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Combustion Research Facility

Fuel Effects on Mixed-Mode Combustion in a DISI Engine

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Abstract:

So-called "Mixed-Mode" combustion can provide increased engine efficiency. It relies on both flame-propagation through a lean/dilute mixture, as well as the controlled autoignition of a lean/dilute end-gas. Both of these controlling processes can be affected by fuel properties, such as the laminar burning velocity, as well as the autoignition behavior of a fuel. It is desirable to quantify the sensitivity to changes in fuel properties. However, to conduct a robust investigation, many thousands of operating conditions must be evaluated. Considering the timescale of rigorous engine experiments, and the timescale for rigorous CFD simulations, neither of these approaches are practical for the scale of investigation which is desired. Therefore, a methodology to use 1-D engine simulations coupled with 0-D chemical kinetic simulations is presented.

The initial results from this modeling methodology indicate that the fuel requirement synergies between stoichiometric SI and mixed-mode combustion are surprisingly strong. Both modes require autoignition resistant fuels to achieve "High Loads." Fuels with high Octane Sensitivity show less sensitivity to intake boosting, thereby extending load range for mixed-mode combustion.

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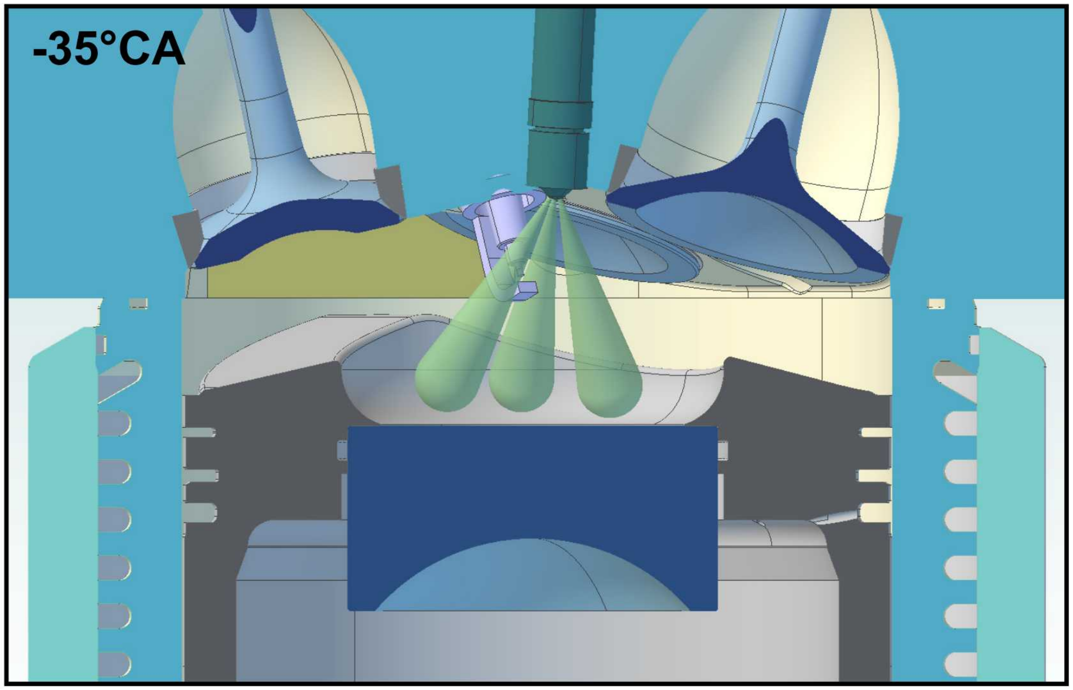
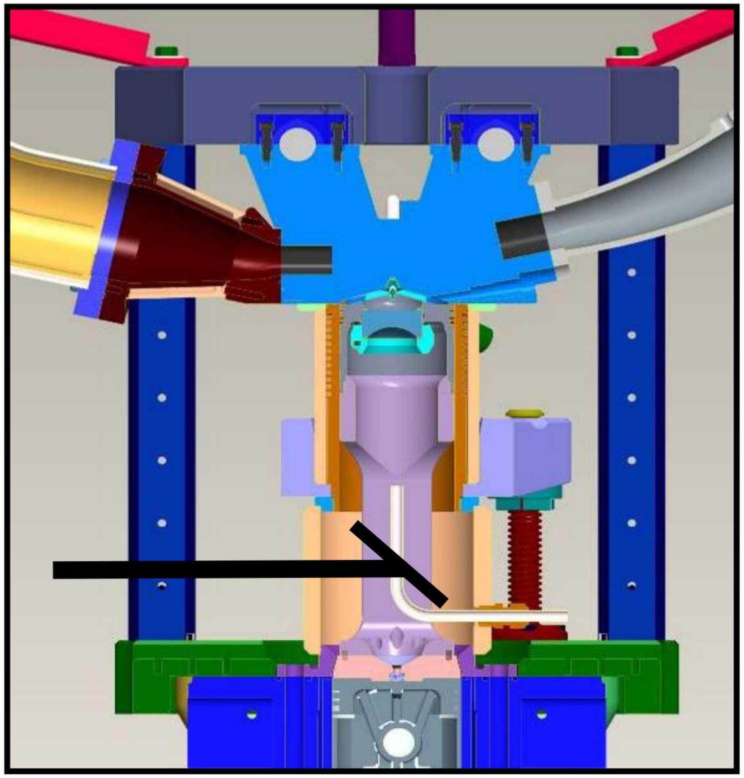
U.S. DEPARTMENT OF ENERGY

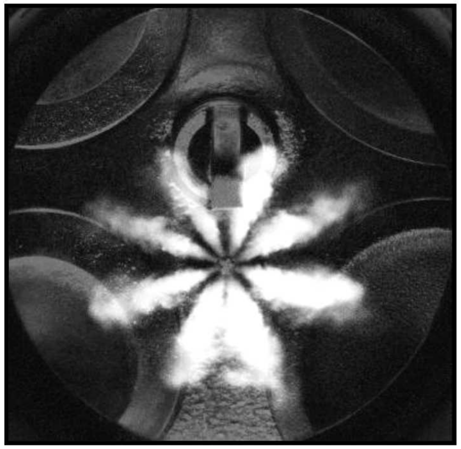
Co-Optimization of Fuels & Engines

Research Engine

- Designed for spray-guided stratified-charge operation ⇒ Piston bowl.
- 8-hole injector. P_{in} = 120 - 170 bar.
- Drop-down single-cylinder engine.
- Automotive size. 0.55 liter swept volume.
- Identical geometry for **All-metal** and **Optical.**



