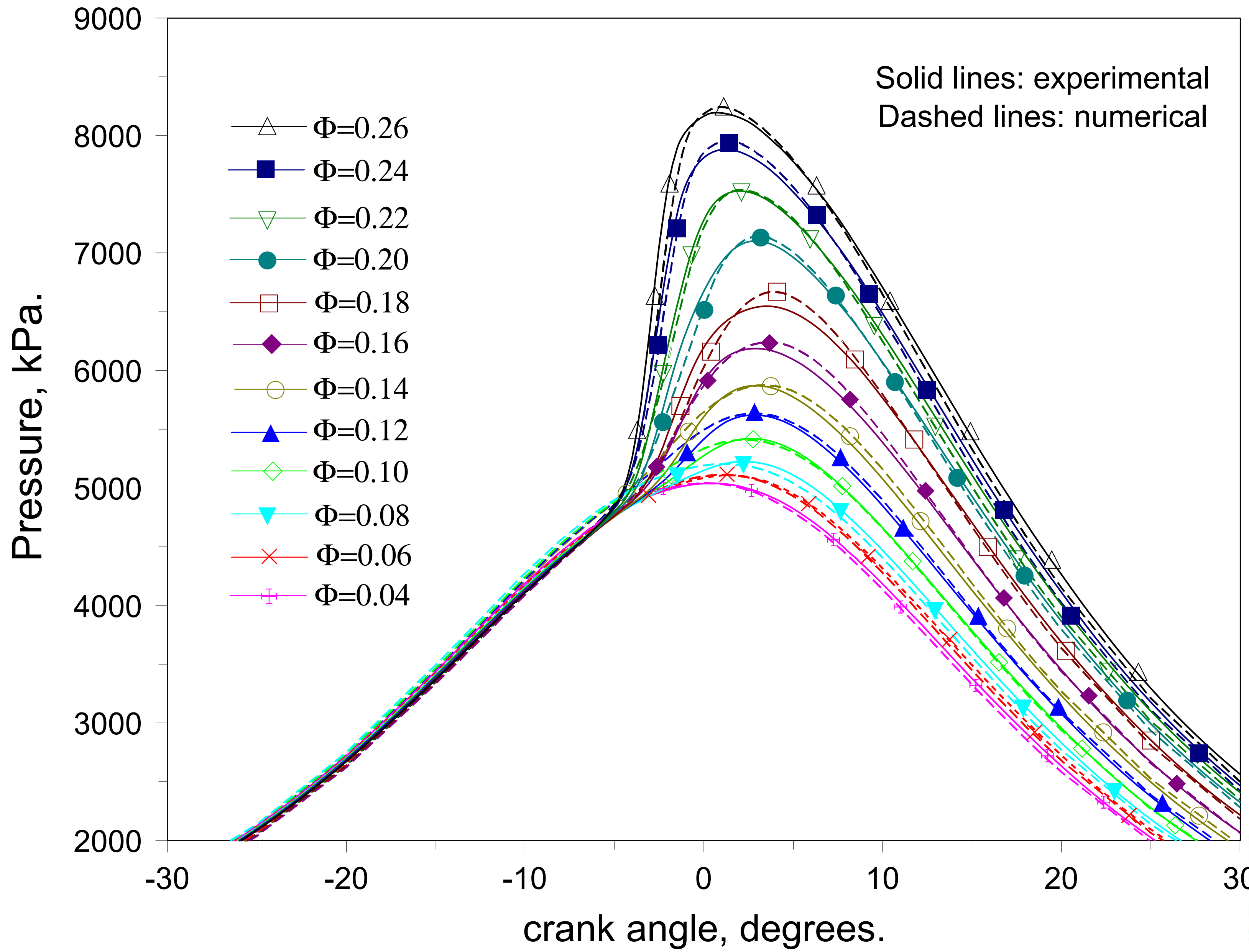
Combustion is very fast and therefore can be analyzed without considering mixing or turbulence

Application of the multi-zone model: Sandia engine running at low equivalence ratio with iso-octane

