Co-Optima Monthly Stakeholder Meeting

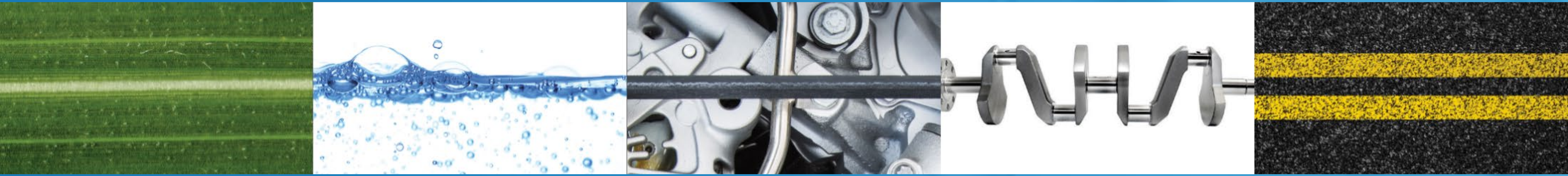
How Can New Simulations and Modeling Tools Accelerate Fuel-Engine Co-Optimization?

SIBENDU SOM – Argonne National Laboratory

October 26, 2021

CO-OPTIMIZATION OF
FUELS & ENGINES

better fuels | better vehicles | sooner



Overview

- Goals
- Models Developed
- Technical Approach
- Main Results
- Key Takeaways

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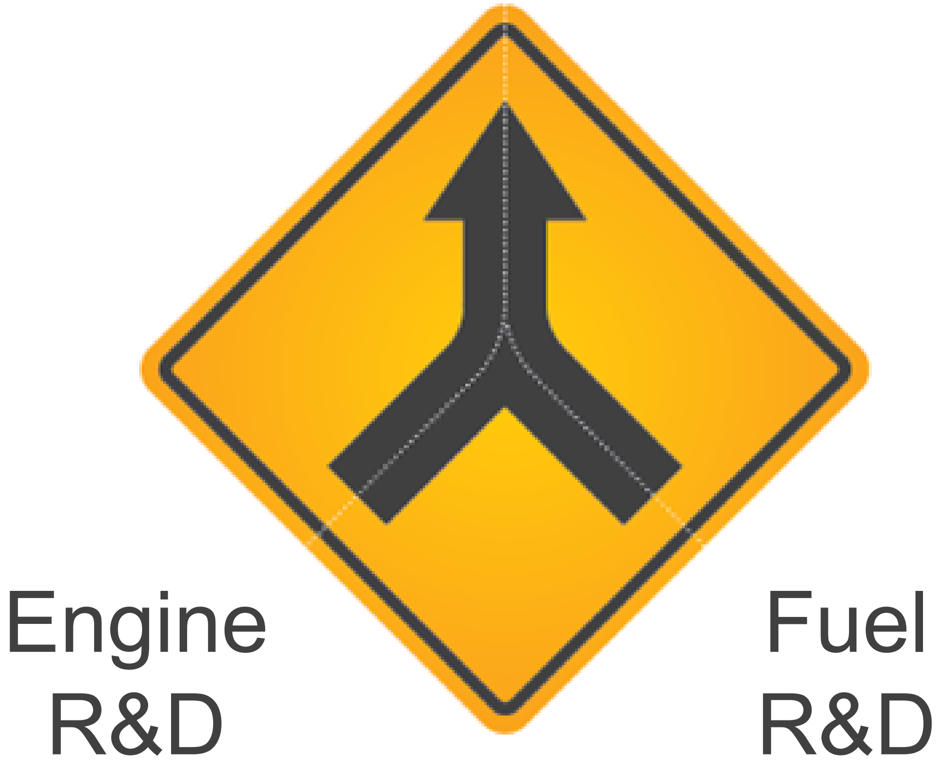
Better fuels. Better engines. Sooner.



On-road transportation from light-duty to heavy-duty

LIGHT-DUTY

- **Near-term:** Turbocharged spark ignition combustion
- **Longer-term:** Multi-mode combustion

MEDIUM / HEAVY-DUTY

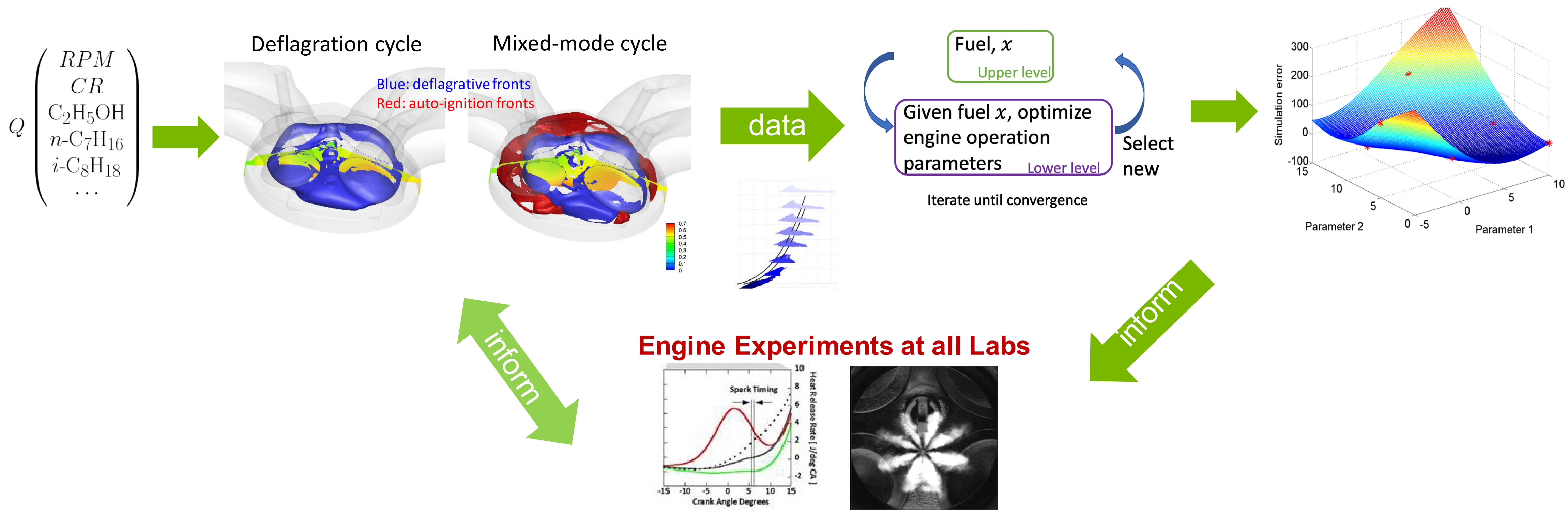
- **Near-term:** Conventional diesel combustion
- **Longer-term:** Advanced compression ignition

Toolkit Team goals

- Provide new insights on fuel-engine interactions through accurate computational fluid dynamic (CFD) calculations.
- Train lower fidelity yet accurate models that enable fuel-engine co-optimization leveraging high-performance computing (HPC) and machine learning (ML) acceleration techniques.
- Provide feedback to experimentalists to run new fuel-engine configurations for hypothesis testing and cross-validation.

Model Development and Validation

Optimization and Data Analysis Development

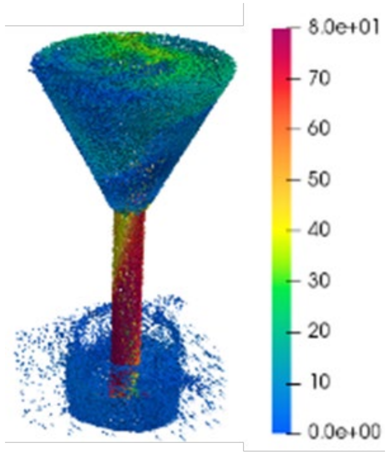


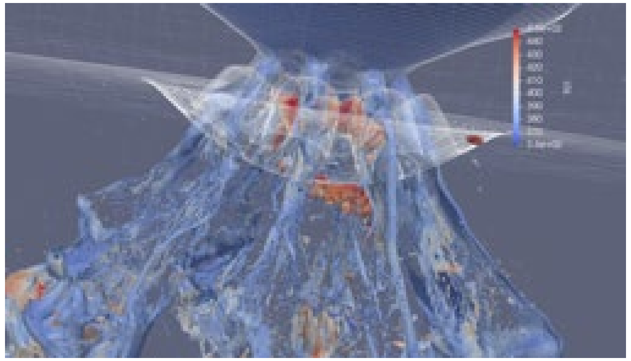
Toolkit Team

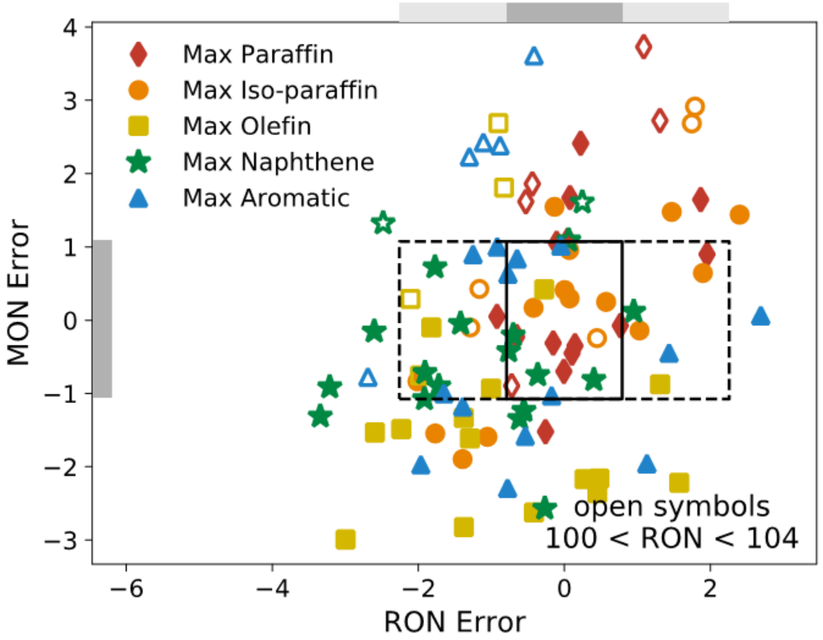
Lab	Team Members
LLNL	Matt McNenly, Nick Killingsworth, Simon Lapointe, Russell Whitesides
NREL	Shashank Yellapantula, Bruce Perry
SNL	Marco Arienti, Everett Wenzel
ORNL	Flavio Chauhy, Dean Edwards
LBNL	Juliane Mueller (TK Deputy)
ANL	Riccardo Scarcelli, Pinaki Pal, Chao Xu, Roberto Torelli, Hengjie Guo, Sayop Kim, Krishna Kalvakala, Ram Vijayagopal, Sibendu Som (TK Lead)

Tools developed leveraging HPC

- New multi-phase flow models: flash-boiling, nozzle flow-spray coupling, multicomponent film vaporization, ducted fuel injection.
- New ignition/combustion models: robust combustion model for traversing through different combustion regimes, flame quenching, pre-spark heat release, pre-chamber flows.
- Neural network for octane prediction from the detailed Co-Optima mechanism (~3,000 species).
- Laminar flame-speed solver for detailed Co-Optima mechanism (several orders of magnitude speedup over Chemkin-Pro).
- Chemkin-Pro engine model for spark-assisted compression ignition (SACI) multimode operation accelerated by 40x using Zero-RK to allow 50,000 fuel blends to be evaluated. Coupled with bilevel optimization.