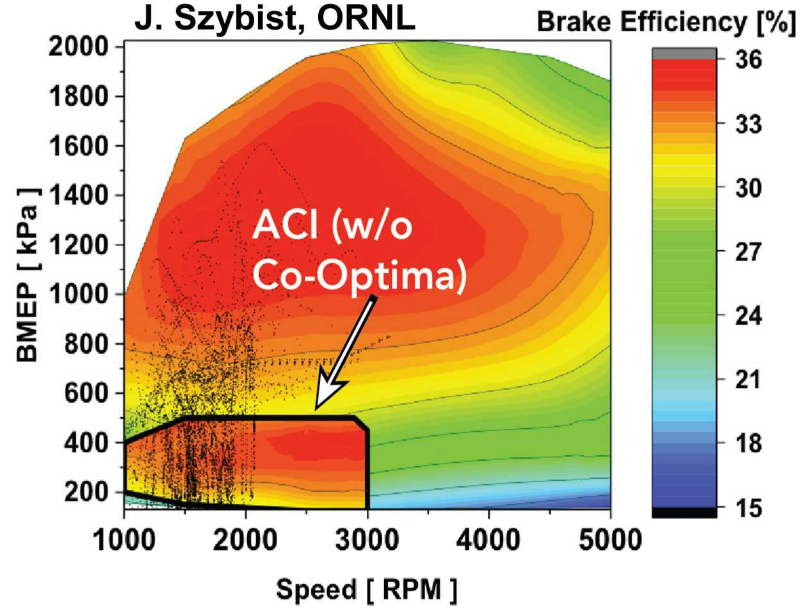


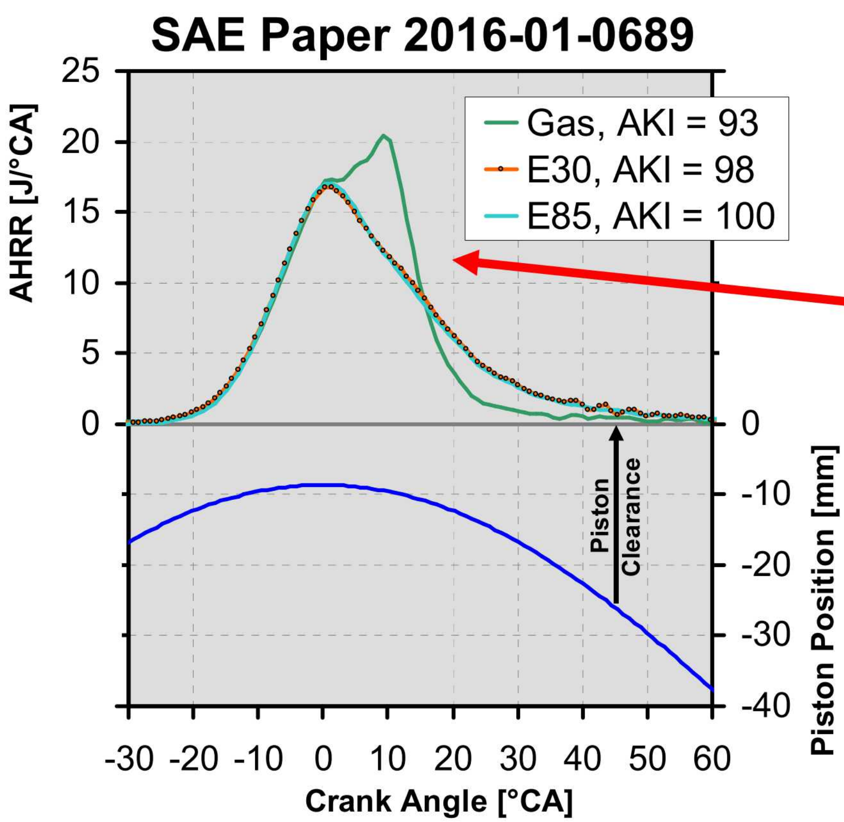


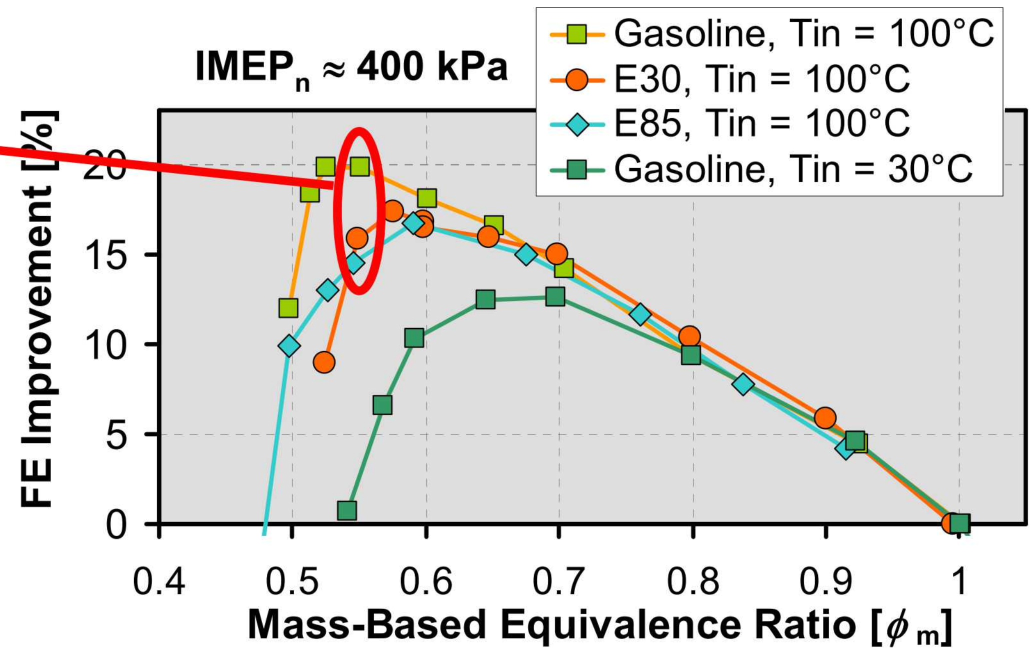
Mixed-mode Combustion for Multi-mode Operation

- Lean operation provides efficiency benefits.
- Can be used at low to medium loads where the engine spends a majority of the time.
- With current hardware, mixed-mode combustion is required for sufficiently short burn duration for $\phi < 0.6$

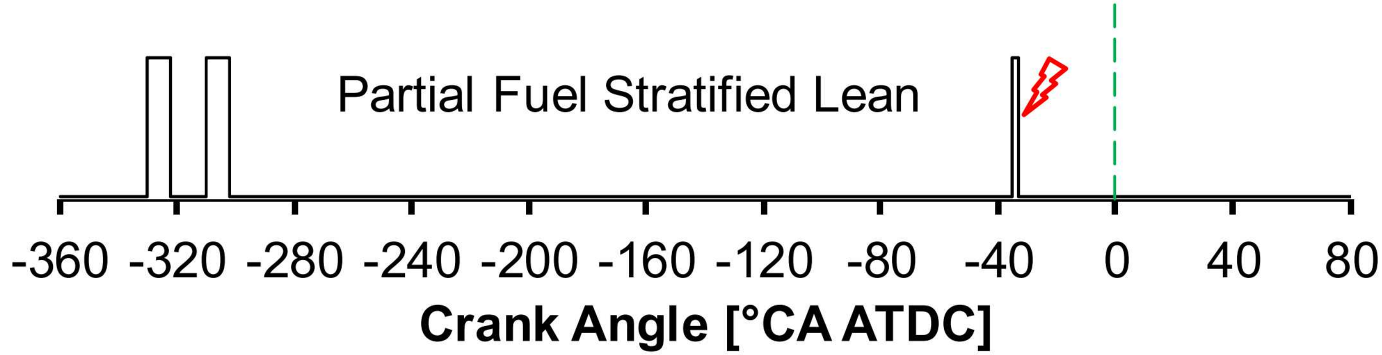
Figure credit:
J. Szybist, ORNL



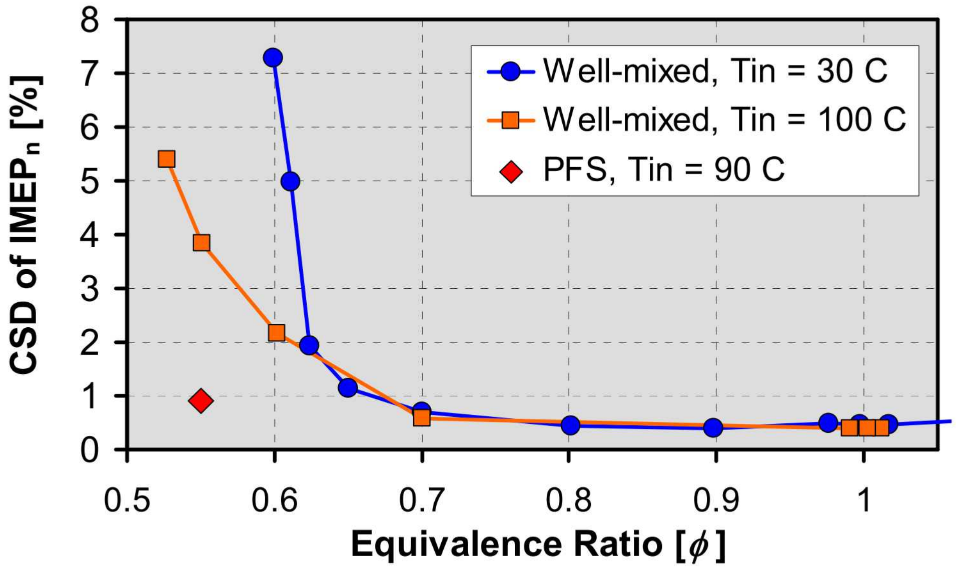




Partial Fuel Stratification for Stable Operation

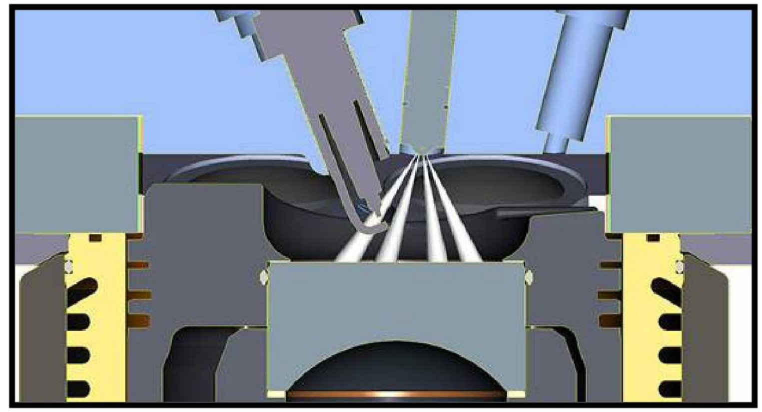


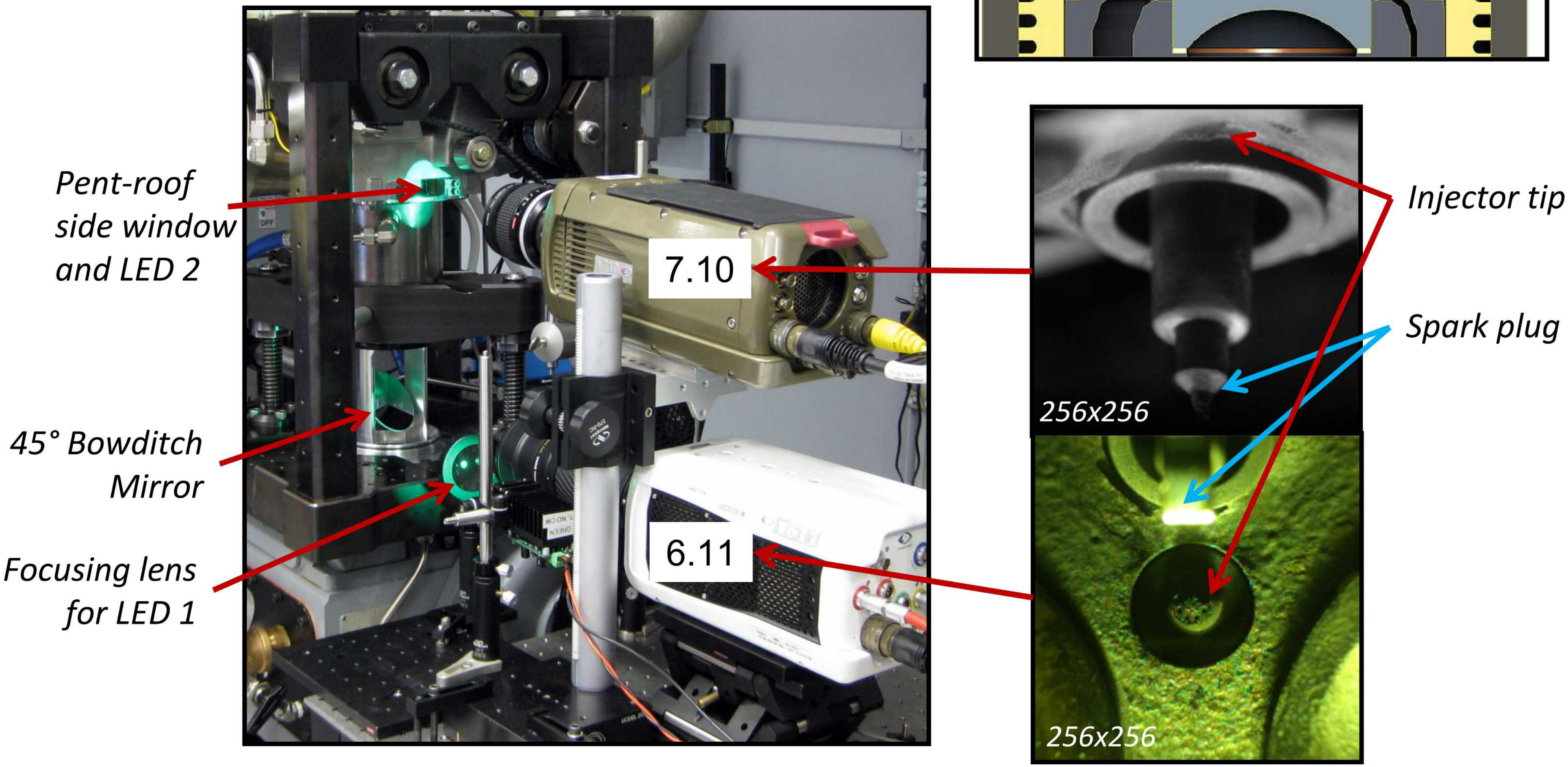
- Need to stabilize deflagration to facilitate mixed-mode studies.
- Use small injection at the time of spark.
- Minimize amount of pilot fuel to minimize NO_x penalty.
- Yet provide sufficient stability for lowest ϕ encountered.
- Most recent data were collected with a relatively small pilot ≈1.5 mg.