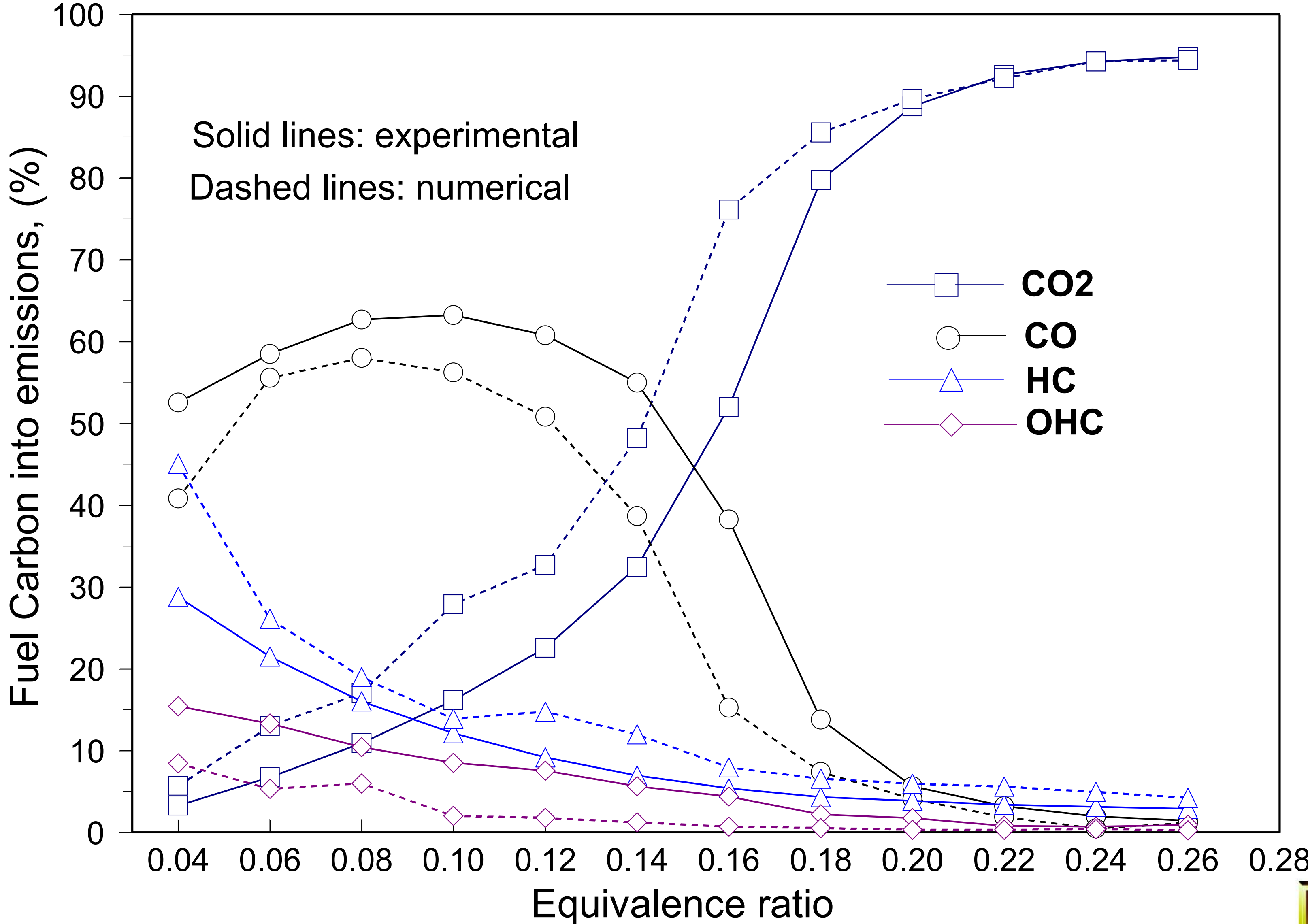


SAE Paper 2004-01-1910

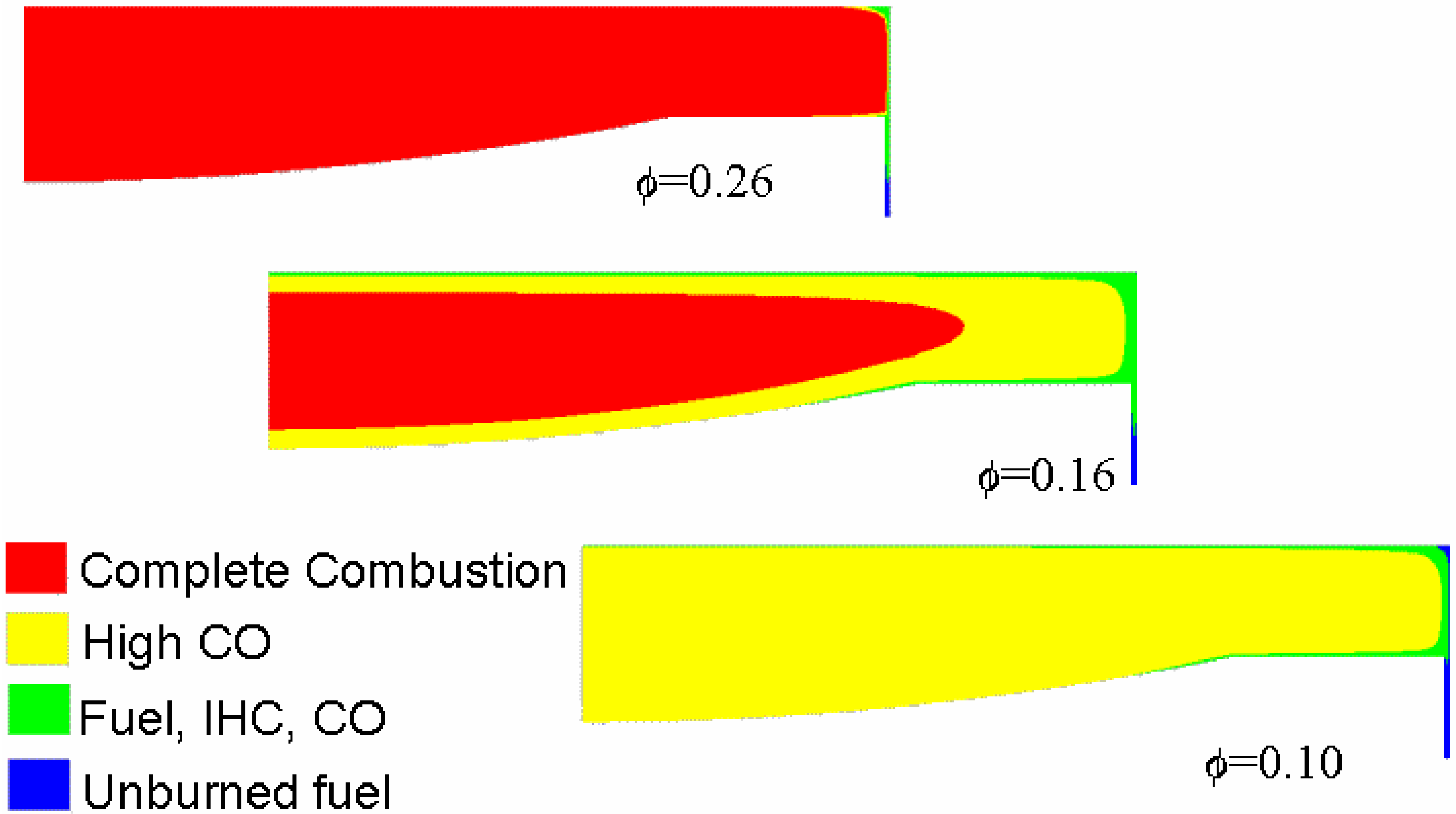
Multi-zone model accurately predicts pressure traces for multiple equivalence ratios from ultra lean to mid load



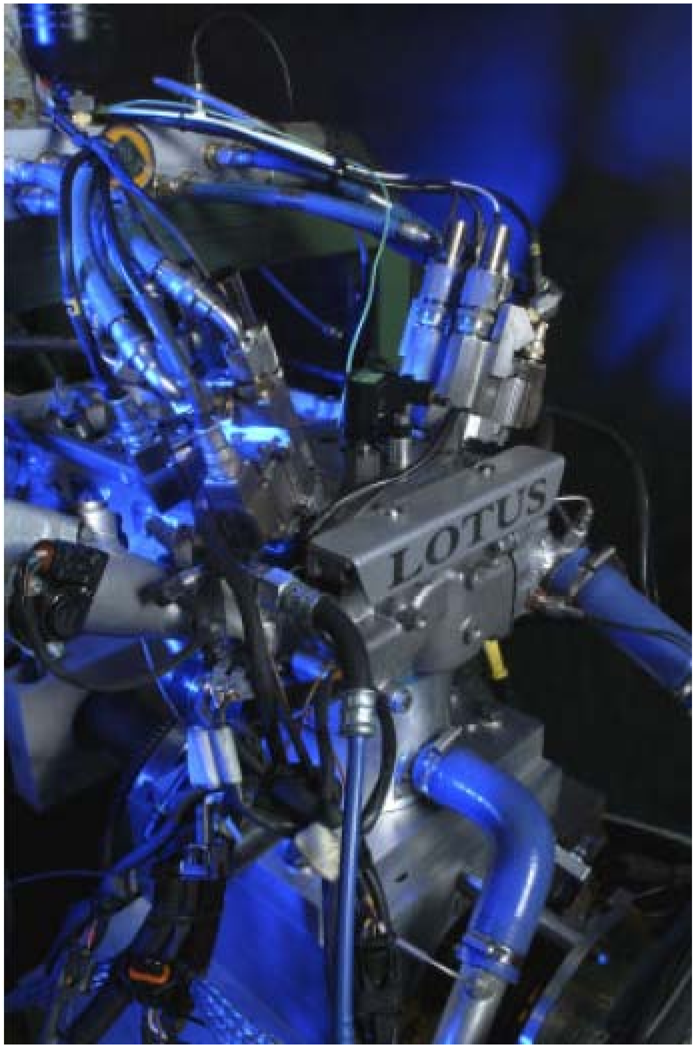
Multi-zone model makes good predictions of emissions over the full range of operation



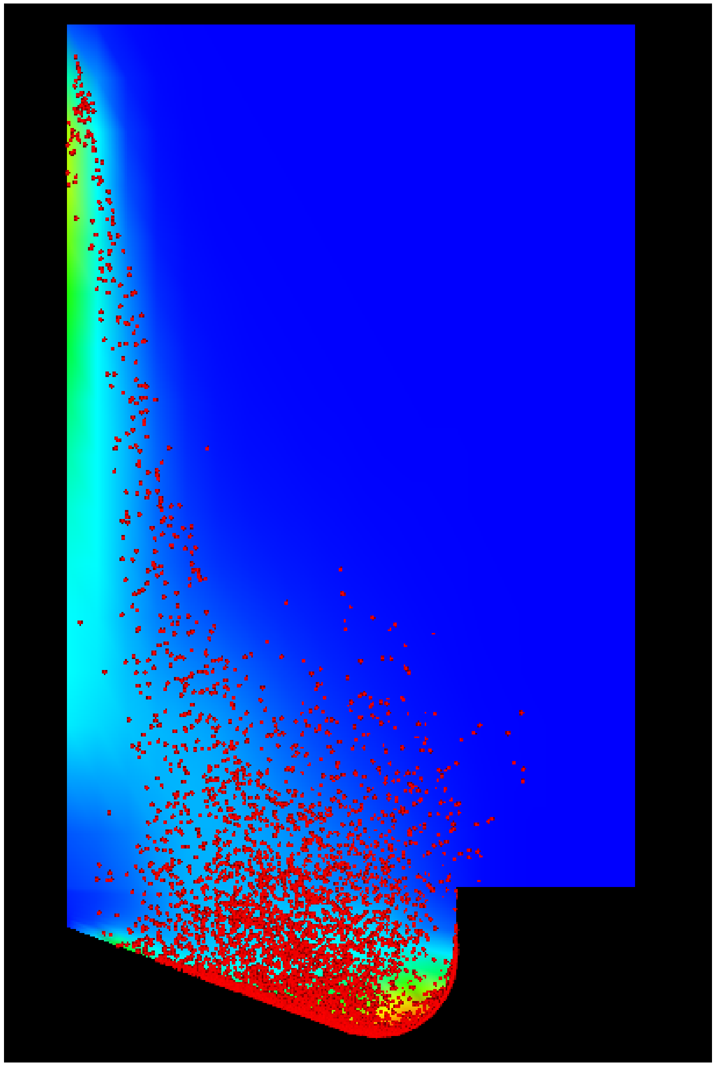
Model can tell us the location in the cylinder where different pollutants originate