CFD-driven analysis of fuel-engine interactions

CFD

Fuel

Multicomponent fuel surrogates
Fuel physical properties
(viscosity, density, HoV, etc. vs. T, P)
Fuel thermochemistry
(~ $O(10^3)$ species, $O(10^4)$ rxns)
Reduced kinetic mechanisms
(~ $O(10^2)$ species, $O(10^3)$ rxns)

Ignition delay (τ_{ig})
Laminar flame speed (S_L)
ϕ sensitivity
RON/MON

Physical Submodels

Spray dynamics
(Breakup, evaporation, etc.)
Wall heat transfer
Turbulent mixing
Turbulent combustion
(flame propagation, autoignition)
Computational efficiency

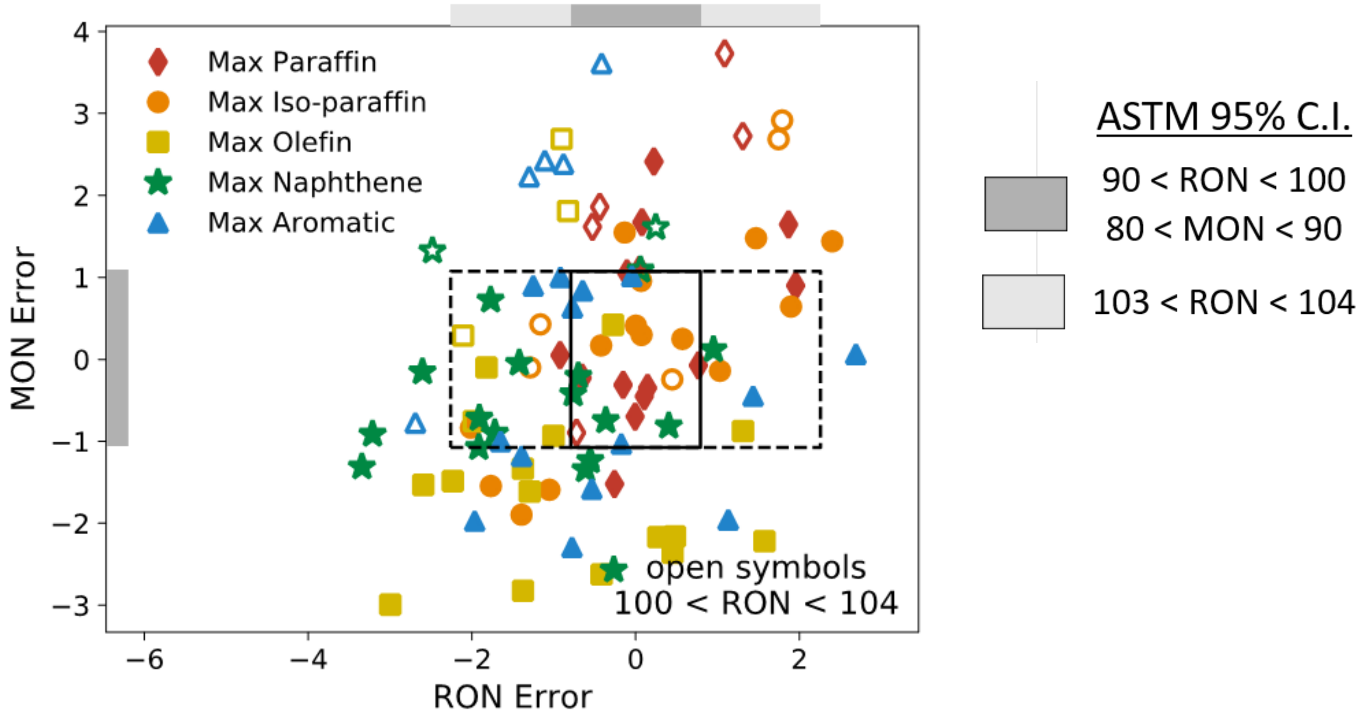
Engine

Real geometry
Combustion mode
(SI, SACI, HCCI, GCI, MCCI)
Operating conditions
(speed, load, etc.)
Boundary conditions
Experimental data

APPROACH Neural network octane prediction model

- Neural network model uses detailed chemical kinetic ignition calculations with fuel properties to predict research octane number (RON) and motor octane number (MON).
- Improved prediction of non-linear blending for high performance fuels.
- Blind predictions made for six high-performance fuel (HPF) blendstocks mixed with 5 new blendstocks for oxygenate blending (BOBs) with a matched octane rating.

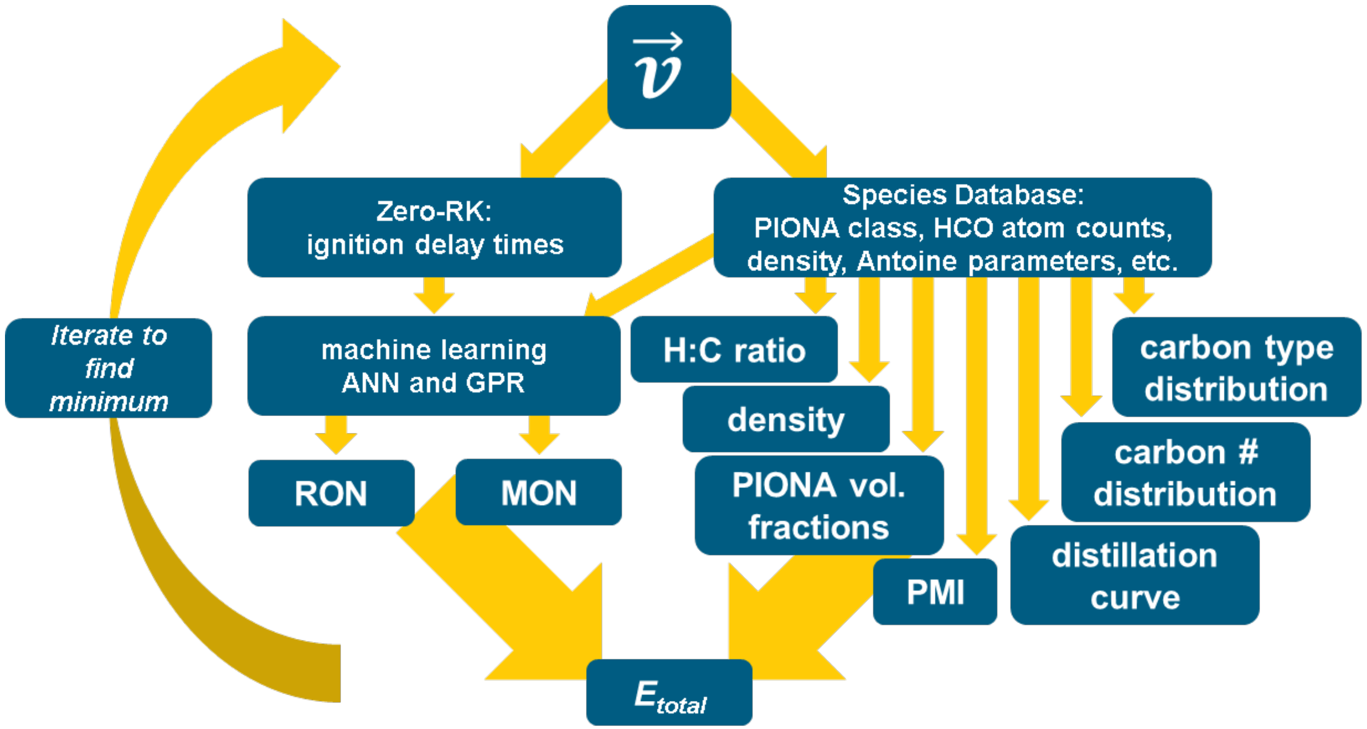
M. McNenly et al. (LLNL)



Neural network performance on 95 new HPF + BOB blends
Mean Abs Error: 1.1 RON and 1.2 MON

RESULTS Automated surrogate fuel designer

- Fuels can be readily designed to match +30 experimental and numerical tests to assess gaps and sensitivities in predictive models.
- A posteriori evaluation of additional key fuel properties:
  - Heat release measurements for rapid compression machine (RCM) and homogeneous charge compression ignition (HCC) engine.
  - Flame speeds.
  - Liquid properties (viscosity, surface tension, enthalpy of vaporization, thermal conductivity).



ANN = artificial neural network
GPR = gaussian process regression

$\vec{v}$ = vector of targets
E_{tot} = total error of objective function
PMI = particulate matter index

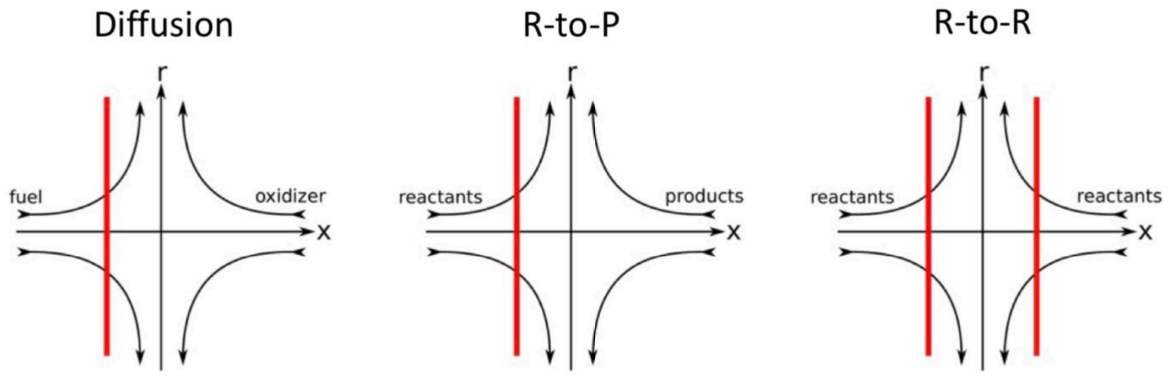
M. McNenly et al. (LLNL)

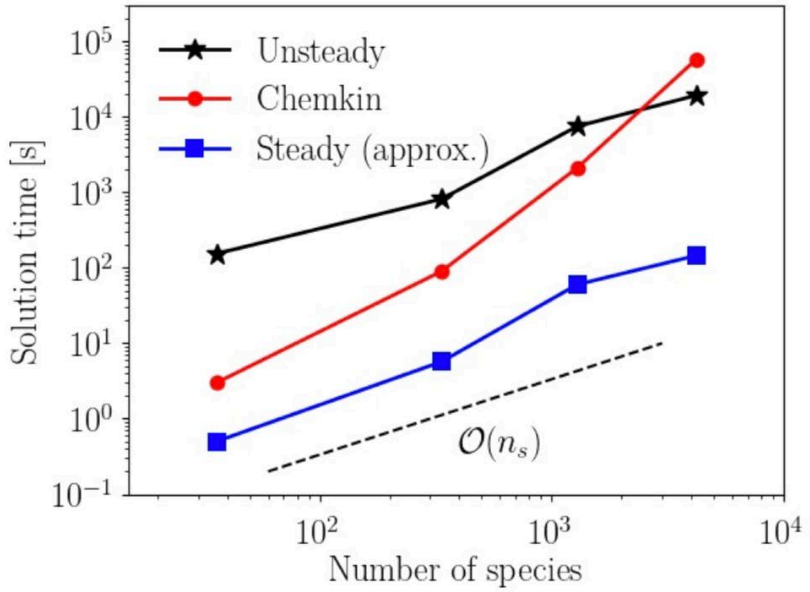
RESULTS

Zero-RK allows virtual fuel exploration and mechanism development

- New models created for: laminar flame speed, counterflow diffusion, perfectly stirred reactors, micro-liter fuel tester, and multi-zone engines.
- Enables previously unattainable computations of flame speeds and extinction strain rates with detailed Co-Optima mechanism (>4000 species).

M. McNenly et al. (LLNL)





Zero-RK

Available at https://github.com/LLNL/zero-rk

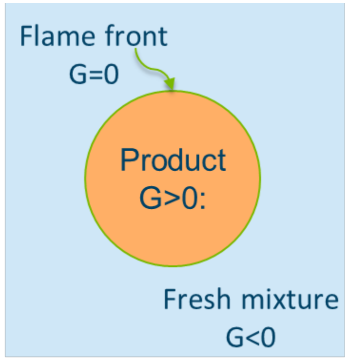
APPROACH Predictive CFD model for SACI engines

CFD model developed and validated for SACI multimode engine.

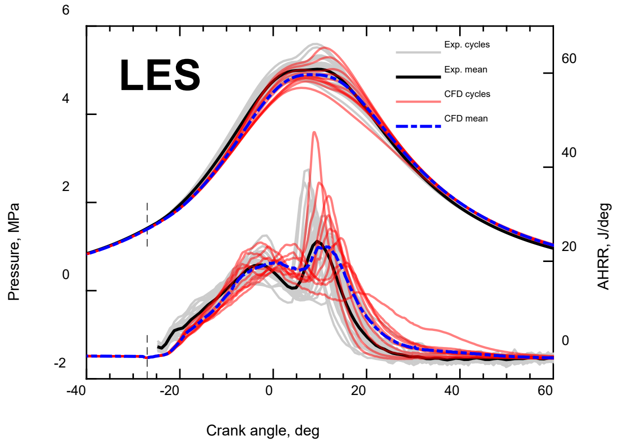
- Hybrid G-equation/finite rate chemistry combustion model with tabulated flame speed to predict flame propagation and end-gas auto-ignition simultaneously.
- Large eddy simulation (LES) to capture cycle-to-cycle variation.
- Model validated against first-principles simulations (DNS) and Sandia direct-injection spark-ignition (DISI) optical engine data for both well-mixed (WM) and partial fuel stratification (PFS) assisted SACI operations.