High-Speed Spray Visualization

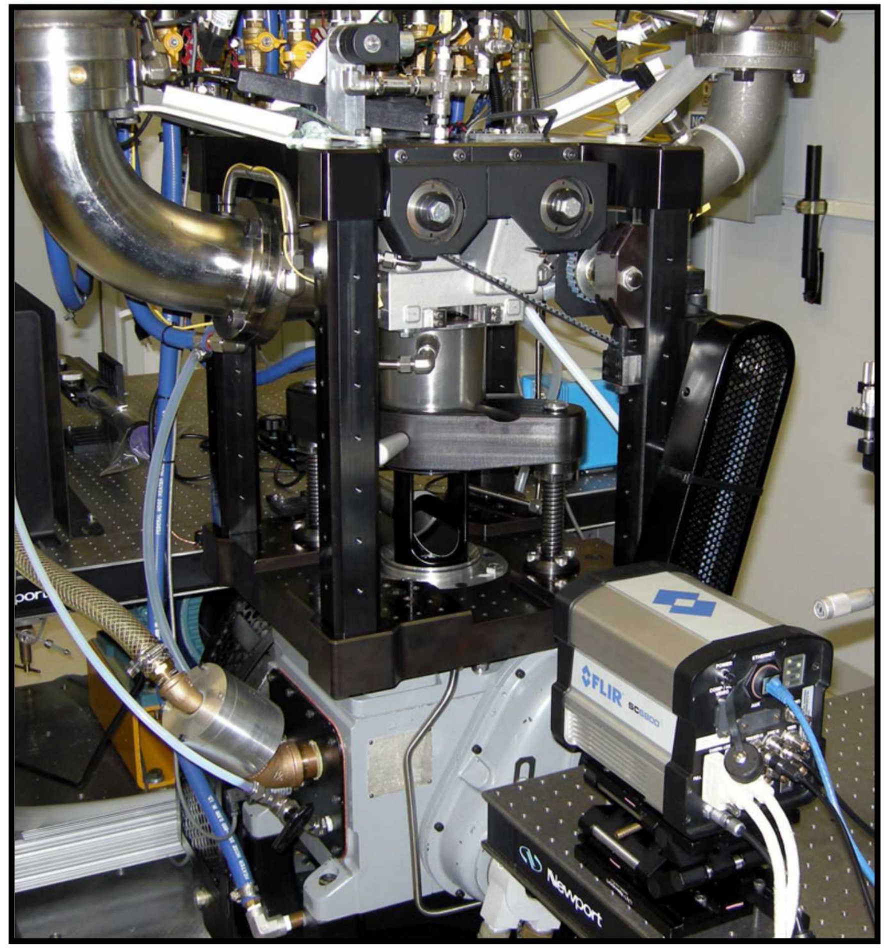
- 60 kHz – 0.1°CA resolution. Dual cameras.
- Requires timings of LED pulses to be offset to avoid reflections.

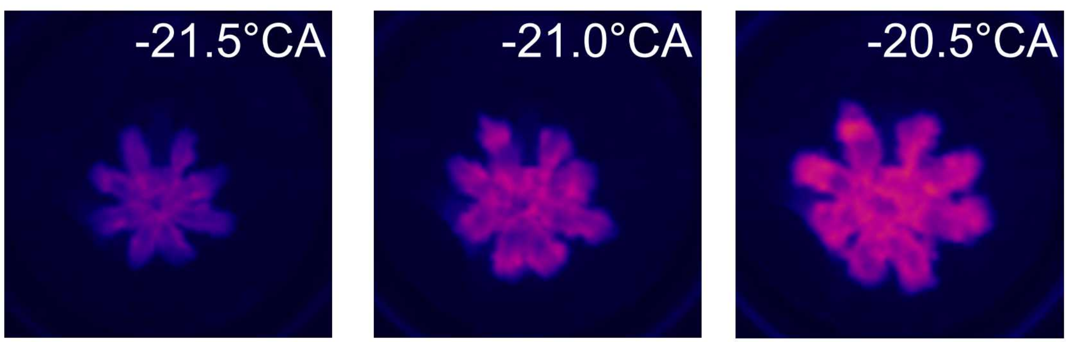




High-Speed Infrared Fuel-Vapor Imaging

- Mid-infrared thermography. Band-pass filter 3.20µm ± 300 nm
- Thermal emission from the C-H stretch band near a wavelength of 3.4µm (thermal-vibrational radiation)
- Well isolated from most other emitting species (in particular H_2O and CO_2)
- FLIR SC6800.
- Relatively high frame rate - 2000 Hz.
- 1 image each 3°CA at 1000 rpm. Phase-shifted repetitions provide 0.5°CA resolution.