Much interest exists on Premixed Charge Compression Ignition (PCCI) engines for high load and improved combustion control



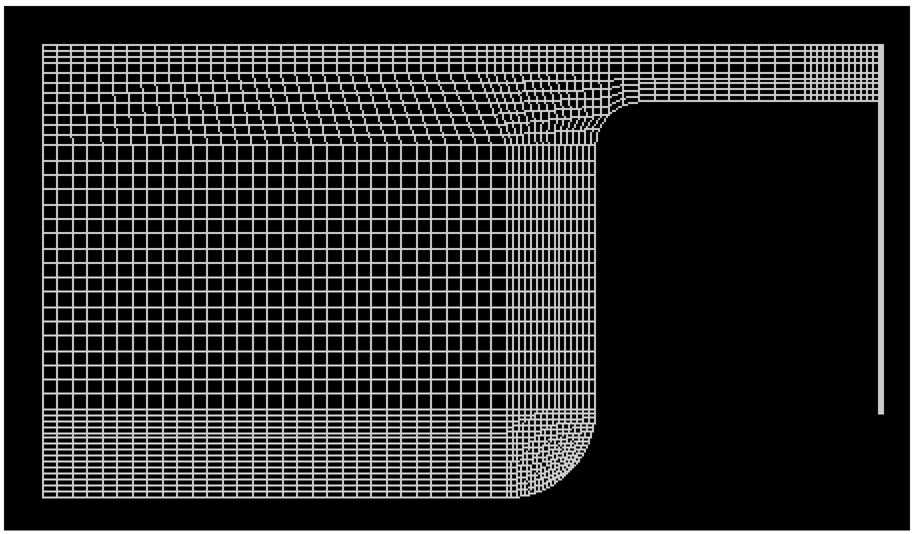
PCCI through high EGR that does not mix well with fresh charge (VVT CAI)



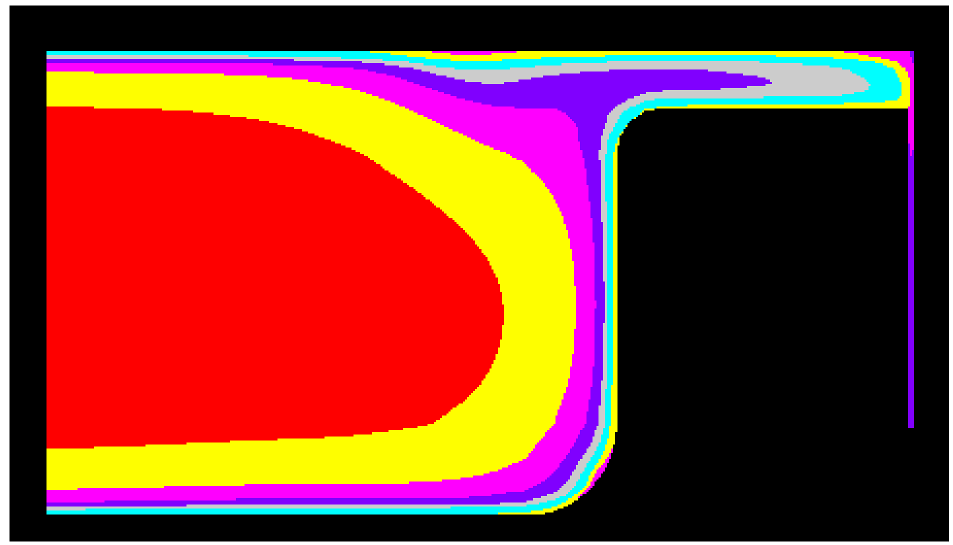
PCCI through early direct injection

Can we extend our sequential fluid mechanics-chemical kinetics model to model PCCI combustion?

High resolution CFD simulation (10^5 cells)



Lower resolution chemical kinetics discretization (10-100 zones)



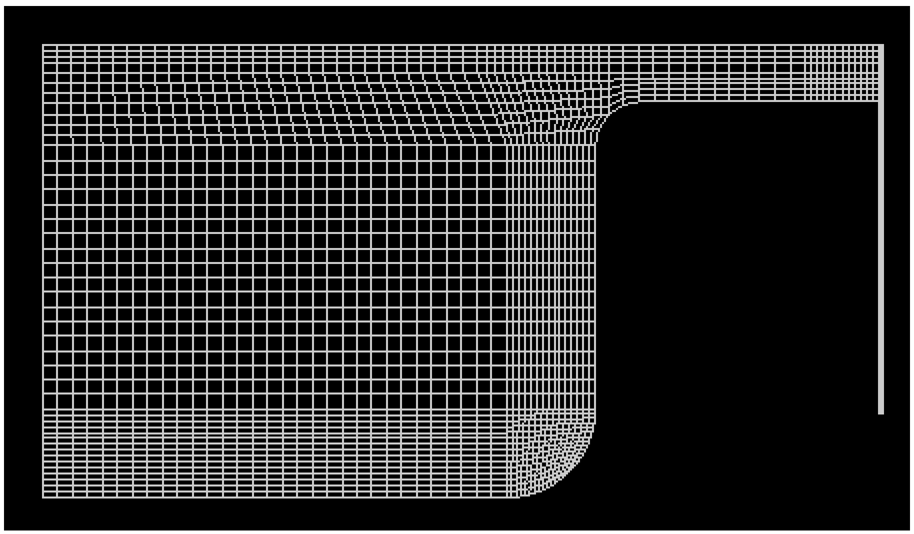
Fluid mechanics sets the temperature distribution where autoignition occurs

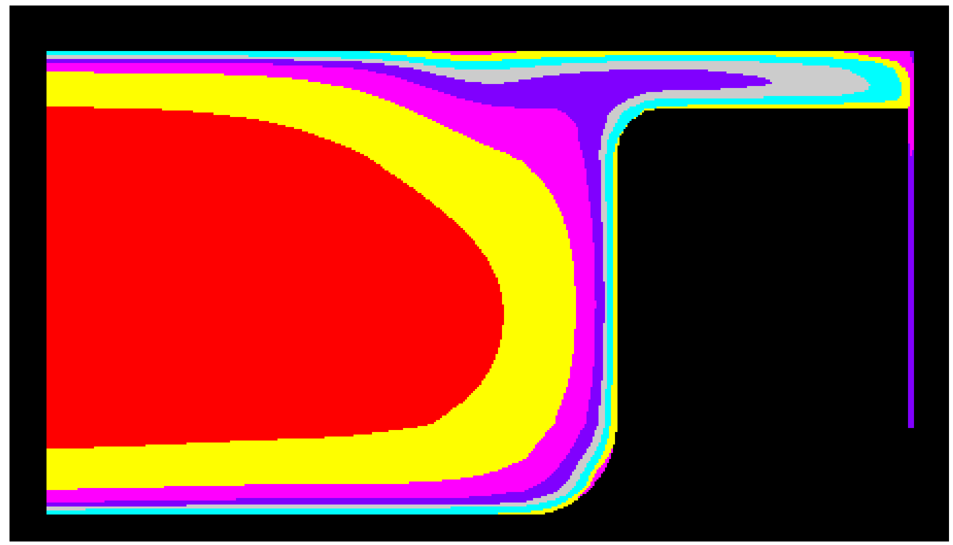
Combustion is very fast and therefore can be analyzed without considering mixing or turbulence