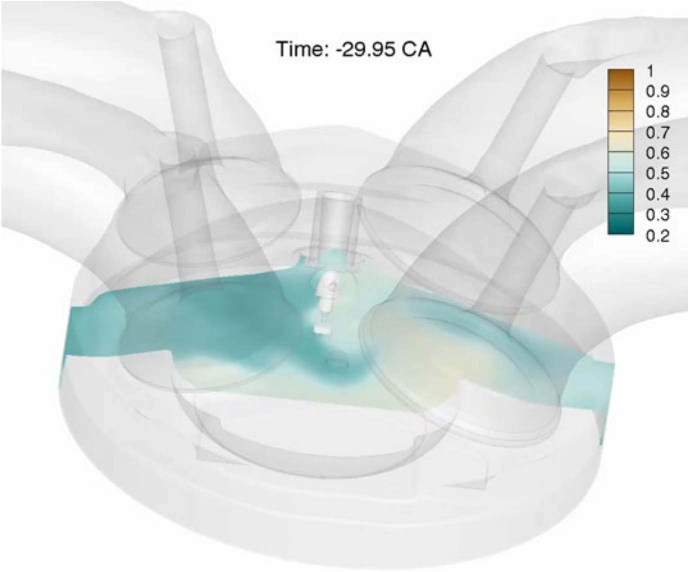
Chao Xu, Sibendu Som (ANL)
Experimental data: Magnus Sjoberg (SNL)

Hybrid combustion model



Pressure and AHRR





Mixing and combustion dynamics predicted by LES

Isosurfaces: Purple: stoichiometric
Blue: flames; Red: auto-ignition

VALIDATION

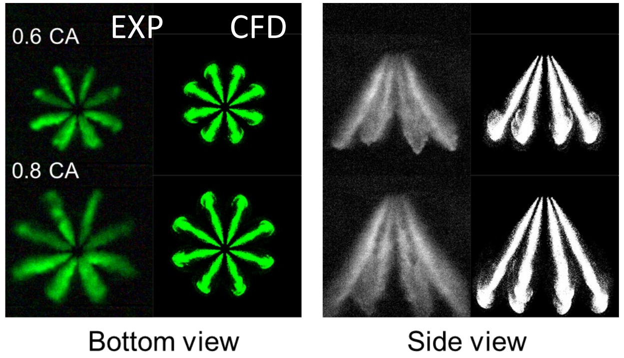
Capabilities in capturing detailed spray, flame structures, and emission

Unique capabilities of the model to capture rich physics in multi-mode SACI engine.

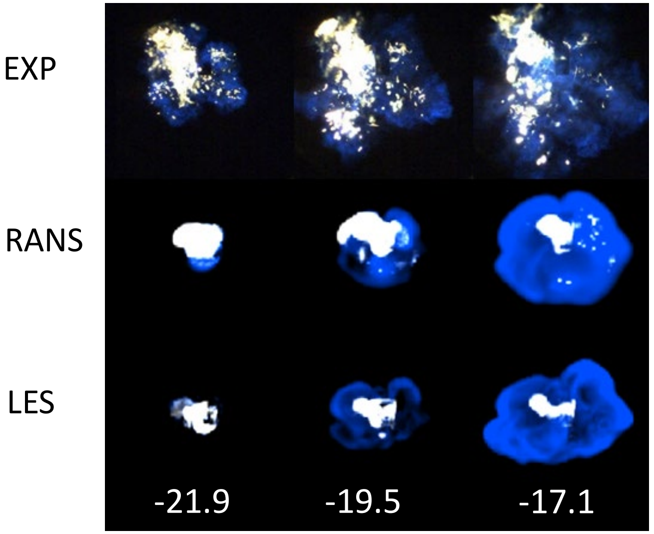
- Reliable spray prediction and validation.
- Detailed flame structure transitioning from diffusion to premixed flames revealed.
- Magnitude and sensitivity of nitrogen oxide (NOx)emission to engine operation mode well captured by detailed chemistry-based NOx model (empirical Zeldovich model fails).

Chao Xu, Sibendu Som (ANL)
Experimental data: Magnus Sjoberg (SNL)

Spray patterns in PFS-SACI

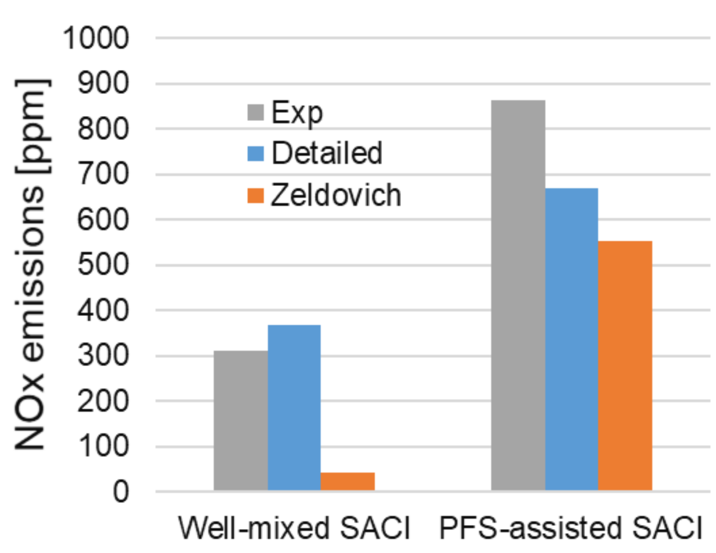


Flame structure in PFS-SACI



Bright: Diffusion flame; Blue: Premixed flame

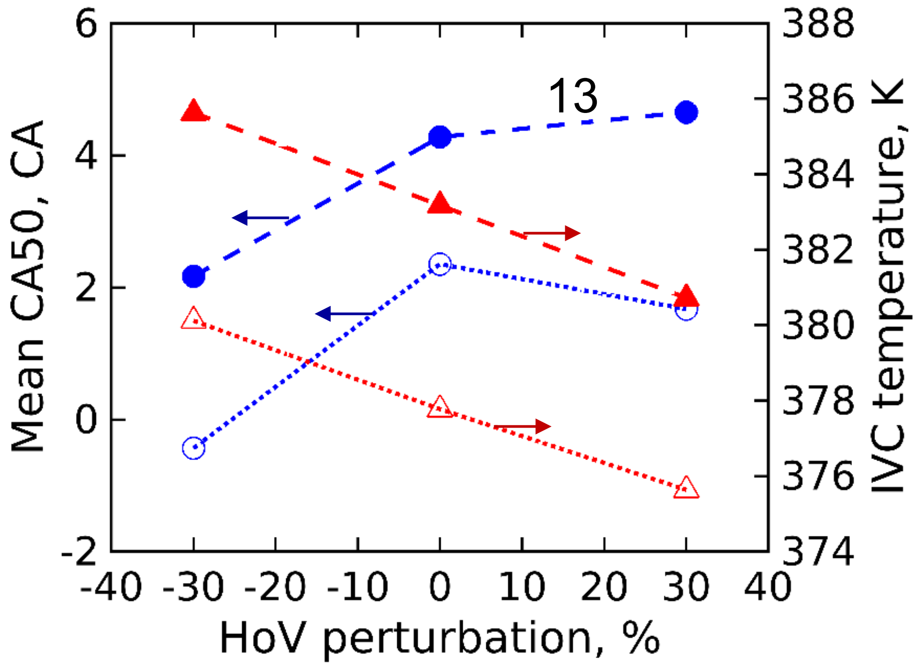
NOx emission in WM- vs. PFS-SACI



Fuel property sensitivity - SACI

- Heat of vaporization (HoV) plays modifies unburned gas temperature and thus combustion phasing; **HoV sensitivity of PFS operation is comparable with well-mixed charge operation.**
- Laminar flame speed (S_L) directly controls initial ramp-up of heat release rate in deflagration and thus affects subsequent auto-ignition; **PFS operation is more tolerant to S_L changes.**

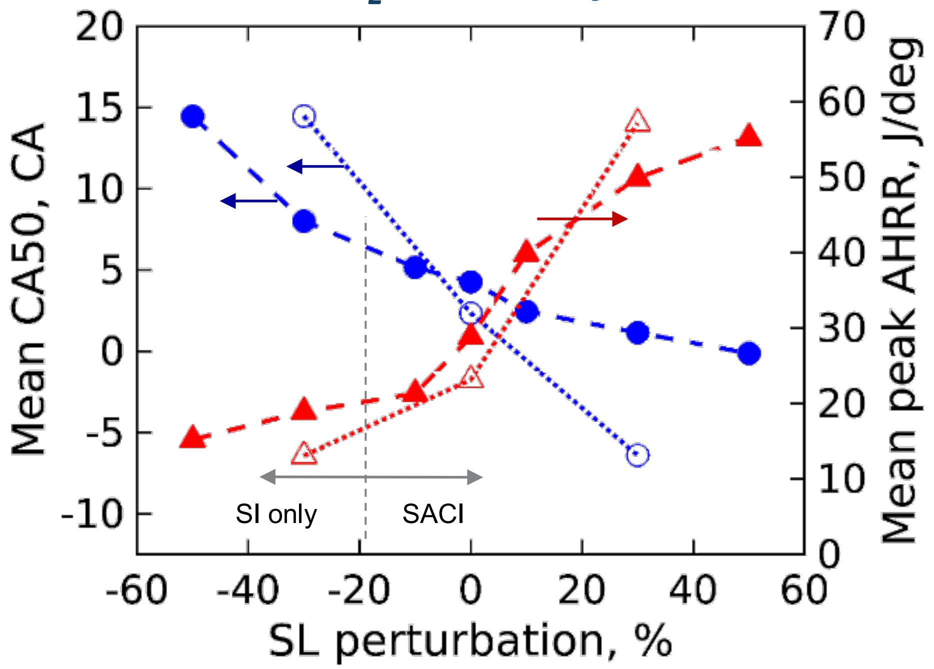
HoV sensitivity



Closed cymbols:
PFS-SACI
(ϕ: 0.5, ST: -27 °CA)

Open symbols:
well-mixed SACI
(ϕ: 0.55, ST: -57 °CA)

S_L sensitivity

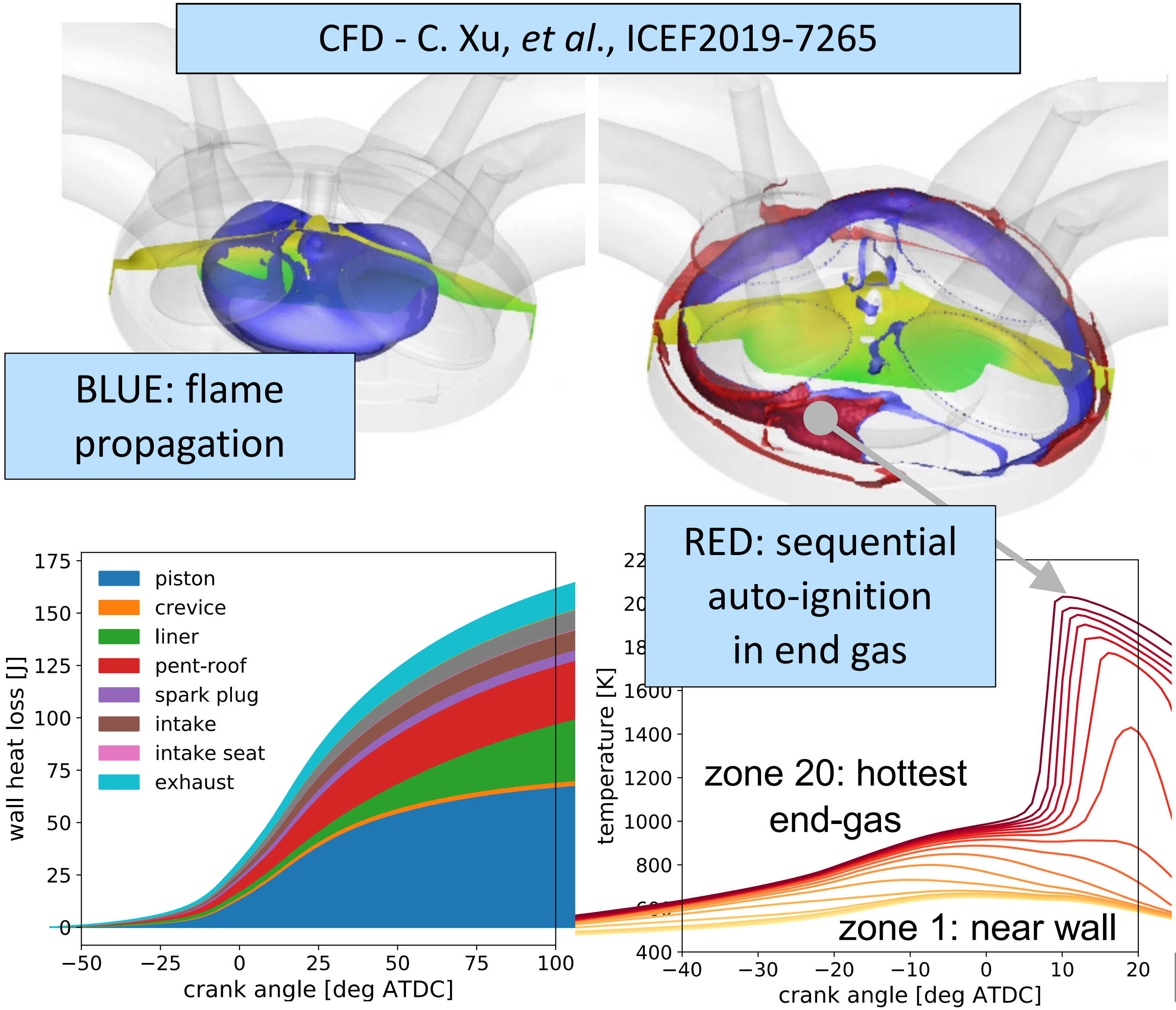


Chao Xu, Sibendu Som (ANL)

Zero-RK engine model trained with CFD and experiments for big co-optimization searches

- Zero-RK models trained with detailed CFD can evaluate the engine-fuel effects of a virtual blend in minutes for multimode and ACI operation.
- New features added:
  - Flame propagation from experiment, CFD, or neural network.
  - Modified heat transfer and species mixing correlations possible with CFD turbulent properties .
  - Multiple wall temperatures to capture hot spots.
  - Evaporative charge cooling.