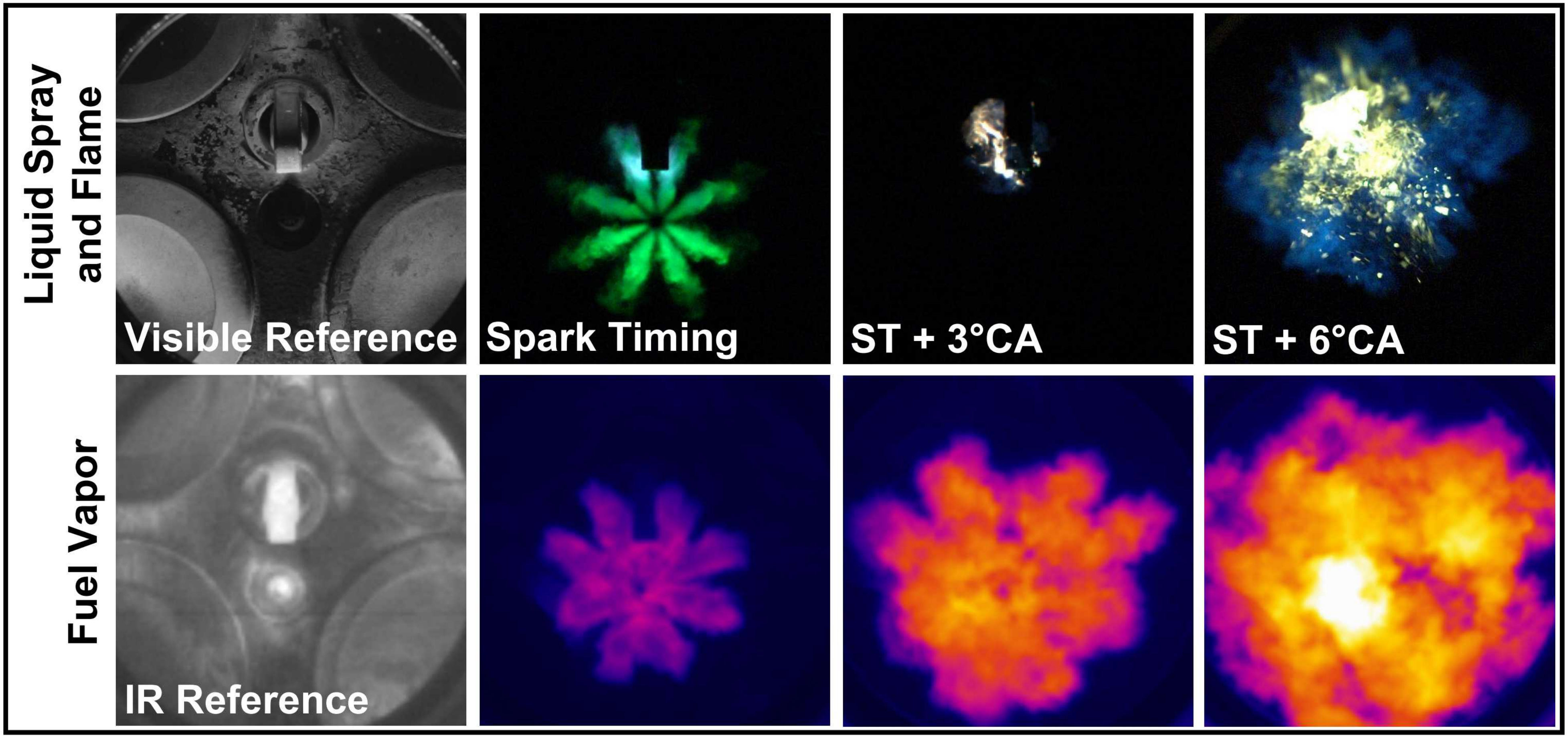




SOI_a = -23°CA

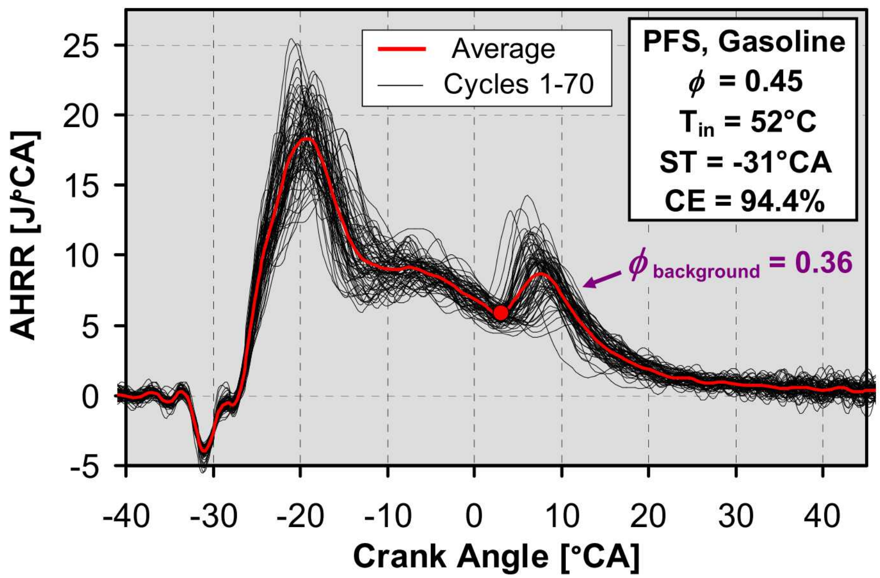
High-speed IR and Flame Imaging

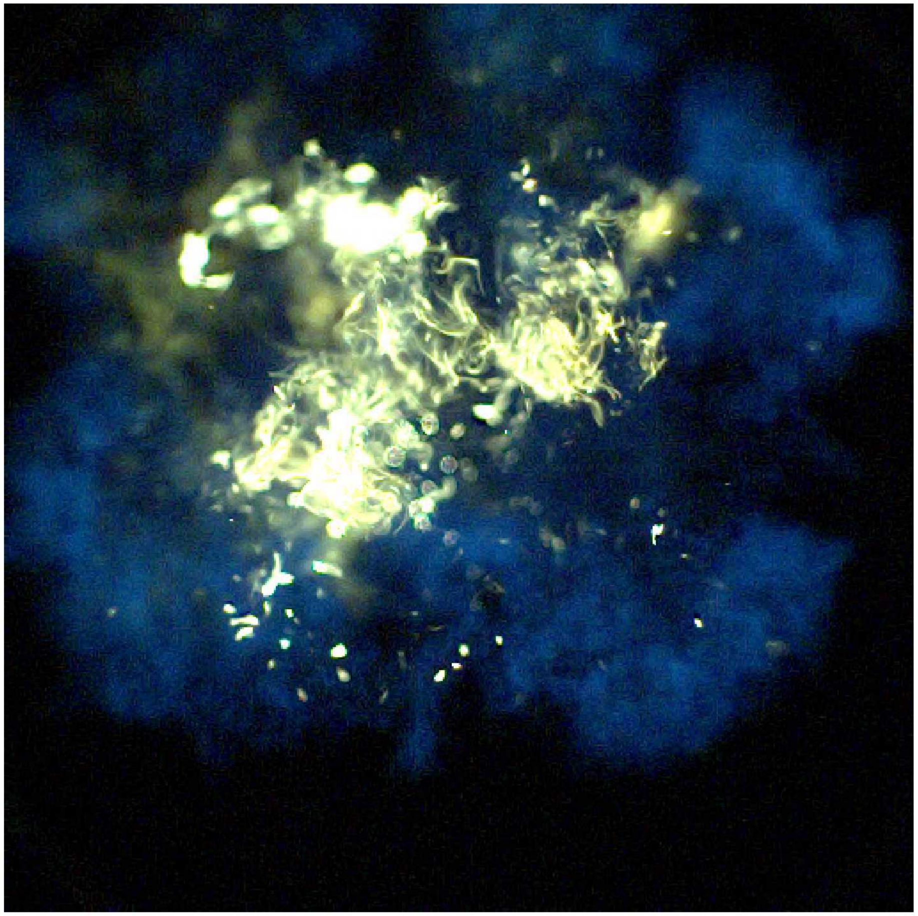
- IR fuel vapor imaging reveals extent of fuel stratification relative to the flame spread. Here, using a large 3.4 mg pilot.



High-Speed Spray and Flame Imaging

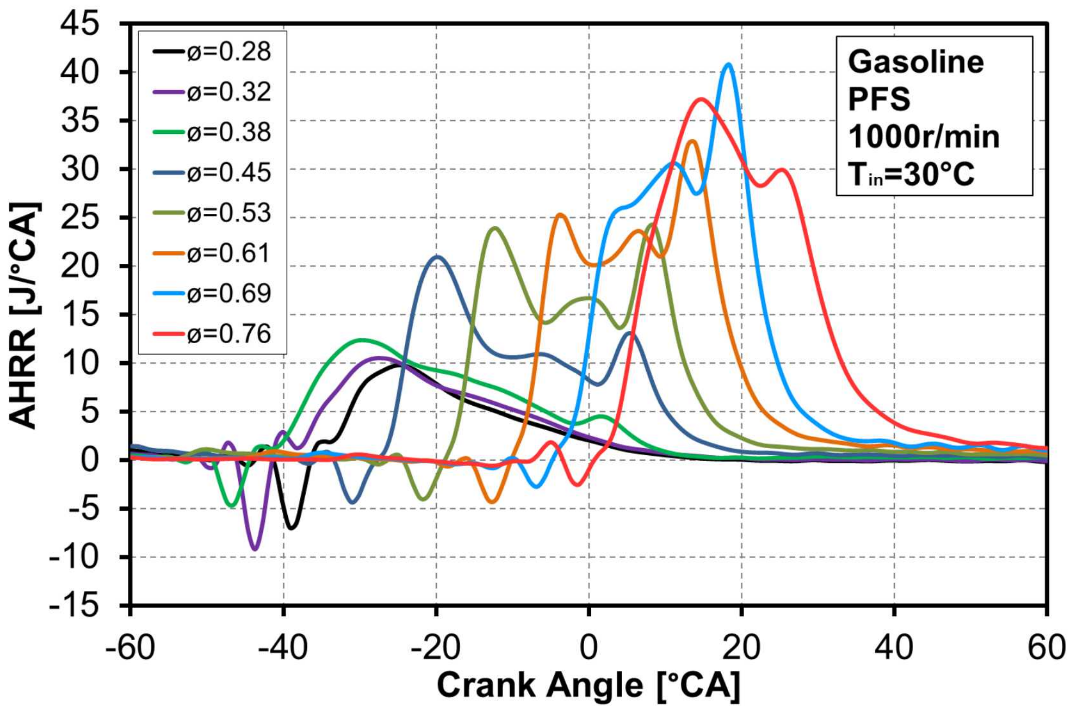
- Liquid fuel vaporizes quickly.
- Flame spread is rapid throughout the piston-bowl area.
  - Consistent with IR imaging showing large area being enriched.
- Flames fronts propagate outside field of view by -20°CA.
  - End-gas autoignition cannot be studied in this configuration.

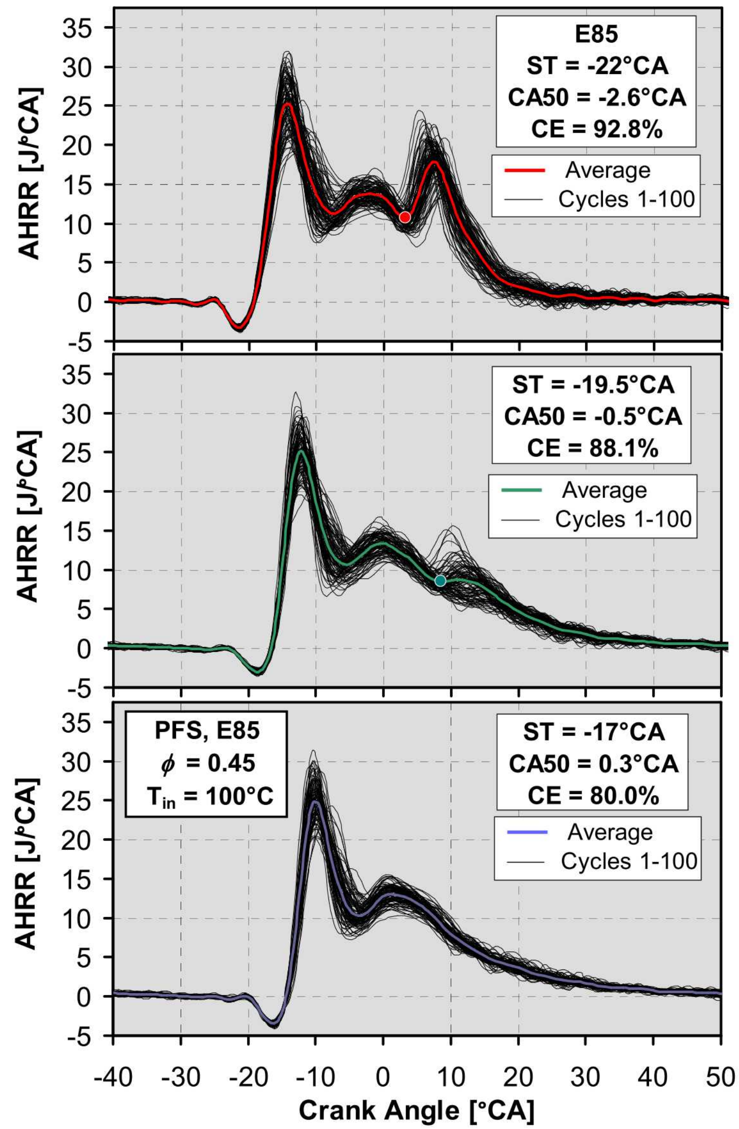




PFS with 3.4mg pilot (330μs inj. dur.)