We can try analyzing PCCI by doing a two-directional mapping, from KIVA to CHEMKIN and from CHEMKIN back to KIVA

High resolution CFD solver handles mixing, advection and diffusion (~100k cells)

Chemistry handled by multi-zone detailed kinetics solver (10-100 zones)

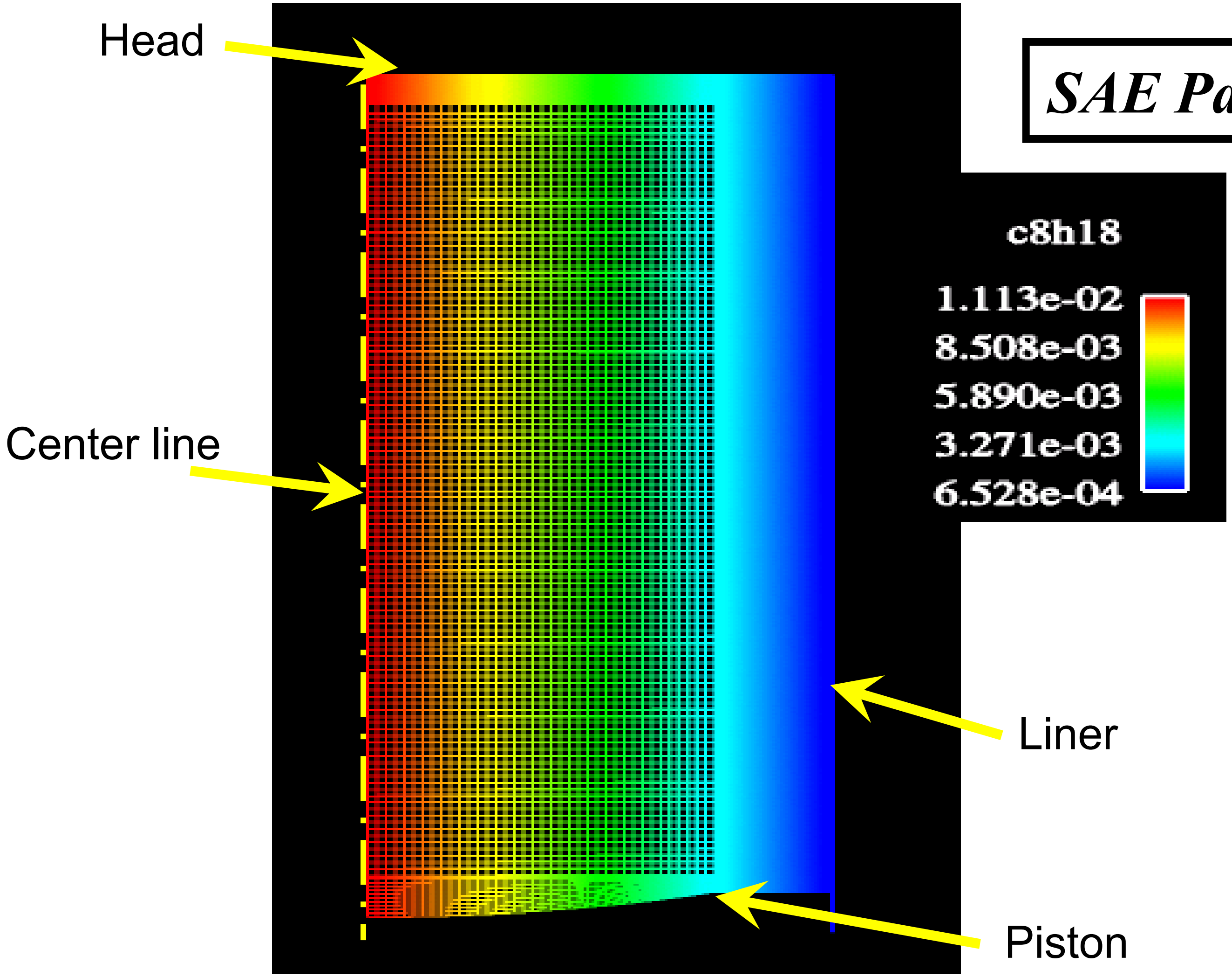




Solutions are mapped back and forth between solvers throughout the cycle

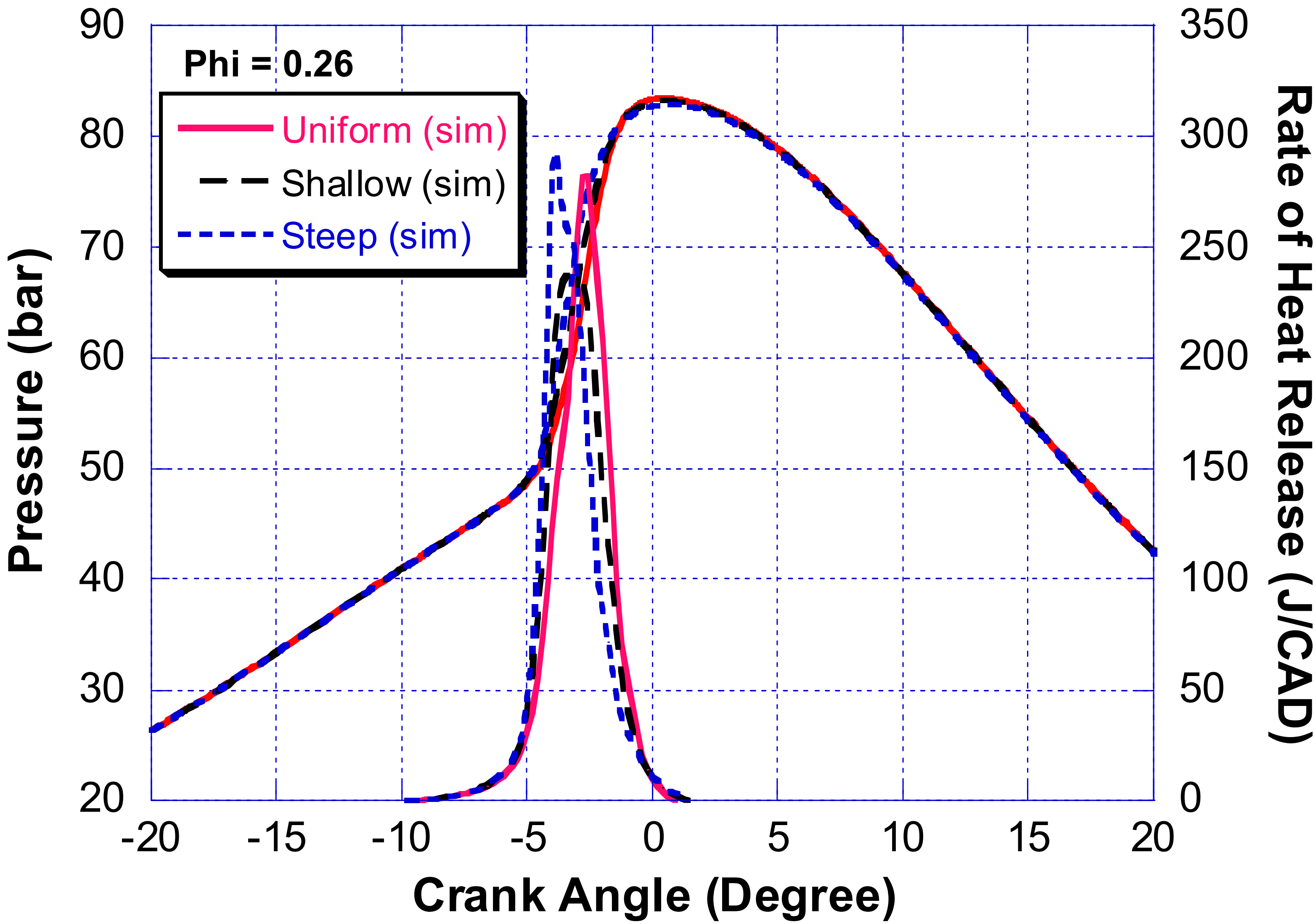
We have applied KIVA-MZ-MPI to analyze partially stratified combustion with a linear fuel distribution at intake valve closing