M. McNenly et al. (LLNL), Chao Xu (ANL)

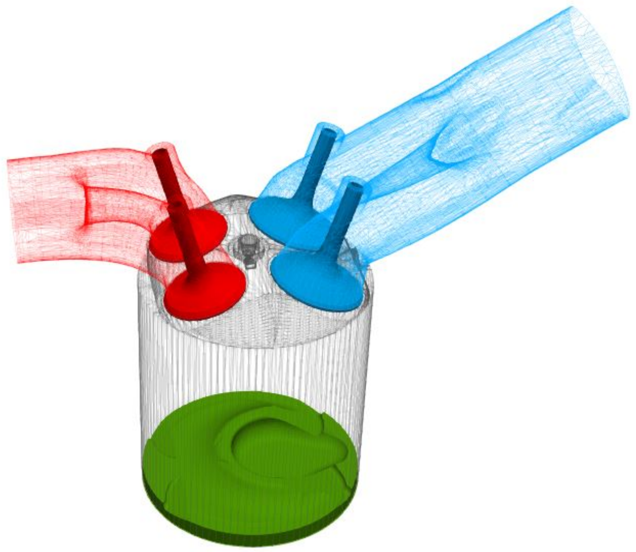


Predicting pre-spark heat release

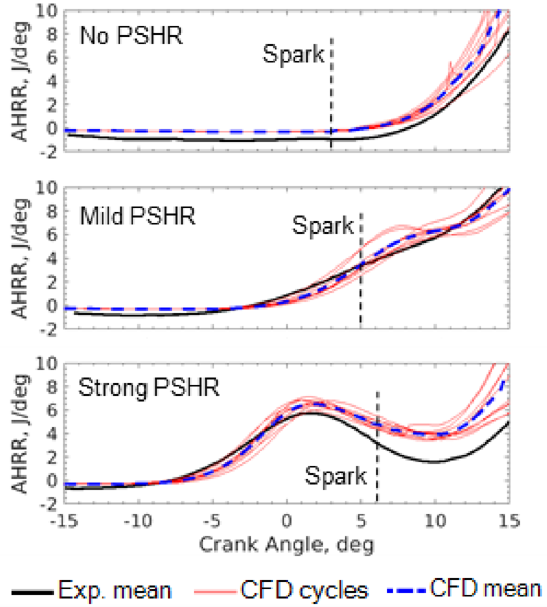
- New approach to capture pre-spark heat release (PSHR) using CFDs.
- Developed and validated combustion model best practices to capture the onset of PSHR accurately.
  - ✓ Engine geometry and experimental data from ORNL's LNF engine using Co-Optima alkylate and E30 fuels.
  - ✓ Integration of chemistry mechanisms by LLNL; validation of spray setup against experimental data by Sandia.
- Previous-cycle residuals are key to the occurrence of PSHR.
  - ✓ Chemistry solver must be kept active during gas exchange.

Hengjie Guo, Roberto Torelli (ANL)
Spray data: Lyle Pickett (SNL)
Engine data: Jim Szybist (ORNL)

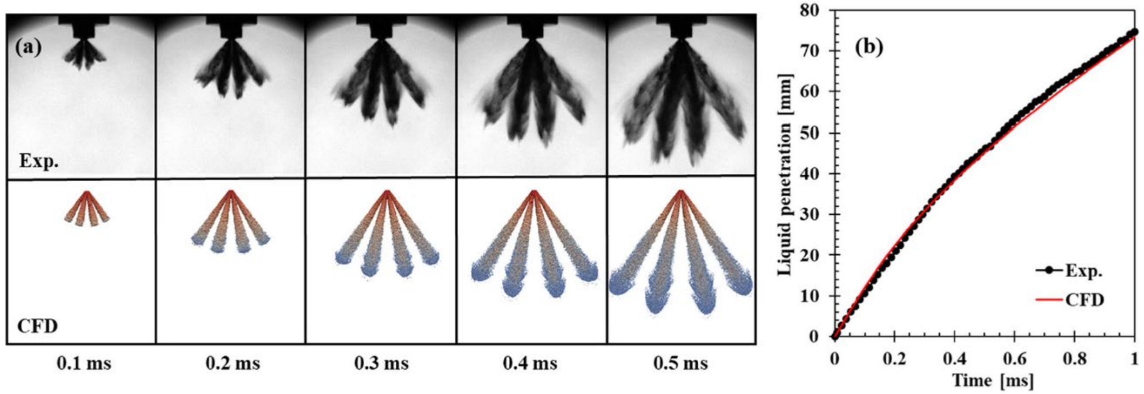
Computational domain



Model validation



Spray model calibration



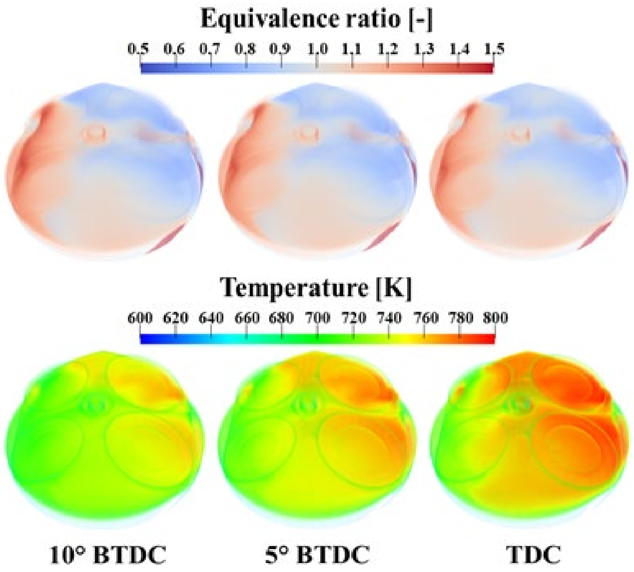
RESULTS

Pre-spark heat release & fuel effects

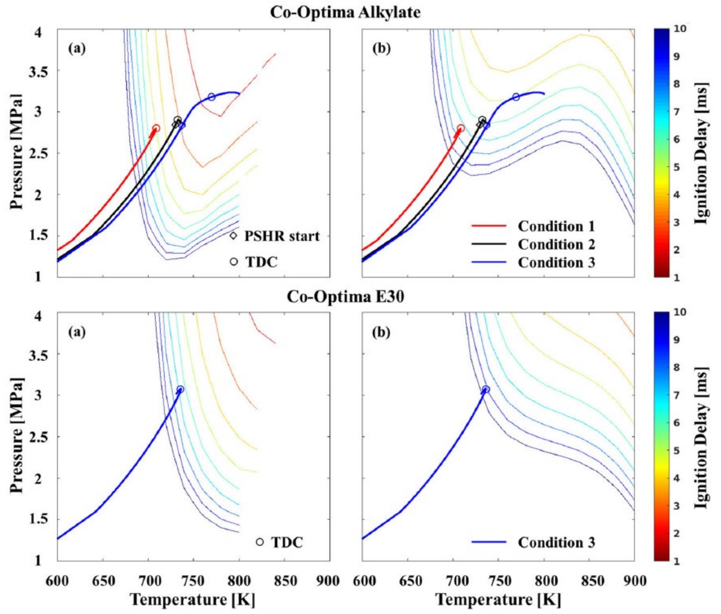
- CFD revealed PSHR begins in fuel-lean regions. Later, its effect becomes more significant in the fuel-rich regions.
- Pressure-temperature (P-T) trajectories explained the trends observed for the different PSHR intensities.
- In-depth analysis reveled the effect of fuel properties: HOV, laminar flame speed, saturation pressure, liquid specific heat.

Hengjie Guo, Roberto Torelli (ANL)
Engine data: Jim Szybist (ORNL)

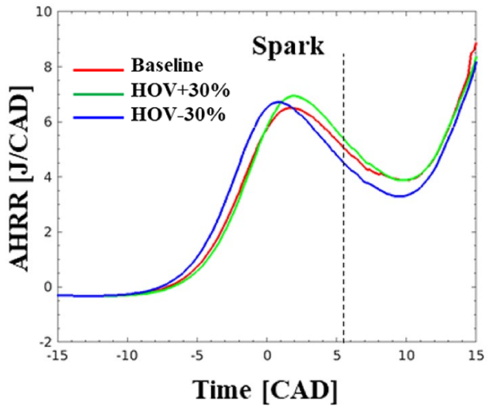
Dynamics of PSHR

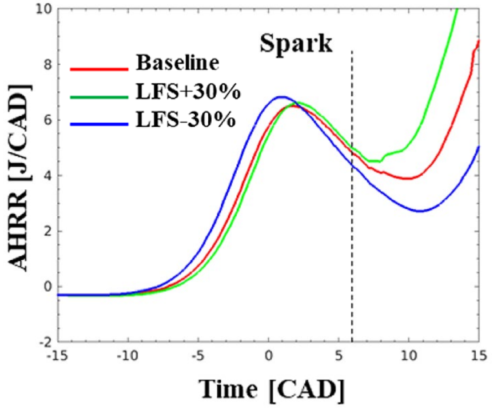


P-T trajectory analysis



Fuel property effects



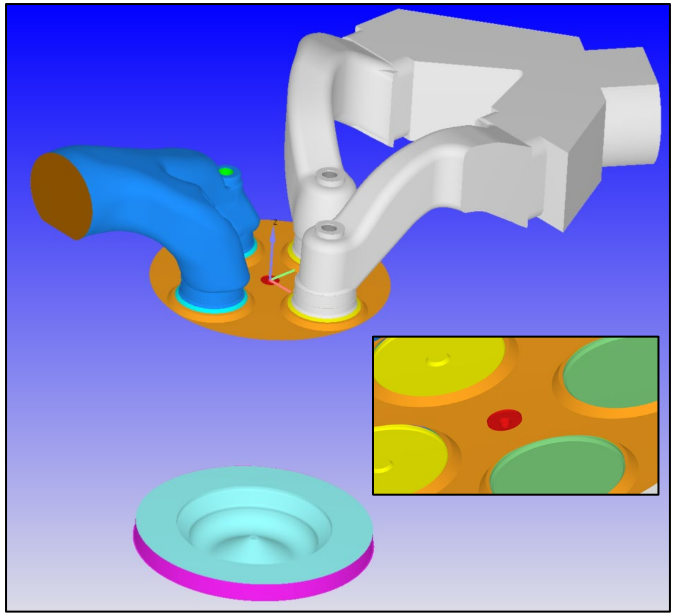


[1] Guo et al, *SAE Technical Paper,* 2021, doi:10.4271/2021-01-0400
[2] Guo et al, *IJER, 2021,* doi:10.1177/14680874211044110

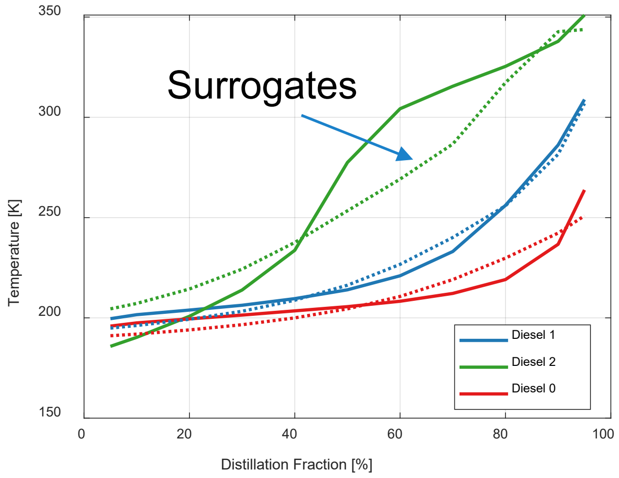
APPROACH Link fuel properties to NOx emissions

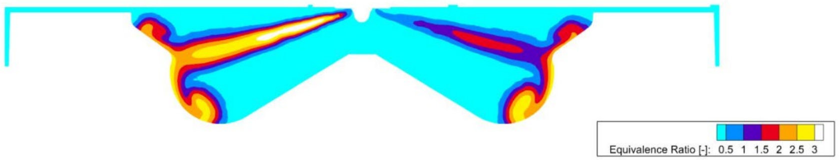
- Cummins ISB 6.7L single-cylinder (MD) engine with step-lipped bowl and 20:1 compression ratio used for experiments and simulations.
- Physical property effects initially explored through development of three diesel fuels (#2, #1, and #0) with increasing volatility but same reactivity.
- Diesel mechanism 319 species 1,797 reactions (including PAH and NOx chemistry) developed by Co-Optima team.