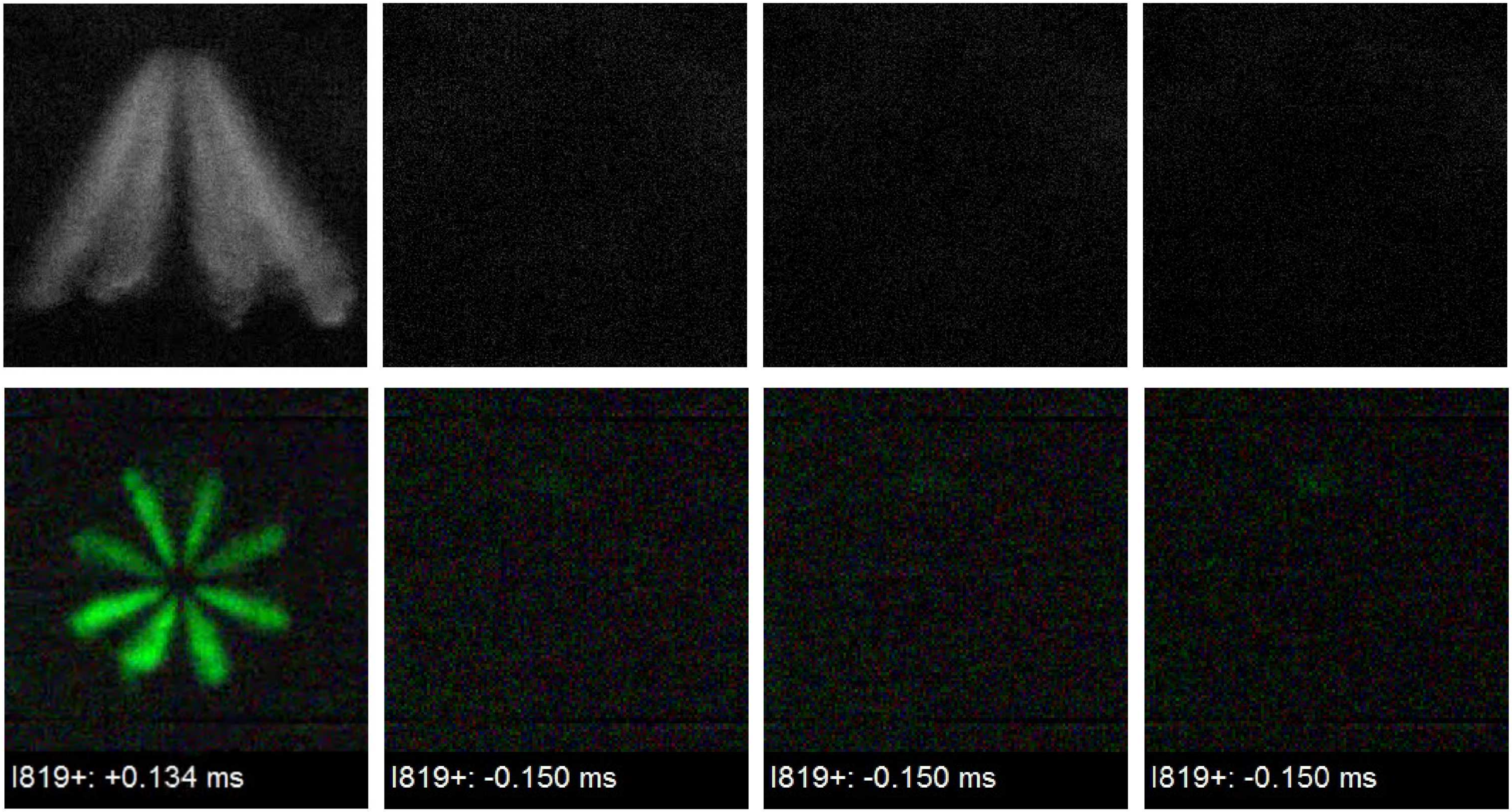
- Large pilot offers good CA50 control down to $\phi_{end\text{-}gas}$ = 0.29
- However, NO_x penalty can be reduced with a smaller pilot injection.





E30 Spray Visualization at 60 kHz

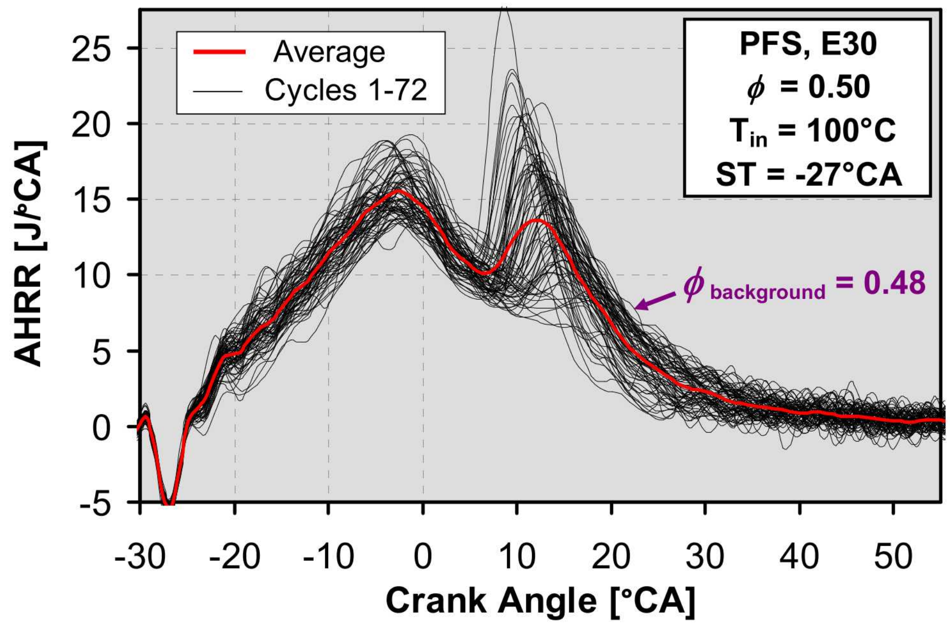
210μs 0.7 mg	220μs 1.4 mg	230μs 2.1 mg	330μs 3.5 mg

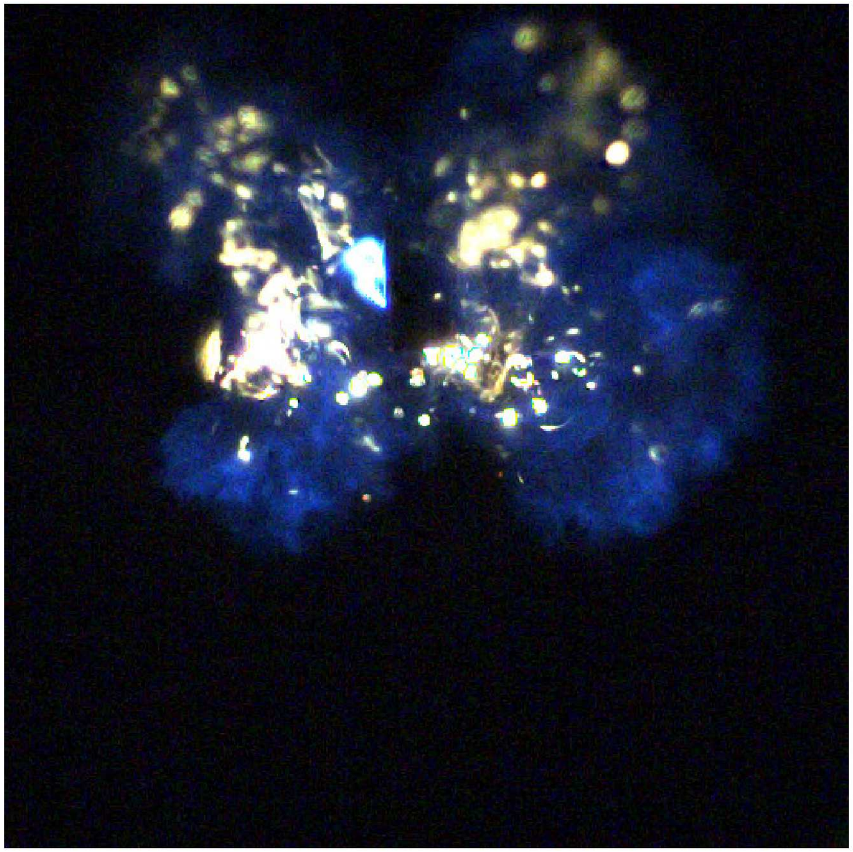


- Explore the use of shorter injection durations. E30 fuel.
- Injection pressure = 170 bar. SOI_a = -28°CA. ρ_{cyl} = 7.2 kg/m^3. T = 680 K.

Spray and Flame Imaging at 20 kHz

- 0.7 mg pilot (210μs inj. dur.)
- Liquid fuel vaporizes quickly.
- Flame spread is relatively slow in the outer parts of the piston-bowl area.
- Highlights importance of flame speed for advanced SI combustion.