SAE Paper 2006-01-1363



Radial stratification imposed from centerline to liner: "Uniform," "Shallow," and "Steep"

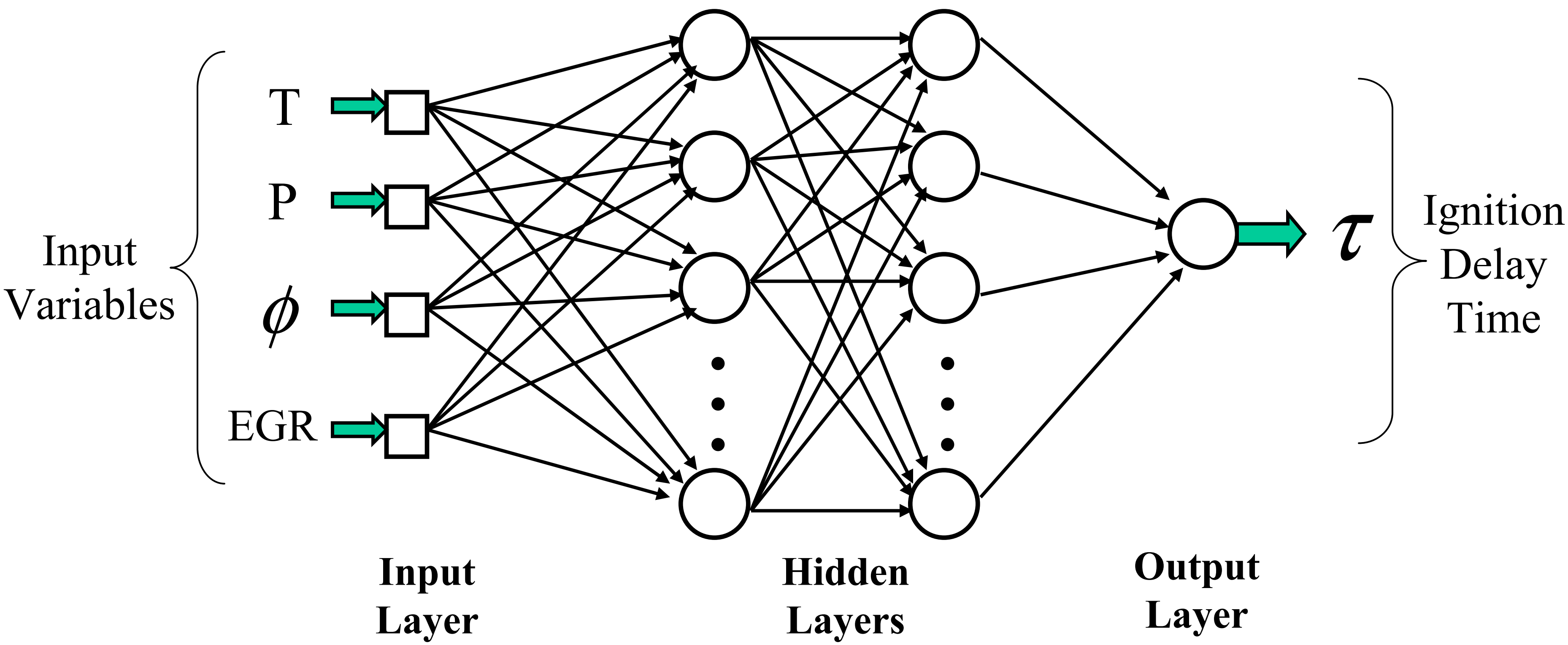
KIVA-MZ-MPI results compare well with the results from a full integration of KIVA and Chemkin



ϕ=0.26

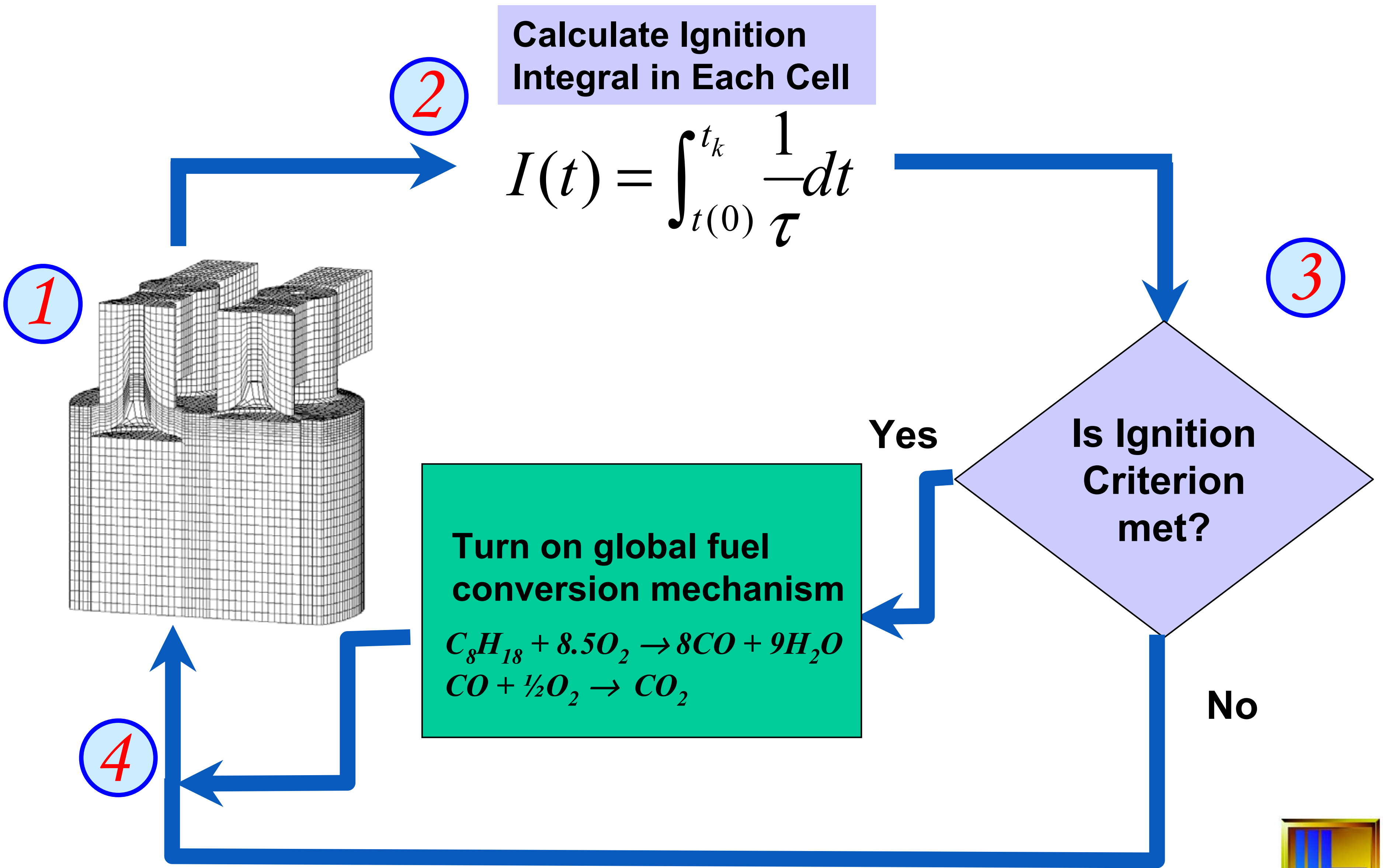
KIVA-MZ-MPI gives significant reduction in computational time, but still requires 1-2 days in 50-100 processors