Flavio Chuahy (ORNL)



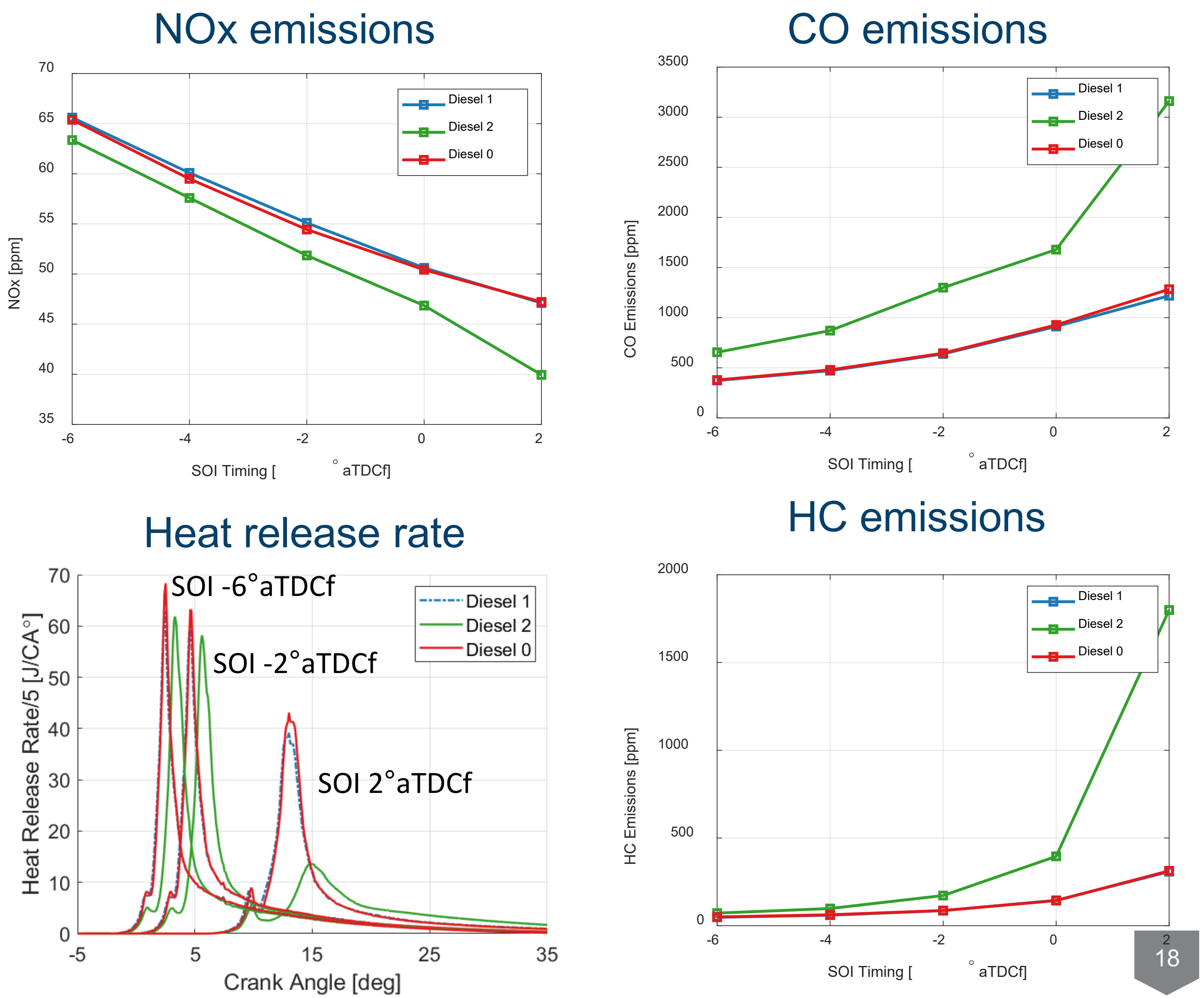
	Diesel #2	Diesel #1	Diesel #0
Density [kg/m3]	844.4	827.0	816.2
H/C Ratio [-]	1.864	1.855	1.892
Cetane Number [-]	45.3	45.3	45.4
Aromatic Content [%vol]	15.1	15.6	14.4
Olefin Content [%vol]	1.0	0.6	0.6
Saturate Content [%vol]	83.8	83.8	85
Kinetic Viscosity [cst]	2.88	1.74	1.44





RESULTS Effect of fuel volatility on NOx emissions

- Large changes in distillation curve resulted in only small changes to NOx.
- Larger changes seen for later injection timings due to later combustion phasing and sensitivity to mixture formation.
- Changes in physical property had small impact as a control lever for NOx at low-load engine operation.



Flavio Chuahy (ORNL)

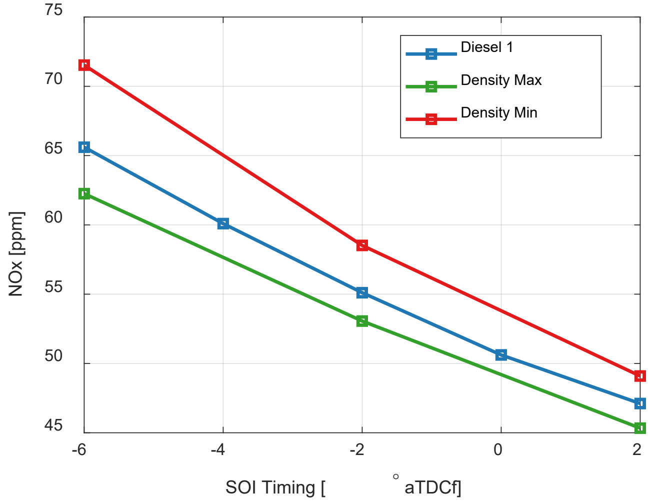
RESULTS Changes in individual fuel physical properties

- Density, surface tension, viscosity, thermal conductivity, HOV, vapor pressure and specific heat were independently modified by a large amount.
- Effect on heat release rate was observed for HOV, vapor pressure, density and specific heat changes.
- Changes in mixture formation were substantial, lower density fuel resulted in richer mixtures and higher NOx (as an example).
- However, changes in NOx were minimal for all property changes, even when property changes were large.

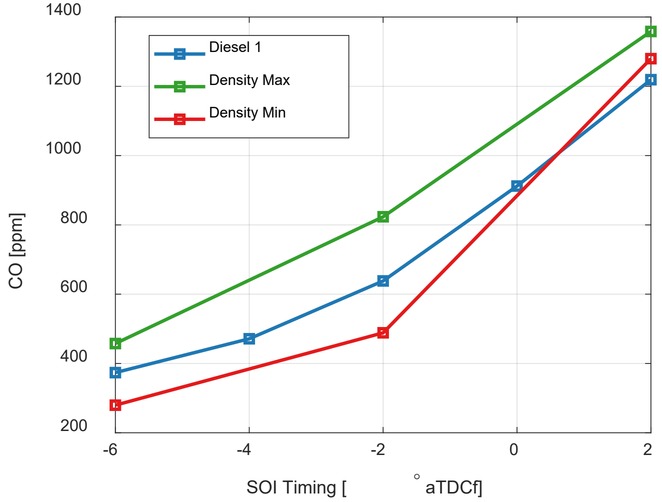
Flavio Chuahy (ORNL)

Example: Density changes

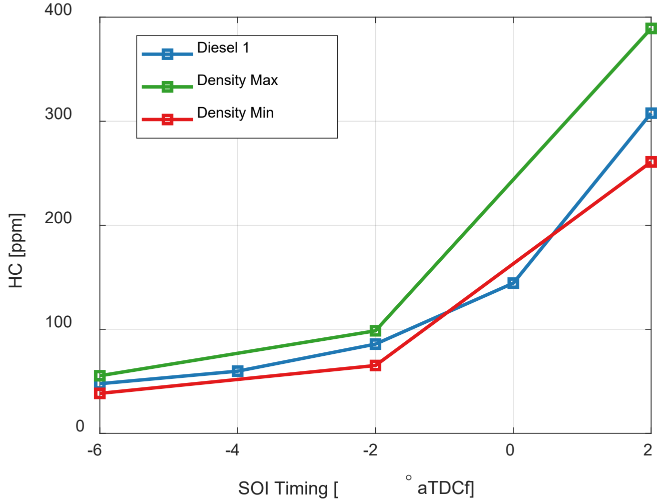
NOx emissions



CO emissions



HC emissions



APPROACH

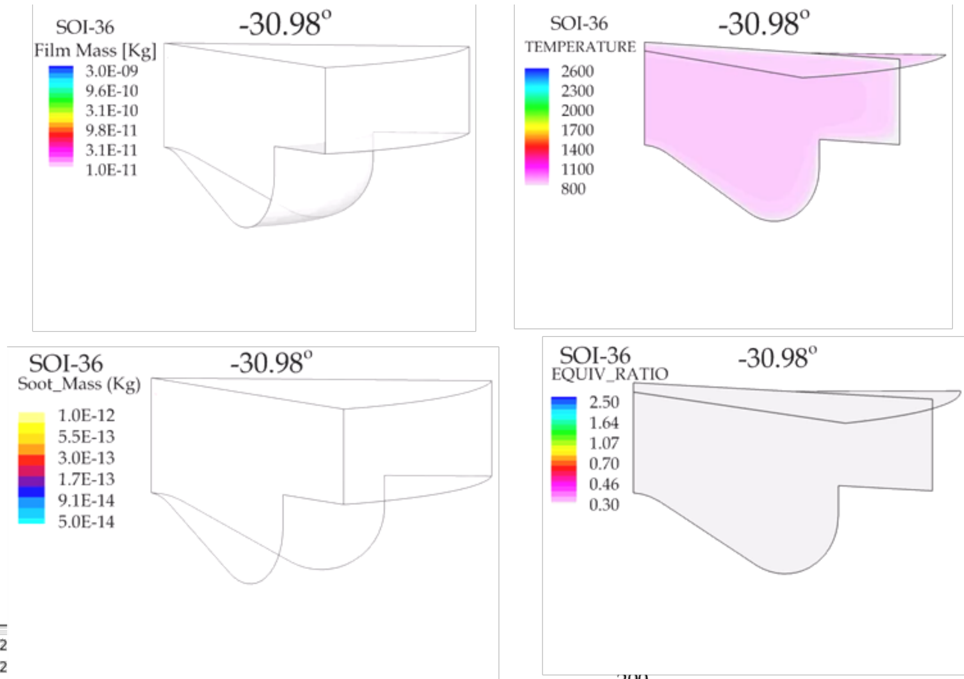
Fuel property effects on HD gasoline compression ignition

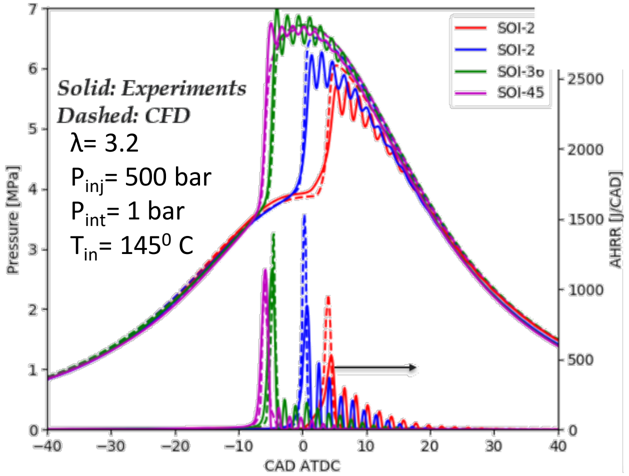
- ANL-CAT HD engine under low-load GCI.
- 240-species LLNL TPRF-E mechanism includes PAH and NOx chemistry together with hybrid method of moments (HMOM) soot model .
- Four fuel stratification levels considered with start of ignition (SOI) timings of -21/-27/-36/-45 ATDC.
- SOI @ -36 CAD ATDC: Cooler in-cylinder conditions at SOI → significantly more fuel film mass → higher soot emissions than SOI @ -27 CAD ATDC.
- SOI @ -45 CAD ATDC: Longer mixing time → more homogeneous mixtures & OH formation → more soot oxidation → lower soot emissions than SOI @ -36 CAD.