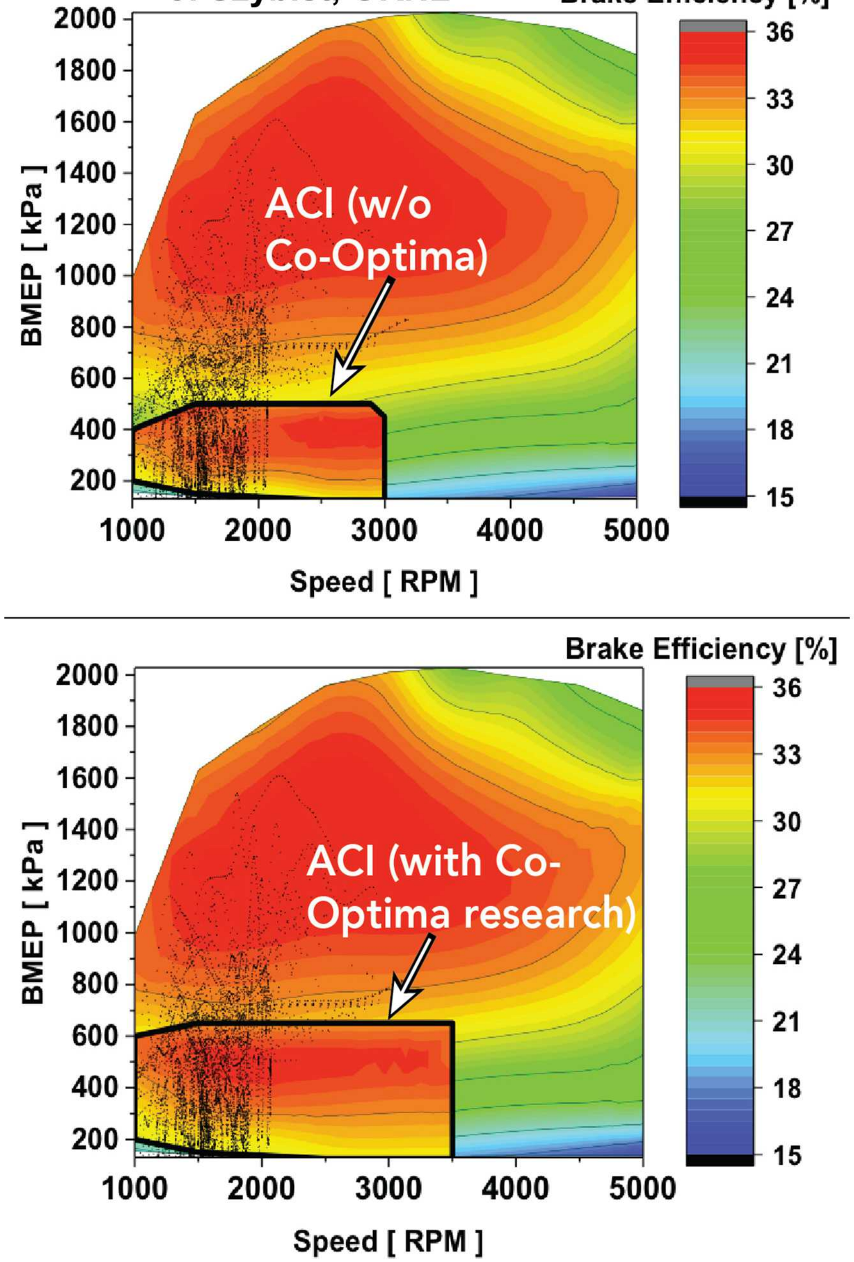




The Co-Optimization Challenge

- The promise of Co-Optima is to identify the optimal combination of fuel and engine combustion.
- For mixed-mode engines, boosted SI provides high-load capability.
- Stoichiometric combustion is often knock limited at high loads.
  - Appetite for higher RON and S.
- What is the fuels appetite for mixed-mode SI combustion?

Figure credit:
J. Szybist, ORNL

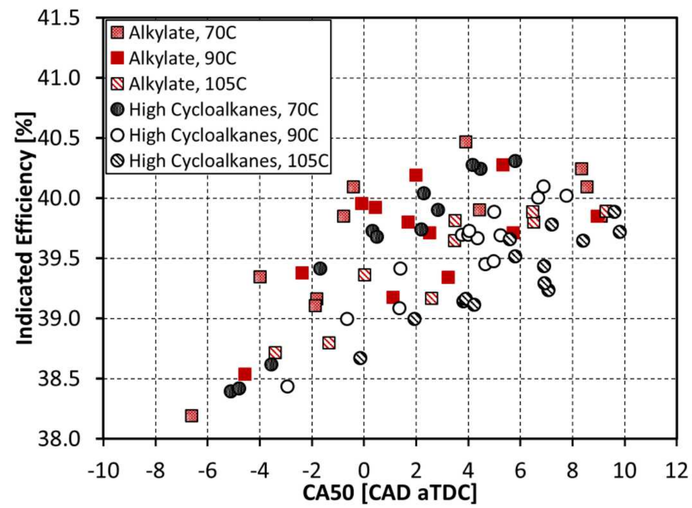


Magnitude of the Challenge

- Exploring the combined fuel-composition / engine-design space is a high-order problem.
- Fuel Parameters: RON, MON, HoV, O-PIONA, Carbon Bond Type Distribution.
- Engine Parameters: Fueling rate, Engine speed, Intake Pressure, Trapped Residuals, Spark Timing, Compression Ratio.
- Result: Greater than 10 independent variables which must be assessed.

Approaches & Throughput:

1. Engine Experiments: ~20 Conditions/day

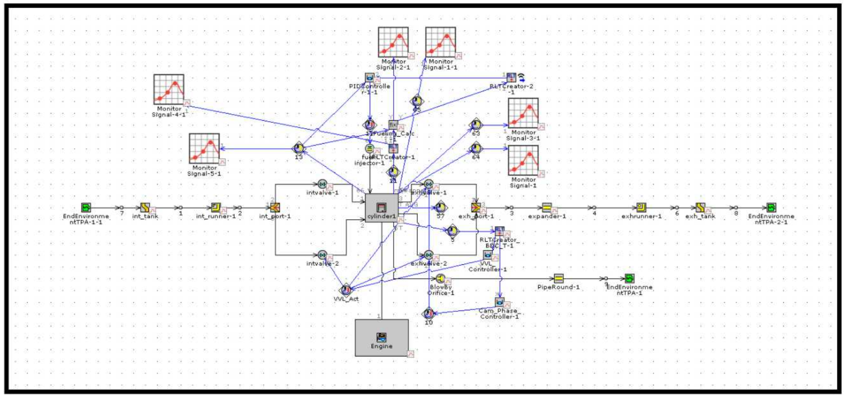


2. CFD: ~1 condition per day

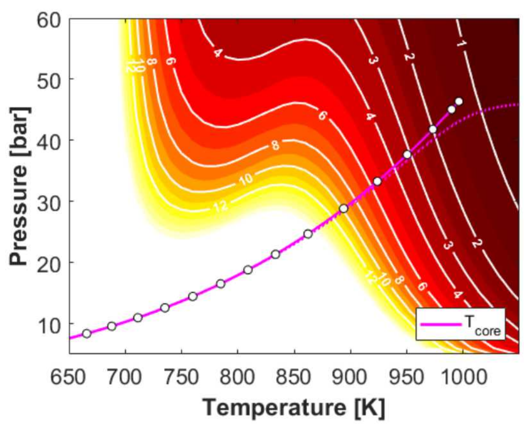
3. Reduced Order Modeling: 100 GT-Power Conditions Per Day; 700 Chemkin Conditions Per Day on a modern PC.
   – Explore this approach here.

Modeling Work Flow

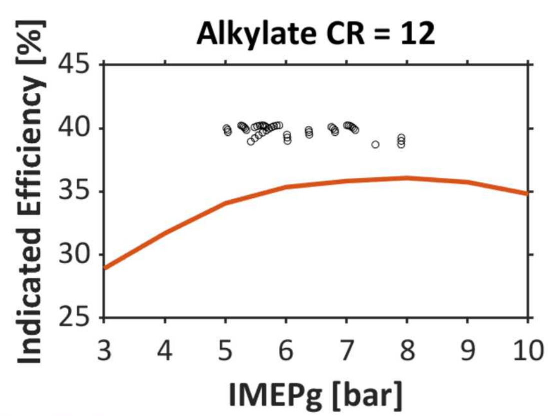
1. Determine Thermodynamic Profiles Using Well-Validated GT-Power Model



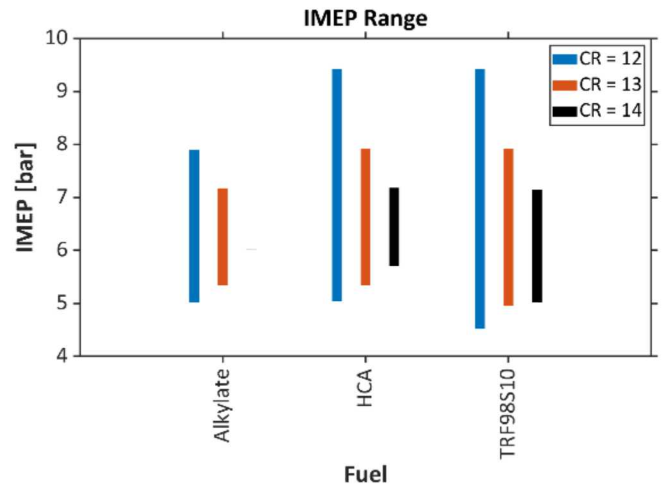
2. Impose Thermodynamic Profiles on Chemkin 0-D Reactor Model



3. Calculate Predicted Autoignition Phasing for Each Operating Condition; Screen Infeasible Conditions

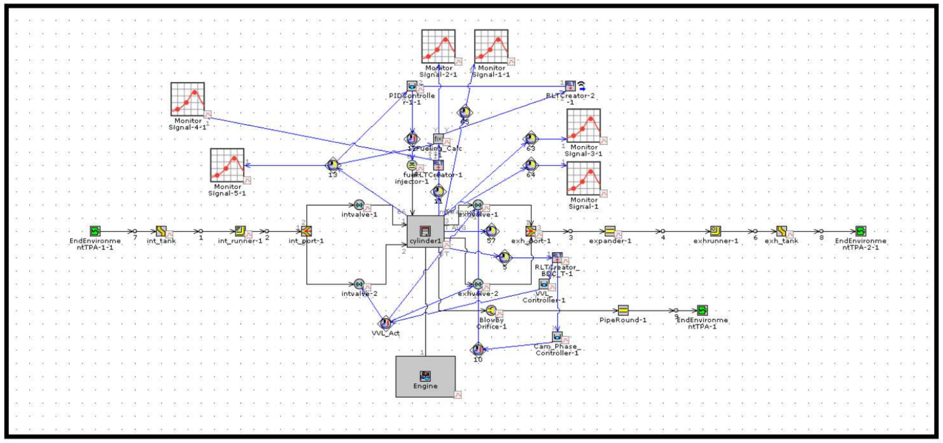


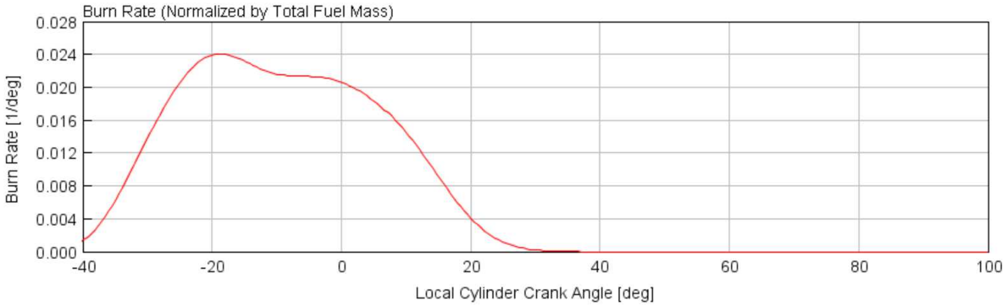
4. Assess Operating Range for Each Fuel and Compression Ratio