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

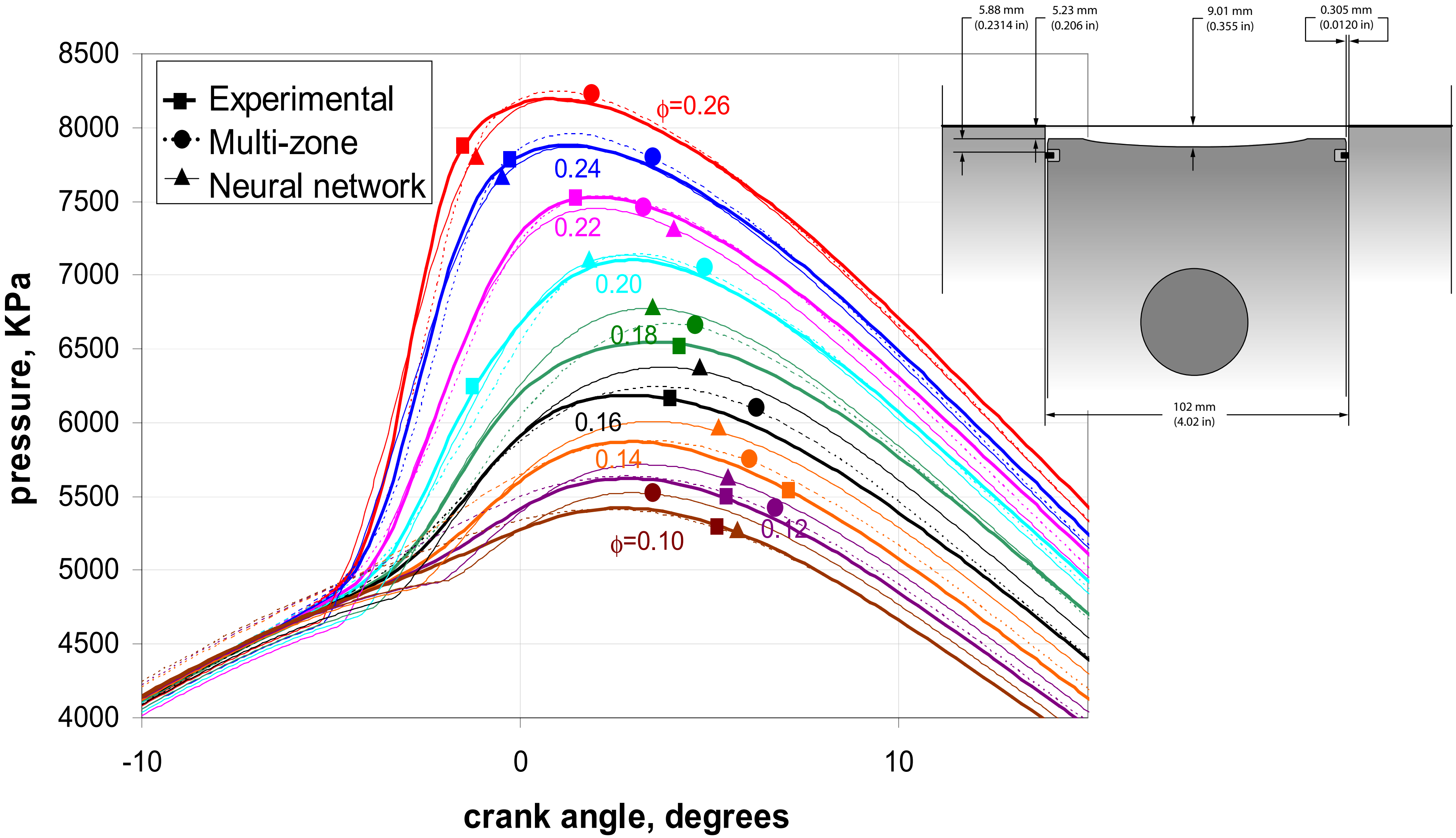


Ignition Condition: $$I(t) = \int_{t(0)}^{t_k} \frac{1}{\tau} dt = 1$$

KIVA3V-ANN greatly reduces computational intensity
Firing cases take ~10% more time than a motored run



Results agree well with experiments and multi-zone model over a wide range of conditions (geometry, ϕ, CR, intake pressure)

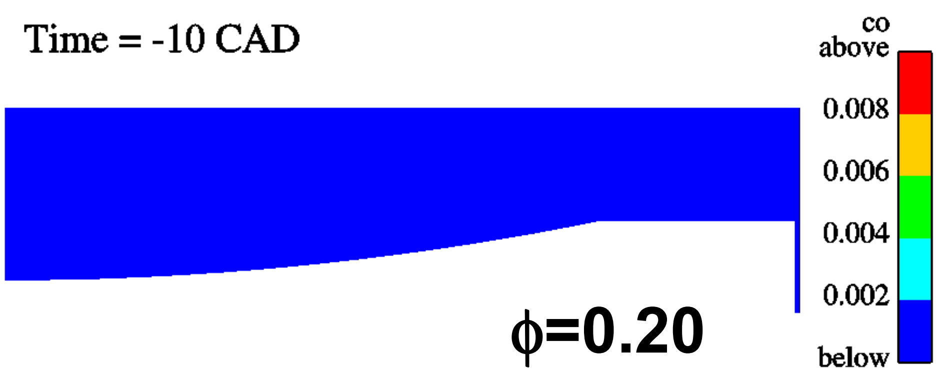


Data from Sandia Livermore, SAE 2003-01-0752,

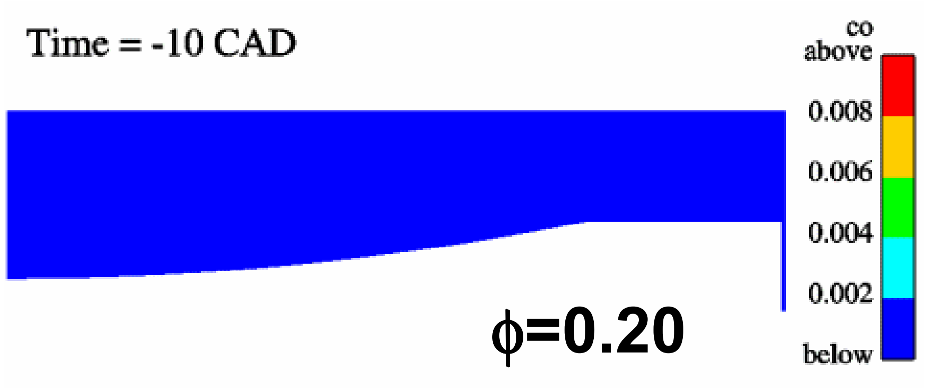
Scalloped piston, iso-octane, ϕ=0.1-0.26, CR=18:1, 120 kPa intake

KIVA3V-ANN predicts similar spatial evolution of combustion as KIVA3V-MZ-MPI for "normal" HCCI