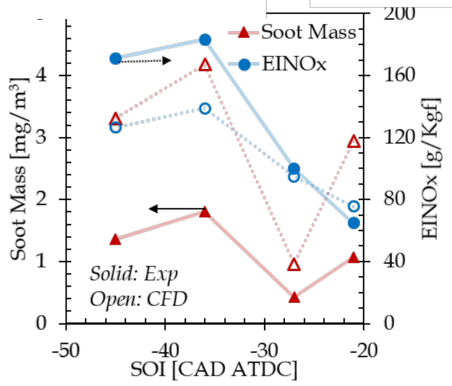
Krishna Kalvakala, Pinaki Pal (ANL)
Expt. data from Chris Kolodziej (ANL)

RD5-87 Surrogate (from LLNL)

Component	Vol %
Ethanol	9.98
Toluene	29.91
N-Heptane	21.03
Iso-Octane	39.08





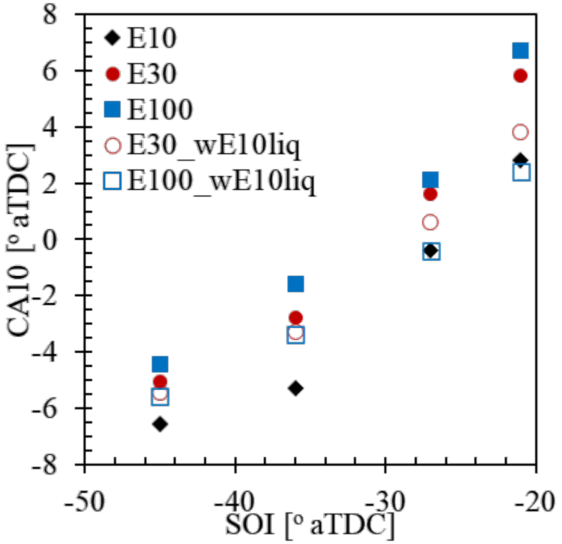


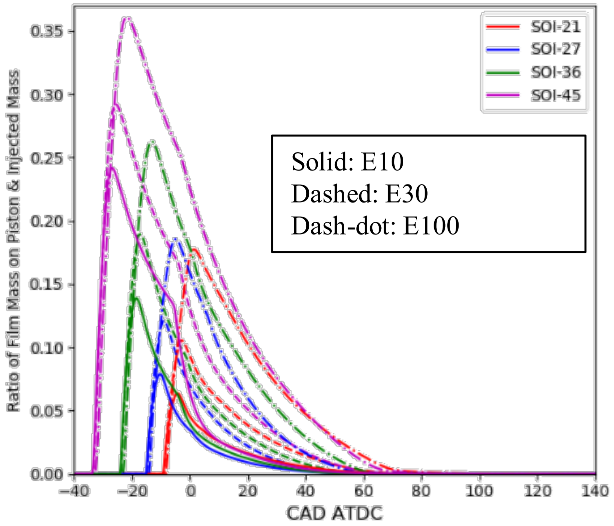
RESULTS

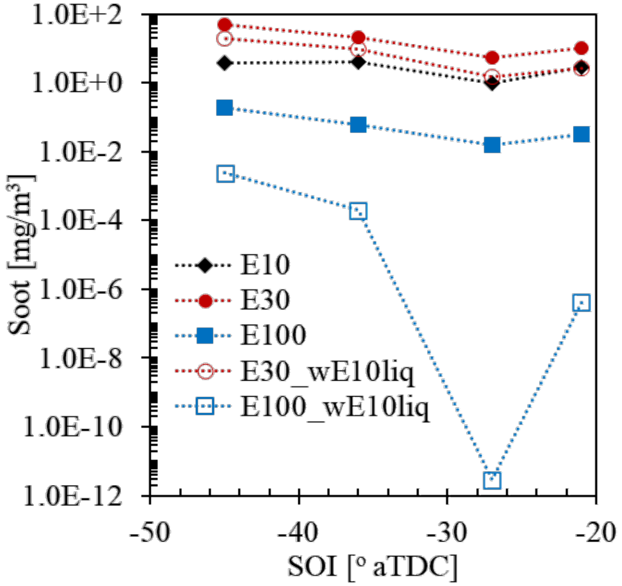
Impact of gasoline-ethanol blending on combustion phasing and NOx/soot emissions

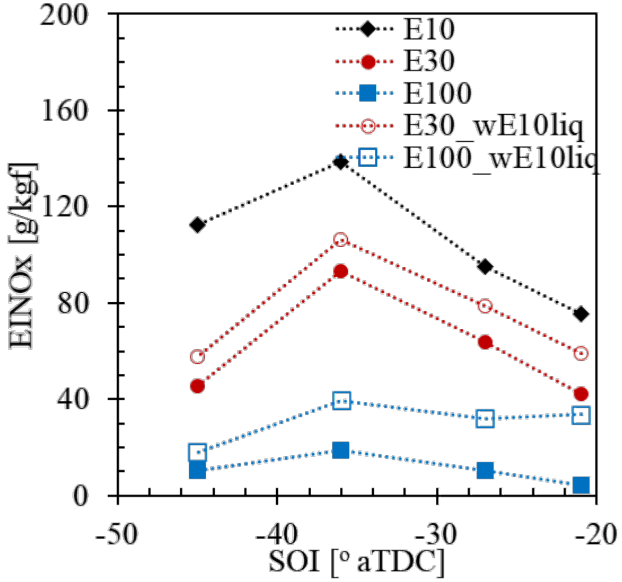
- E30 and E100 exhibit retarded combustion phasing relative to E10 due to fuel chemistry.
- Soot emissions show non-monotonic trend w.r.t. ethanol content as a consequence of strong coupling between fuel chemistry and physical properties (mainly HOV and viscosity).
- E30: Higher fuel film mass (due to higher HOV) + higher acetylene formation (due to more ethanol) → high soot emissions than E10.
- E100: Higher fuel film mass (due to higher HOV) but very low sooting fuel (no aromatic content in E100) → lower soot emissions than E10.

Krishna Kalvakala, Pinaki Pal (ANL)







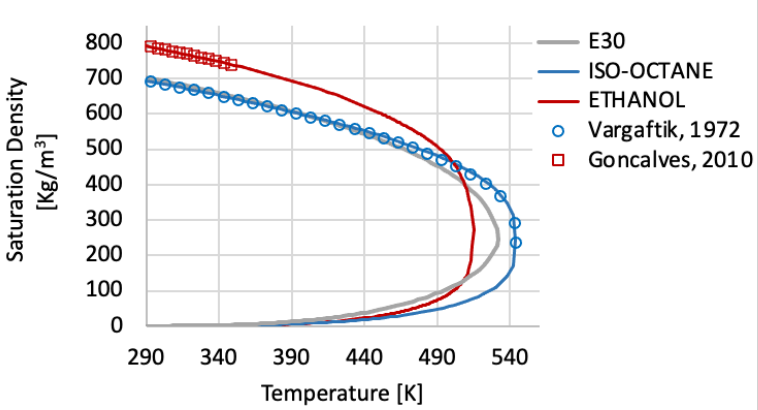


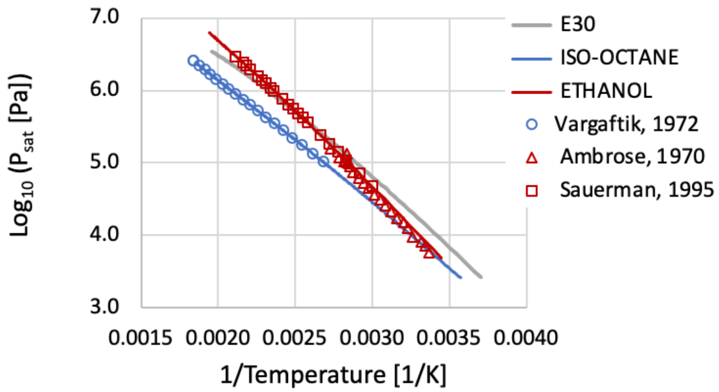
Connect thermo-physical properties to spray characteristics via high-fidelity simulations

- Proceed with a methodology that minimizes the dependence on calibration from conventional fuels.
- Create a small number of validated case studies using the real properties of the liquid/vapor/gas system (with SNL research code CLSVOF).
- From data, develop sub-models to cover gaps found in the engineering-level simulations.

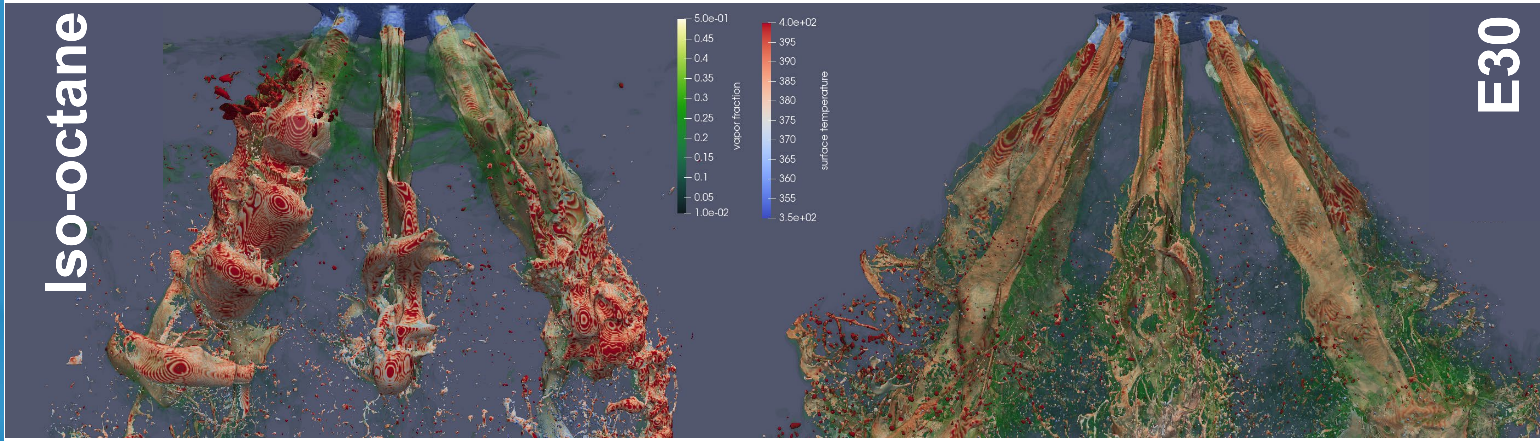
Marco Arienti et al. (SNL)

- Many fuel blends do not behave like ideal mixtures.





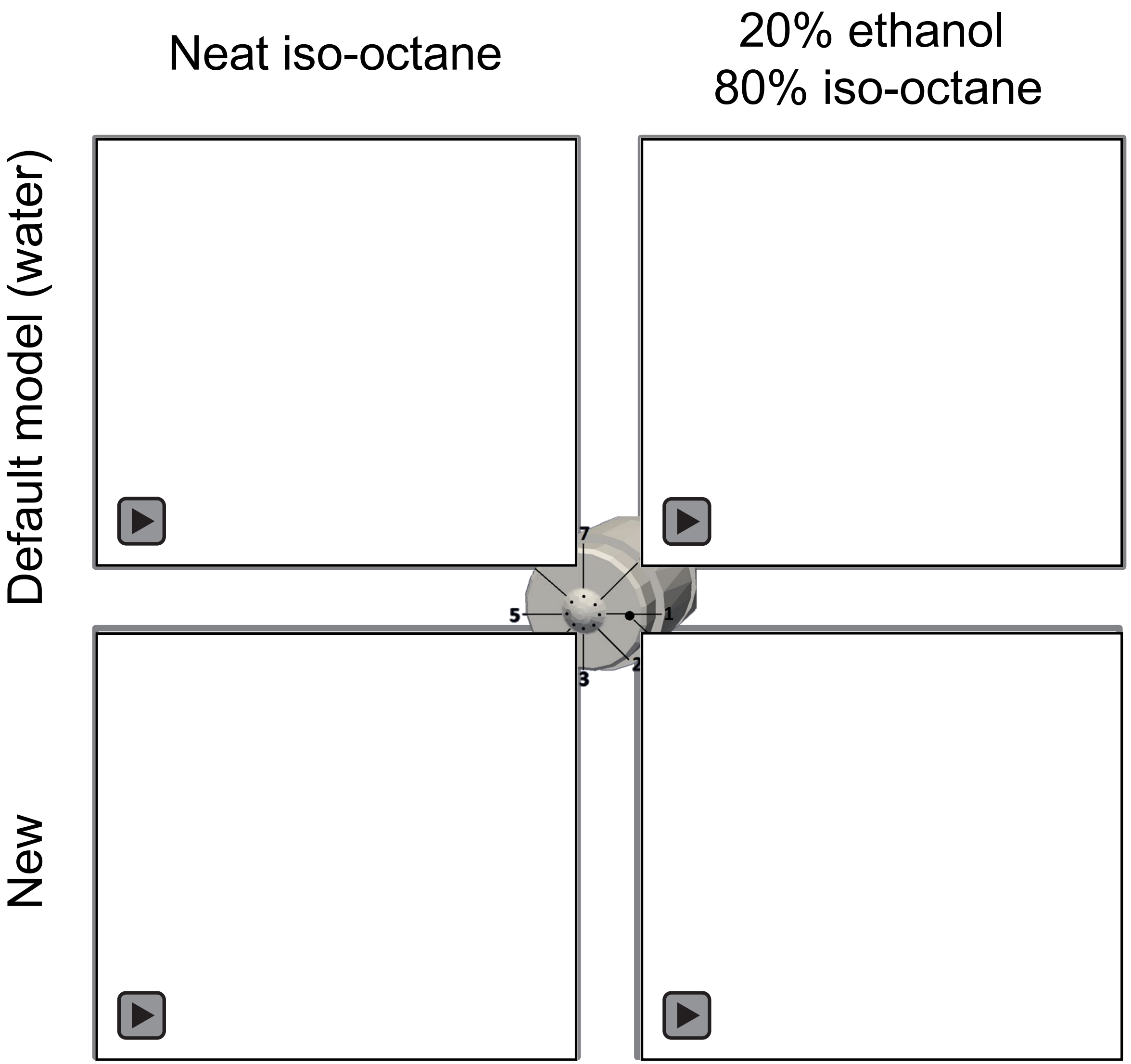
- The primary atomization process is non-linear: focus on how sprays are affected by thermo-physical properties.