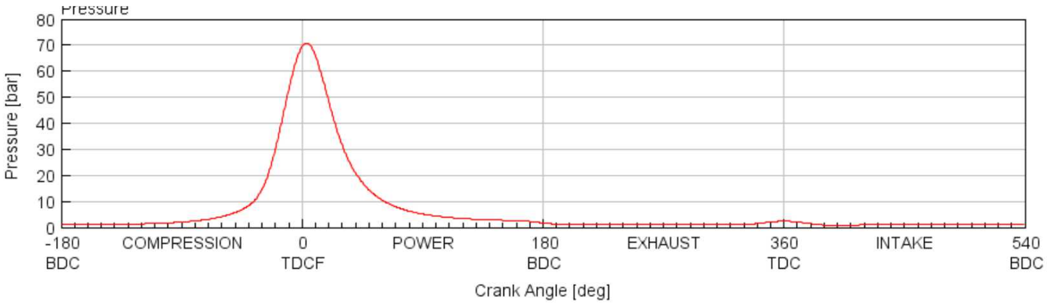


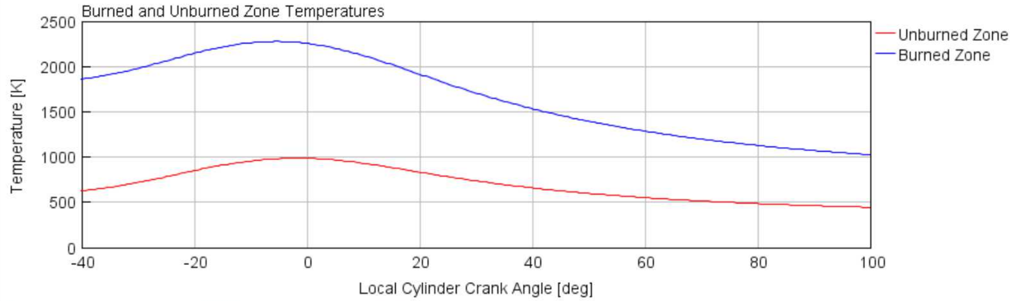
Calculate Thermodynamic Profiles Using GT-Power

- First, validate GT-Power model.
- To explore new conditions, impose new boundary conditions and burn profiles
  - Burn profiles prescribed by multi-Weibe functions (3)
- Explore a range of plausible operating conditions parametrically
  - CR: 12, 13, 14
  - CA50: -10 to 15°CA aTDC
  - BDC Temperature: 85 – 130 °C (trapped residuals)
    - $[O_2]$ covariant
  - ϕ_m: 0.45, 0.55
  - Intake Pressure: 1.0, 1.3 bar
  - Engine Speed: 1000, 1400, 2000 rpm
  - Focus on 1400 rpm for this presentation.



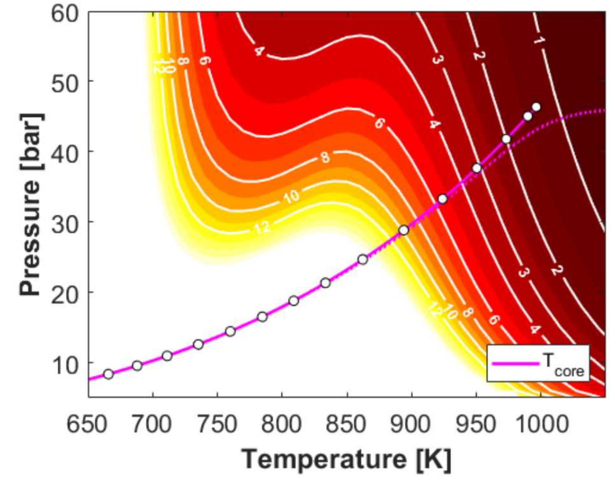


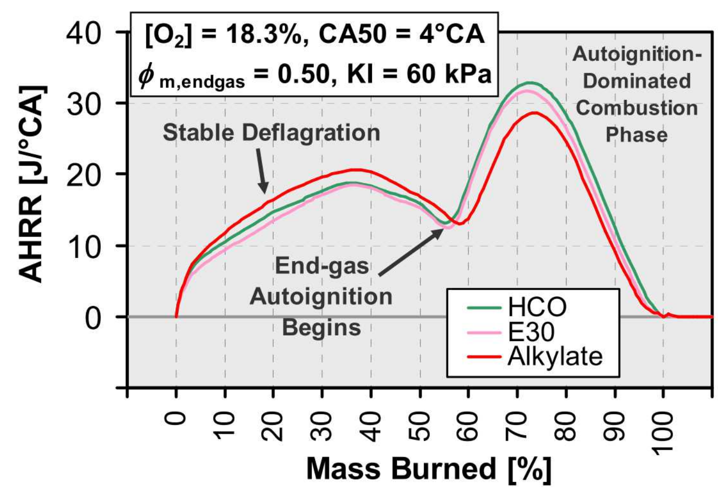




Calculate Autoignition Phasing in Chemkin

- Chemkin-Pro Homogeneous Reactor Model
- Pressure history and initial conditions imposed from GT Power
  - Simulates adiabatic compression
- Trapped residuals included (N_2, CO_2, O_2, H_2O, NO, Fuel)
- Imposed pressure history reflective of in-cylinder conditions without autoignition (compression and deflagration-only)
  - Useful for determining onset of autoignition.
  - But not for any behavior that occurs after autoignition (peak rates of heat release, knock).
- Need multi-zone and/or 3D CFD for assessing fuel effects on peak HRR.





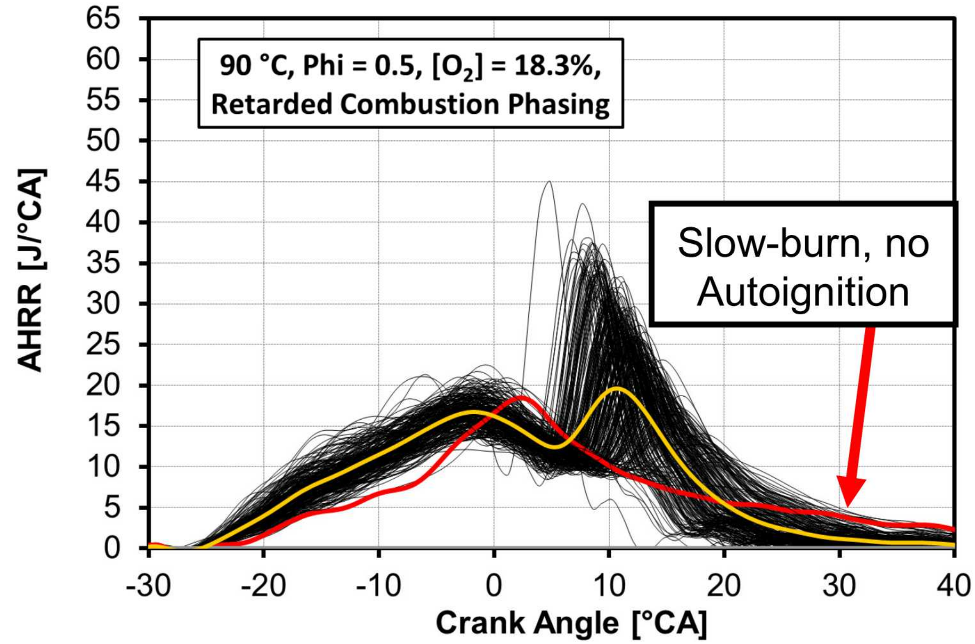
Initial Fuels Matrix

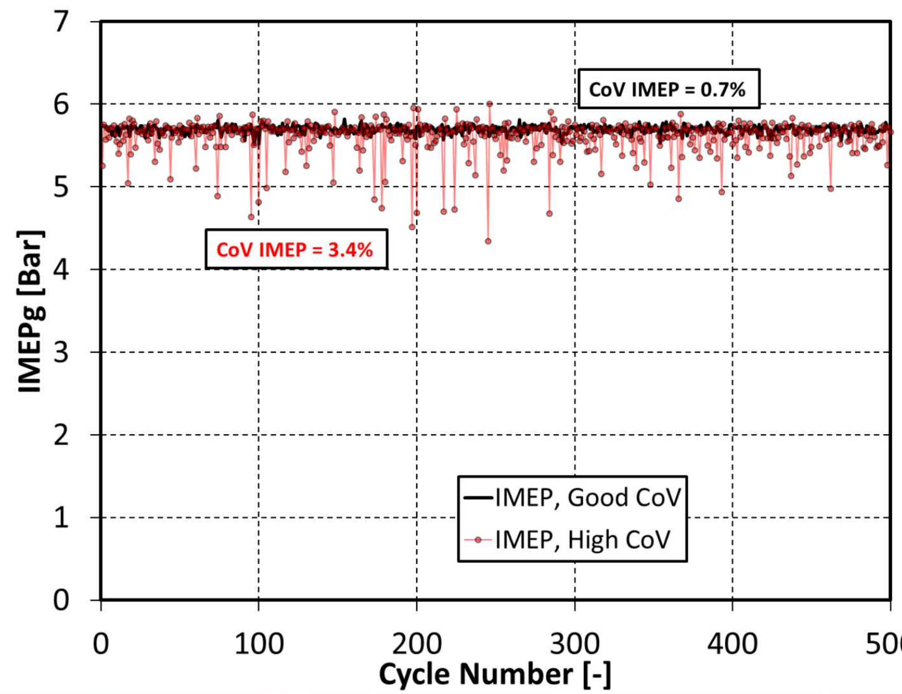
- LLNL Co-Optima Gasoline Surrogate Mechanism used.
  - Including NO_x chemistry.
- Two Co-Optima Core Fuels: RON = 98, S: 1, 10
- Toluene Reference Fuels: RON: 98 - 83, S: 7, 8, 10
- Primary Reference Fuels: RON: 98 - 81, S = 0.