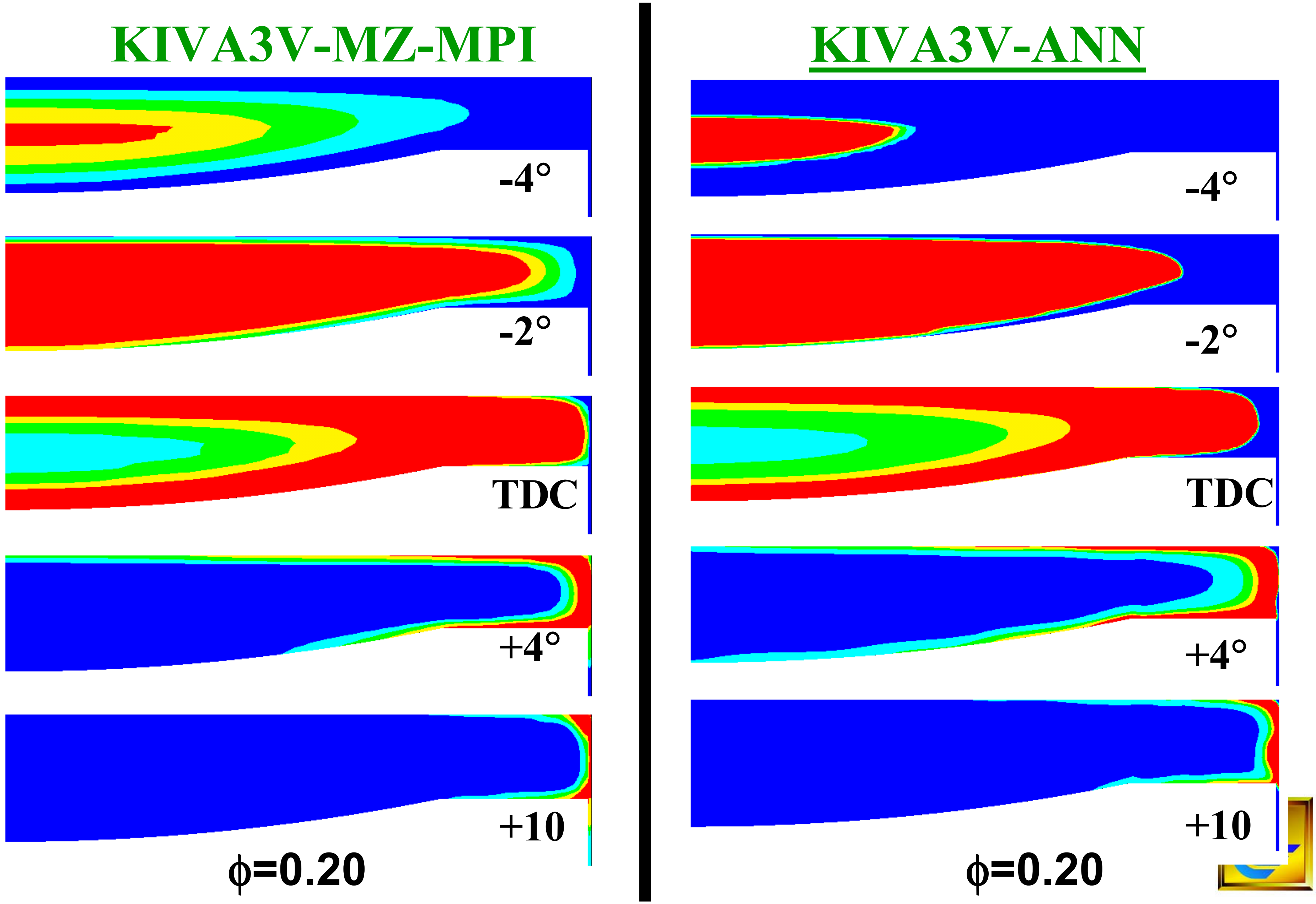
KIVA3V-MZ-MPI



KIVA3V-ANN

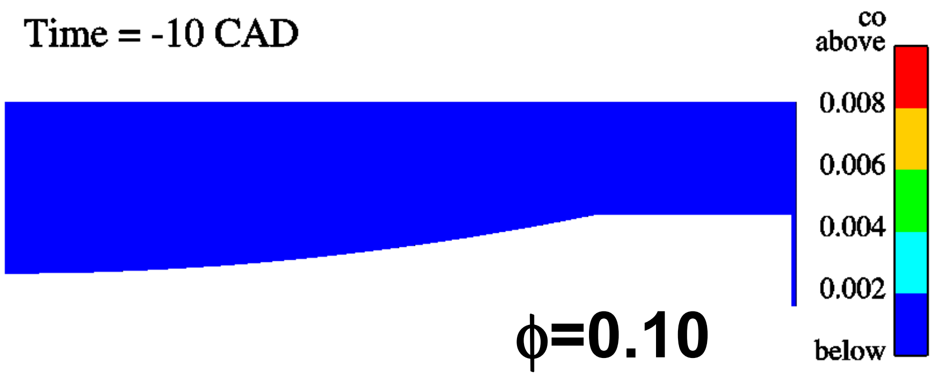


KIVA3V-ANN predicts similar spatial evolution of CO during combustion as KIVA3V-MZ-MPI for “normal” HCCI

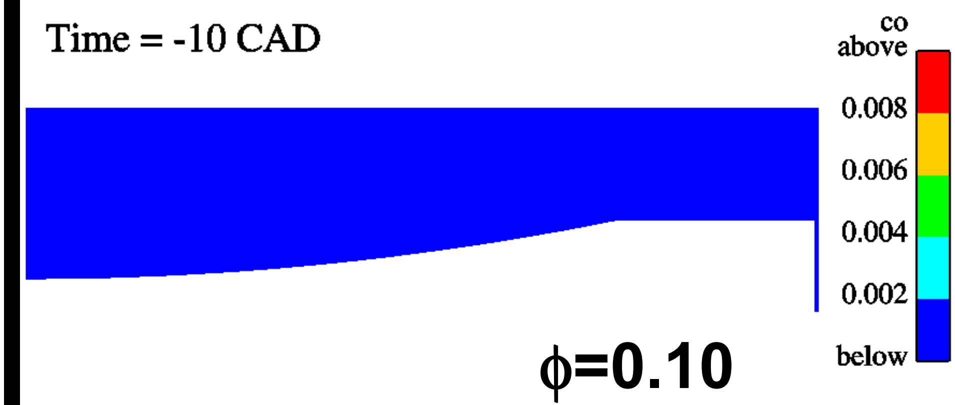


At ϕ=0.10, KIVA3V-ANN predicts high CO emissions because reaction mechanism misses the oxidation of CO in the central core