RESULTS

Improved sensitivity of CFD flash-boiling model to fuel blend composition

- The new thermally-limited bubble growth (TLBG) model helps distinguishing the effect of fuel composition on spray cone angle.
- The new model is available in CONVERGE as user-defined function.
- More progress possible by correcting the sound speed evaluation of the liquid-vapor mixture.



Marco Arienti et al. (SNL)

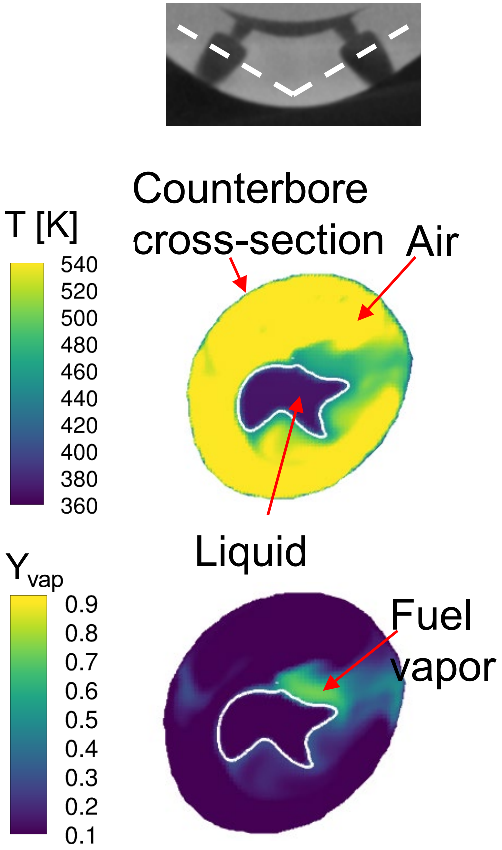
Arienti et al., "A thermally-limited bubble growth model for the relaxation time of superheated fuels," International Journal of Heat and Mass Transfer 159 (2020) 120089.

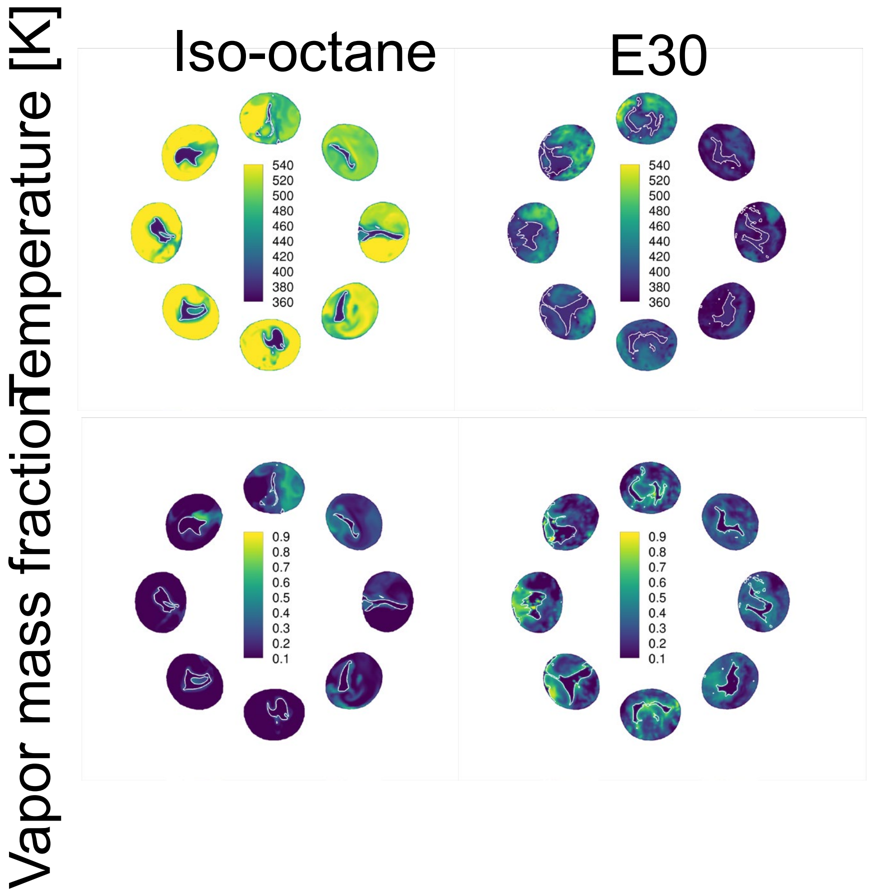
RESULTS

Case study: Differences between neat iso-octane and E30 for GDI at end of injection

- Observed differences between two two fuels in spray angle and jet structure; much enhanced evaporation with E30.
- Differences are particularly clear toward the end of injection as hot gas is entrained.
- But with E30 the temperature increase at the liquid surface is mitigated by the cooling effect of evaporation.

Marco Arienti et al. (SNL)



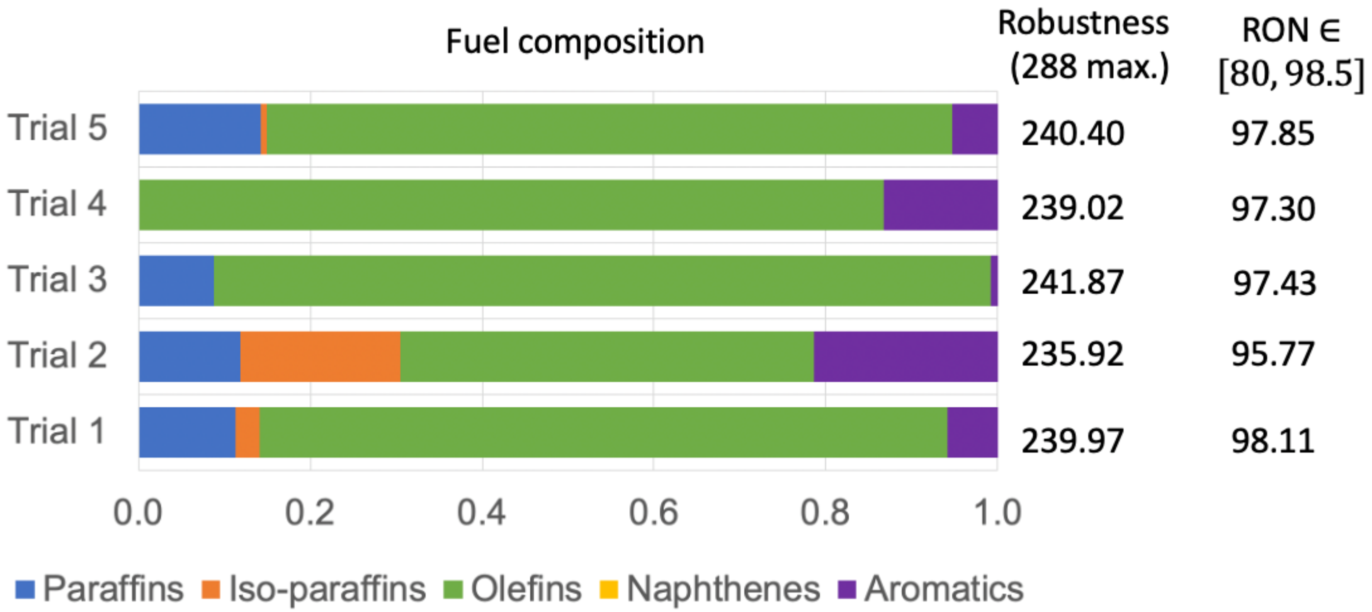


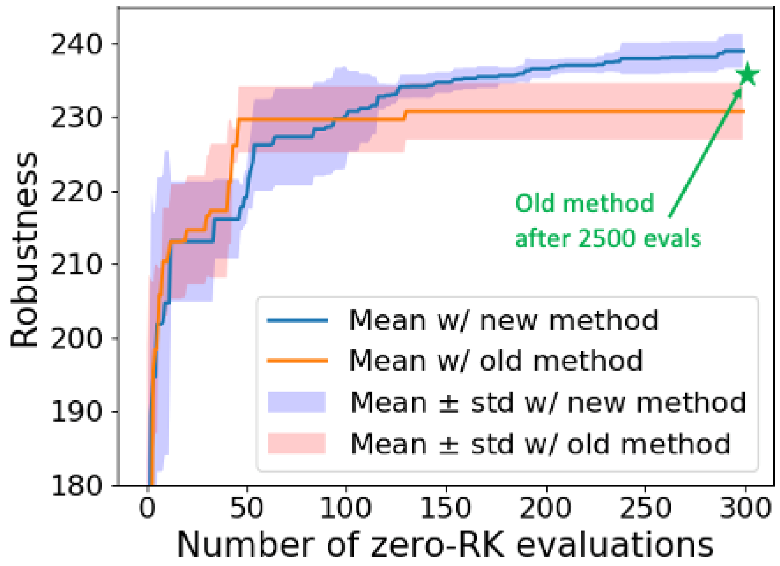
1. *Arienti et al., "Effects of detailed geometry and real fluid thermodynamics on Spray G atomization" Proceedings of the Combustion Institute 2021.*
2. *Arienti and Wenzel, "Detailed evaporation modelling for gasoline direct injection: iso-octane vs. E30," ACS Fall 2021.*

RESULTS Improved optimization tools for fuel search

- Optimization target: Maximize robustness of fuel mix.
- Constraint on RON: 80 to 98.5.
- 5 trials with the GP optimizer.
- 9 fuels components.
- Different fuel compositions lead to similar robustness -> multiple similar local optima present.
- GP finds better solutions faster than evolutionary algorithm.

Juliane Mueller (LBNL)

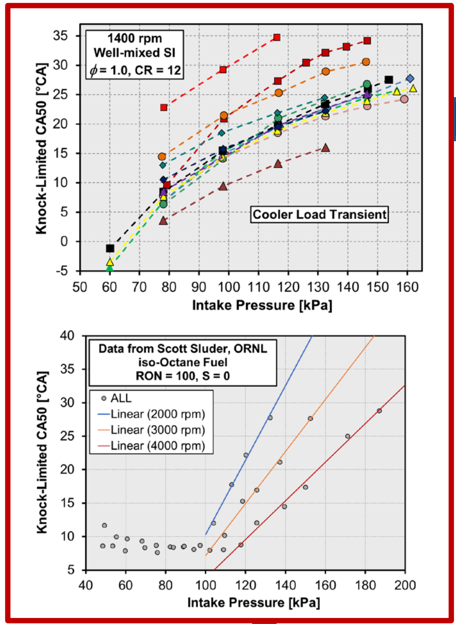




APPROACH

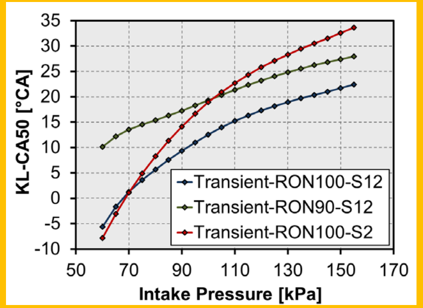
Developed framework to predict effect of fuel type on fuel economy – stoichiometric and multimode

Experimental engine data for many fuels, operating conditions & engine thermal states



Determine knock limits for hypothetical fuels

Regression model

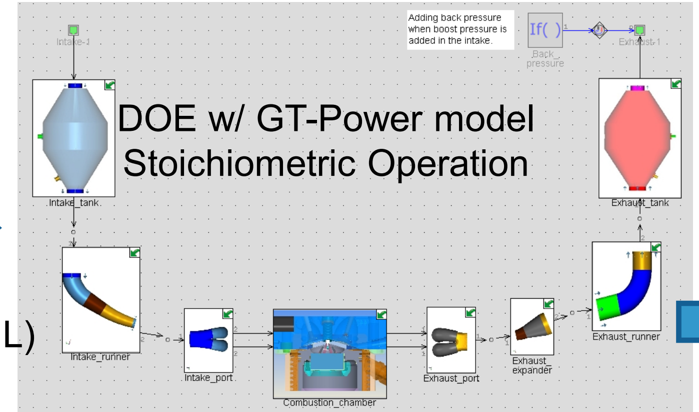


KL-CA50

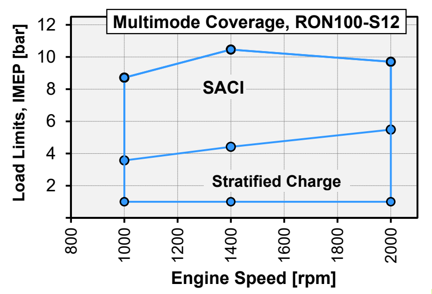
Fuel Consumption Rate

Gaussian Process Regression model

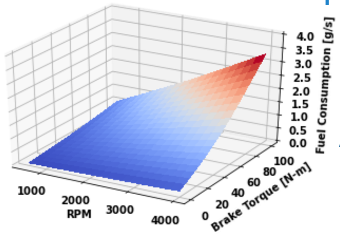
Torque, Fuel Flow



Multimode Coverage



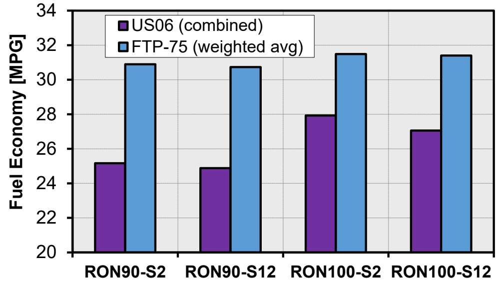
Fuel-Flow Rate Map



Drive Cycle Simulation

AUTONOMIE

Fuel Economy



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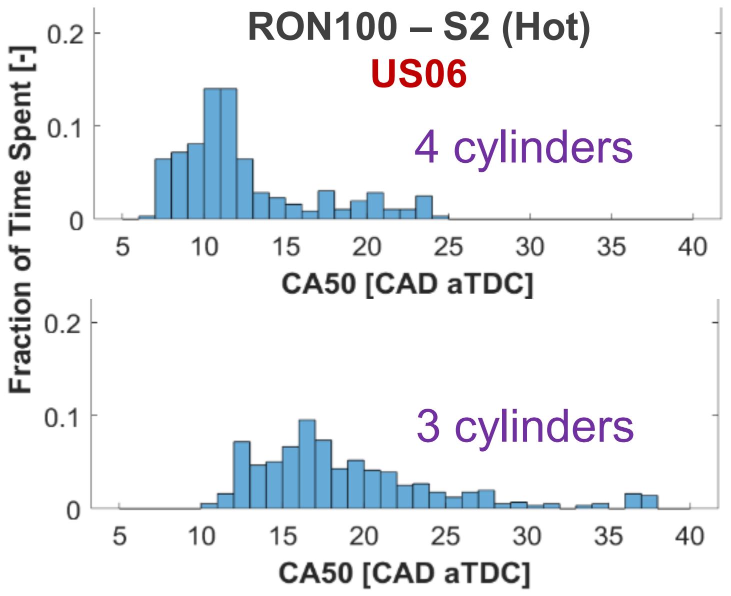
RESULTS

Fuel effects on the benefit of enhanced thermal management

- **Downsizing provides fuel efficiency benefits for FTP-75 and HWFET, but not for US06.**
  - Higher IMEP ⇒ more knock limited.



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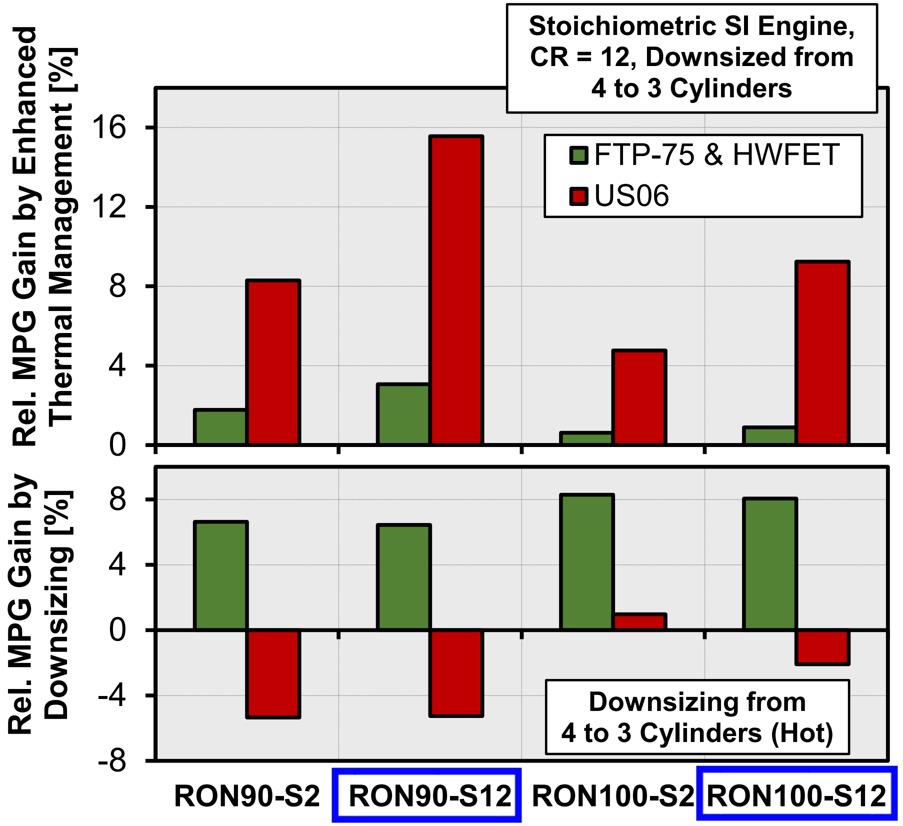
- **Autonomie predicts that enhanced thermal management provides most benefit for more aggressive driving (US06).**

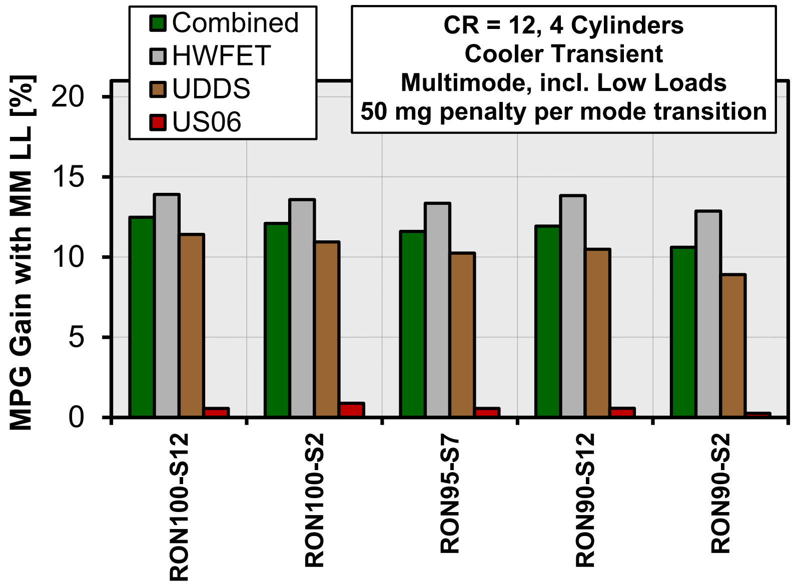


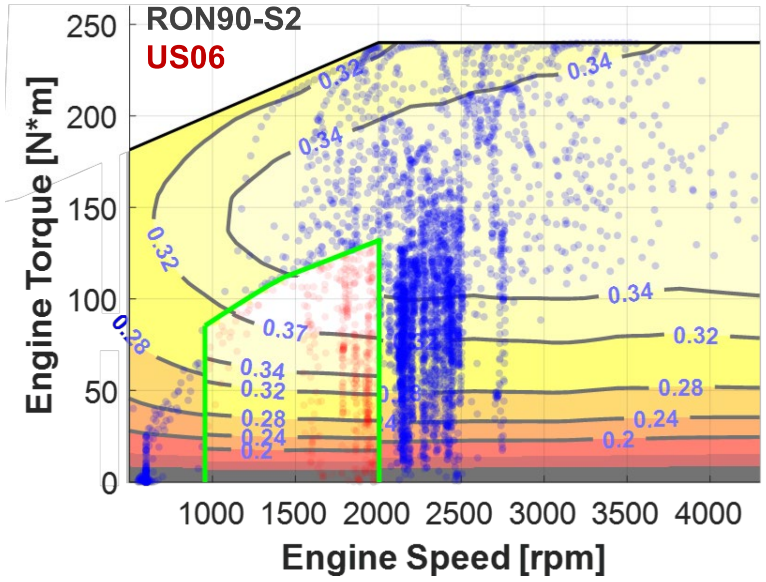
Here, the S=12 fuels provide greatest benefit.

RESULTS

Benefit of multimode varies with drive cycle and fuel type

- Multimode shows essentially no benefit for US06, which uses higher engine speeds.





Nick Killingsworth (LLNL)
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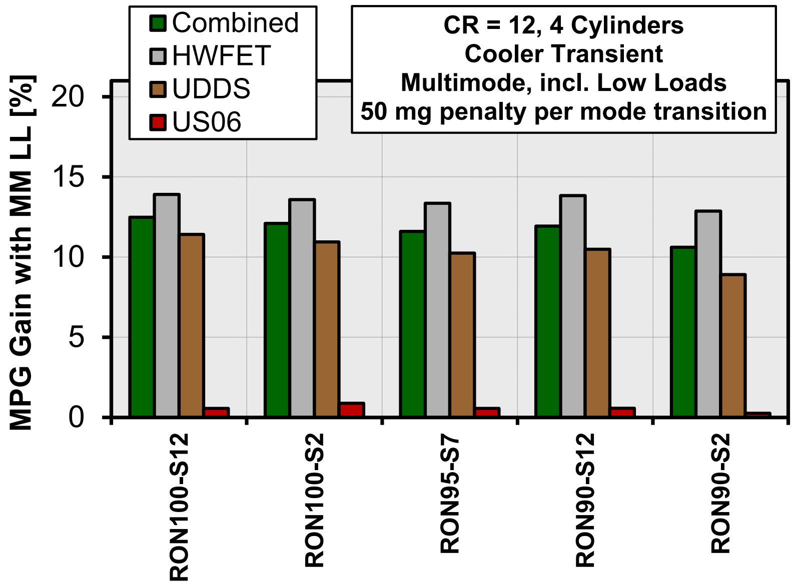
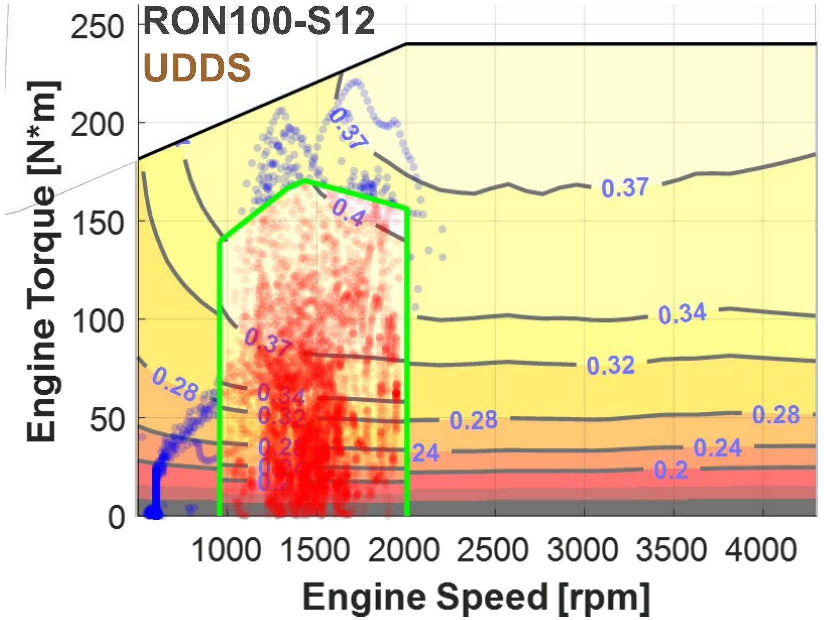
RESULTS

Substantial fuel-economy benefits from multimode operation for HWFET & UDDS

- Multimode operation provides 9 – 14% MPG Gains for HWFET & UDDS cycles.
- Here, the higher SACI load limit of high-RON high-S fuels provides benefits.





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Some takeaways

- Initially computational tools to study physics at the fuel-engine interface for LD and HD were not available.
- Physics based models/sub-models for improved predictions of fuel-engine phenomena developed and implemented in industry standard-use software.
- Reduced kinetic mechanisms for several molecules available for CFD.
- Engine models for multiple platforms such as CFR, CAT, Navistar, Cummins, Ford, and GM, have been developed and validated (at different levels of fidelity) and may be available for public dissemination.
- Lower-order open-source tools also developed and available.
- Initiation of PACE (computationally focused) accelerated Toolkit Team’s prediction capabilities.
- Additional three years would have enabled us to perform true co-optimization.

Acknowledgements

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