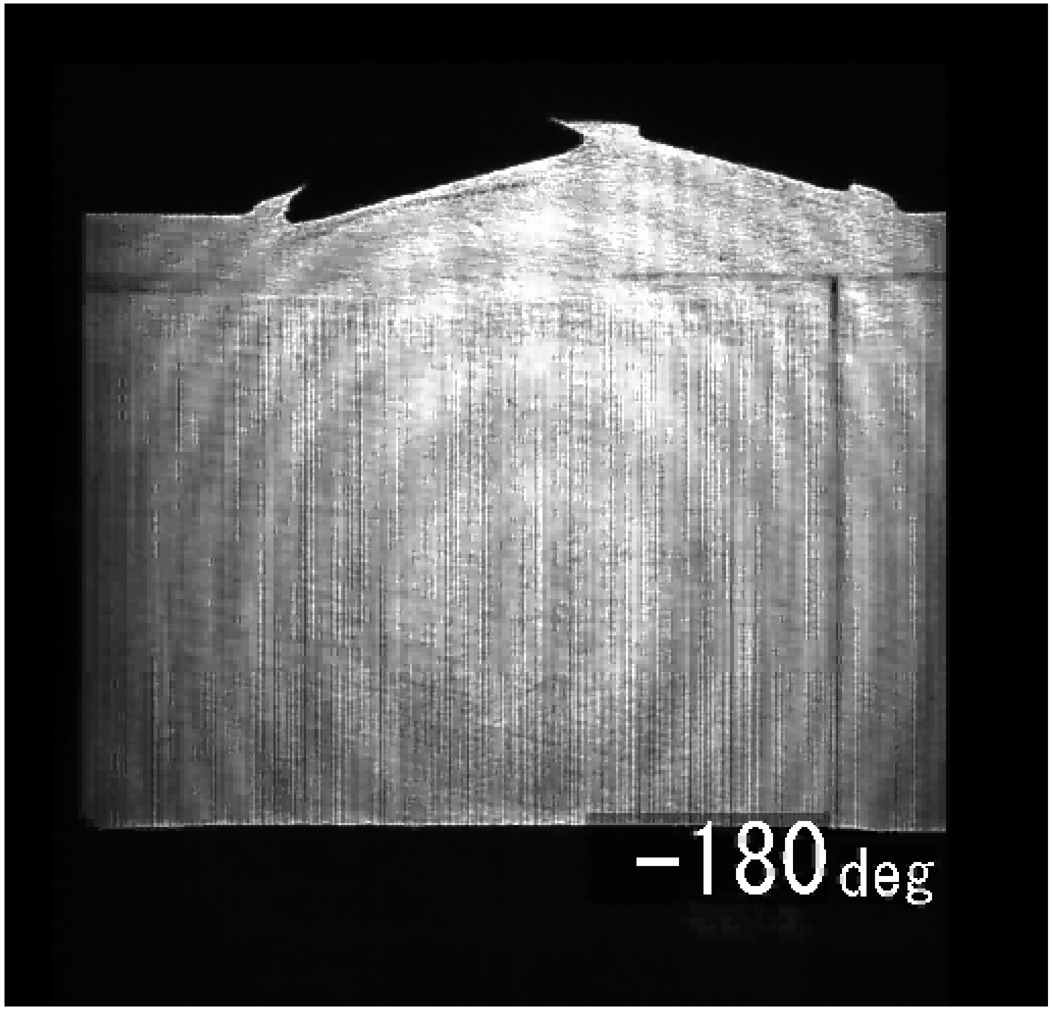
Kiva3v-MZ-MPI



Kiva3v-ANN



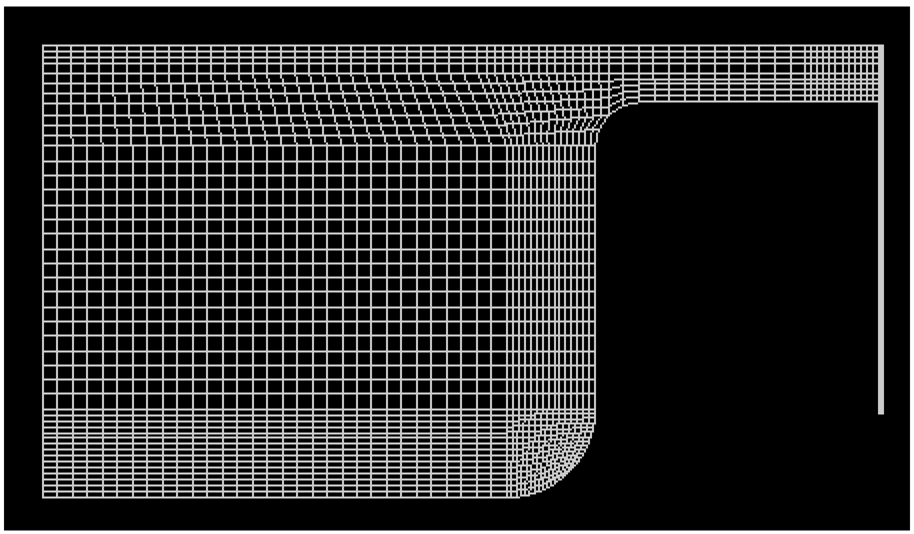
Summary: HCCI is dominated by chemical kinetics, and can therefore be well characterized by a computationally efficient segregated fluid mechanics-multi-zone chemical kinetics model

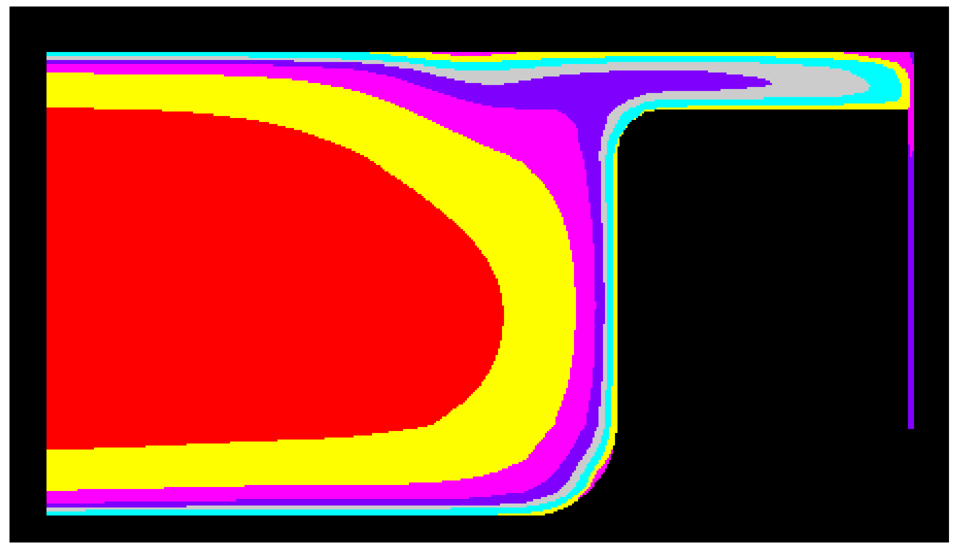


Summary: Our new fully integrated parallelized fluid mechanics-chemical kinetics code (KIVA3V-MZ-MPI) considers the effect of mixing and therefore applies to partially stratified combustion

High resolution CFD solver handles mixing, advection and diffusion (~100k cells)

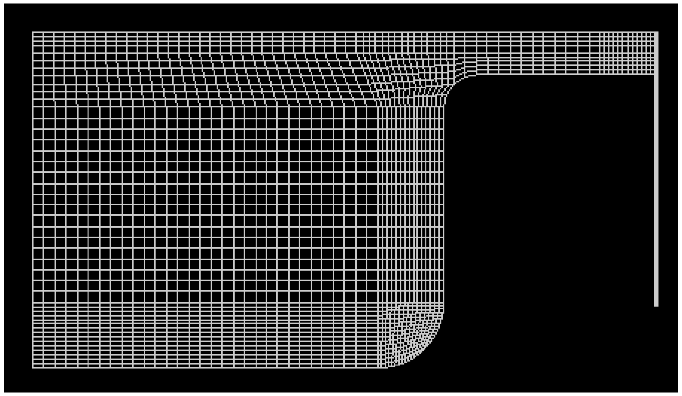
Chemistry handled by multi-zone detailed kinetics solver (10-100 zones)





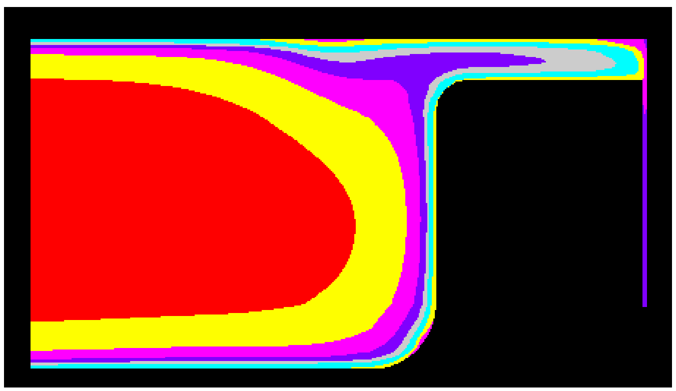
Solutions are mapped back and forth between solvers throughout the cycle

Summary: We are developing accurate HCCI and PCCI analysis techniques with greatly improved computational efficiency



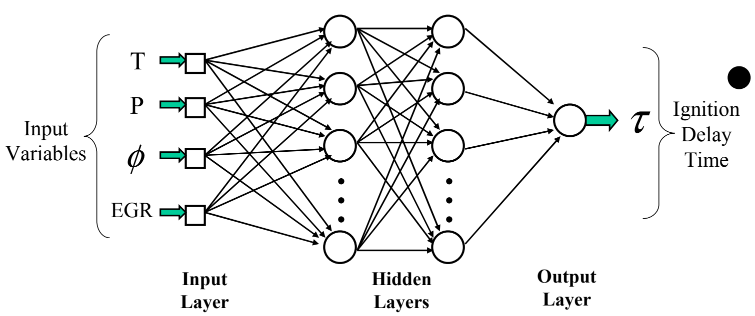
- **Direct integration of KIVA and Chemkin**

  Years of computing time in single processor computer



- **Multi-zone KIVA-Chemkin**

  Days of computing time in single processor computer



- **KIVA-Artificial neural network**

  Hours of computing time in single processor computer