#	Name	RON	S
1	Alkylate	98	1
2	High Cycloalkanes	98	10
3	TRF98S10	98	10
4	TRF98S7	98	7
5	TRF95S7	95	7
6	TRF92S8	92	8
7	TRF87S7	87	7
8	TRF85S7	85	7
9	TRF83S7	83	7
10	PRF98	98	0
11	PRF95	95	0
12	PRF91	91	0
13	PRF89	89	0
14	PRF87	87	0
15	PRF85	85	0
16	PRF83	83	0
17	PRF81	81	0

Interpret Chemkin Results: Operating Limitations

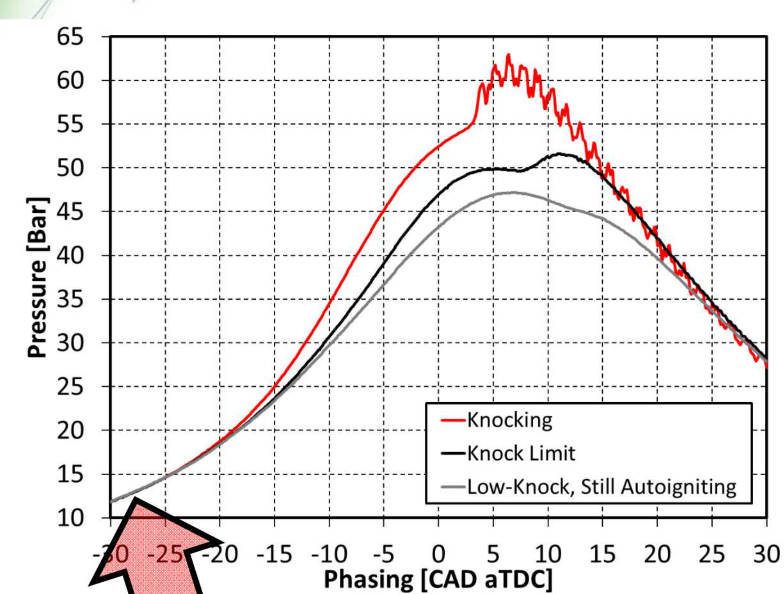
- Chemkin results yield time of autoignition for charge.
  - Converted to crank-angle phasing.
- Autoignition phasing compared to imposed burn profile to determine autoignITING mass fraction.
- Need to be cognizant of physical limits and screen conditions which are inoperable.
  - Too much autoigniting mass ➔ knocking.
  - Too little autoigniting mass ➔ slow combustion, high CoV IMEP.
  - Too advanced phasing ➔ loss of spark control authority, poor thermal efficiency.
  - Too retarded phasing ➔ high CoV autoignition phasing and IMEP.

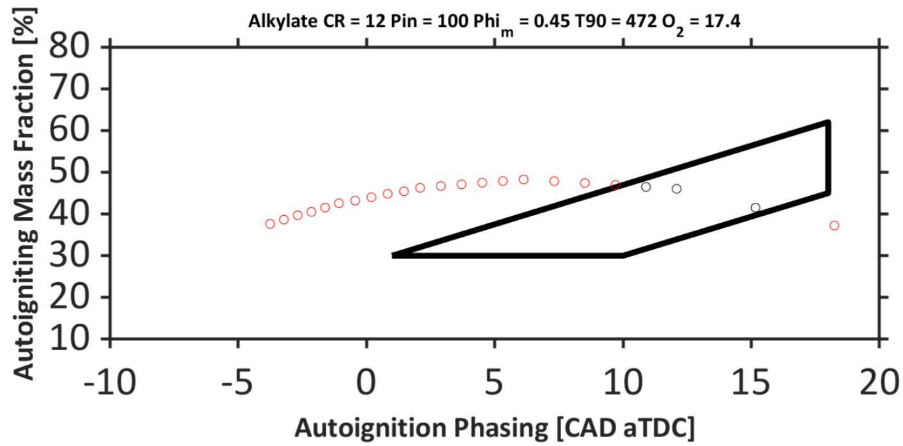




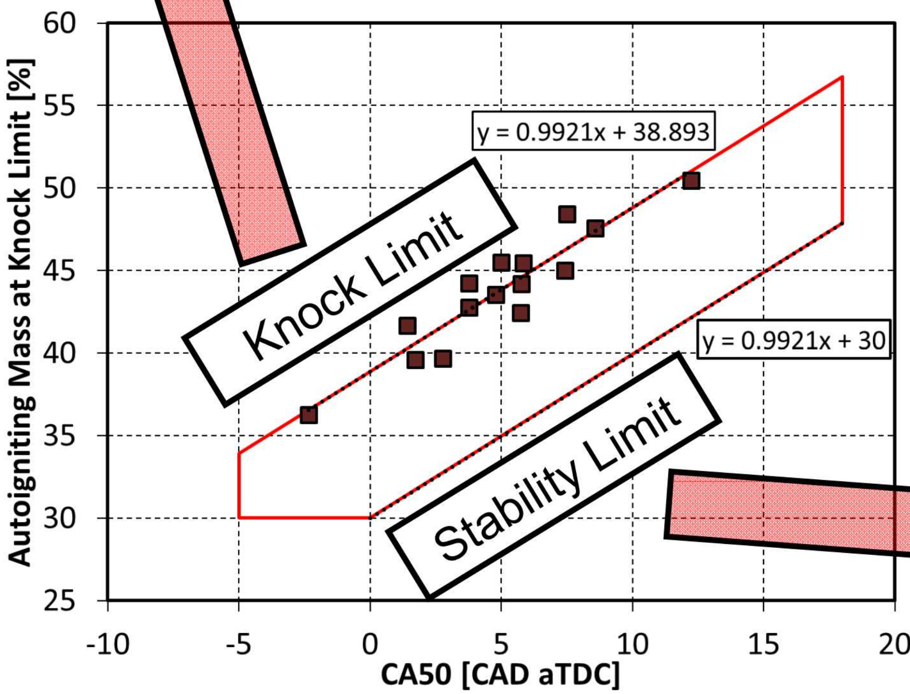
Interpret Chemkin Results: Operating Limitations

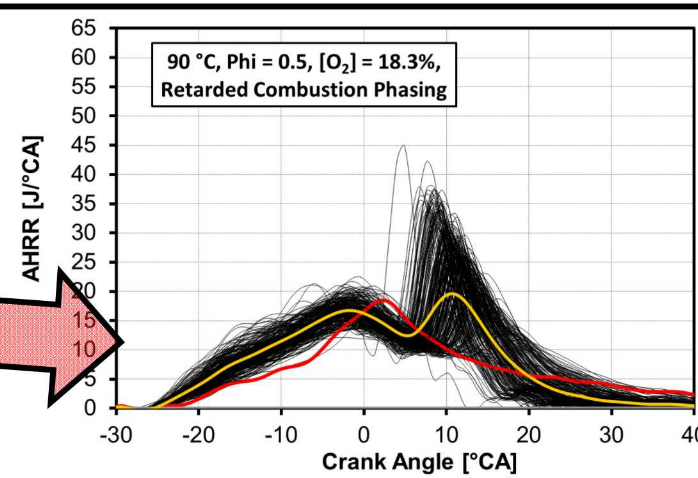
- Operating limits create a space of operability
- Each fuel and operating condition tested for intersection with this operability space





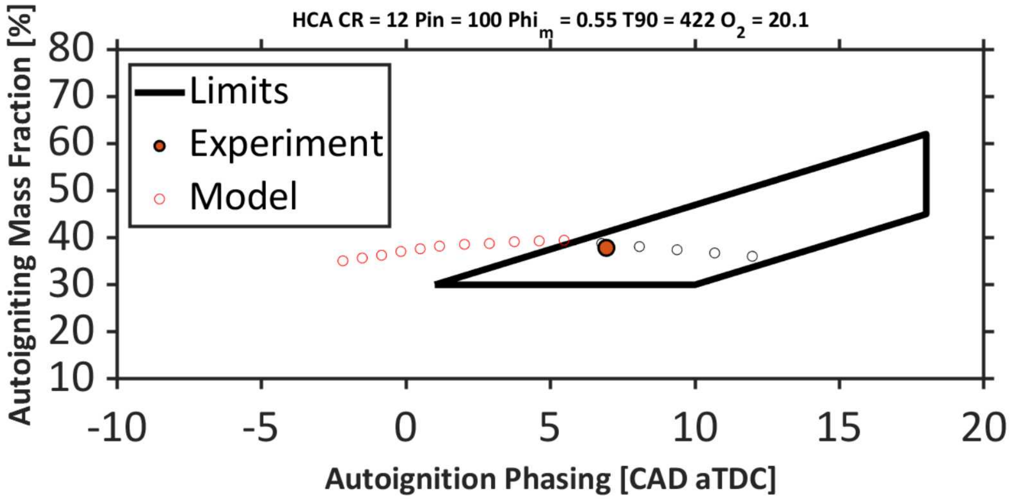
Note: Limits specified in terms of CA50 as this aligns with the available engine data, but more intuitive to think about autoignition phasing, so plotted in this manner

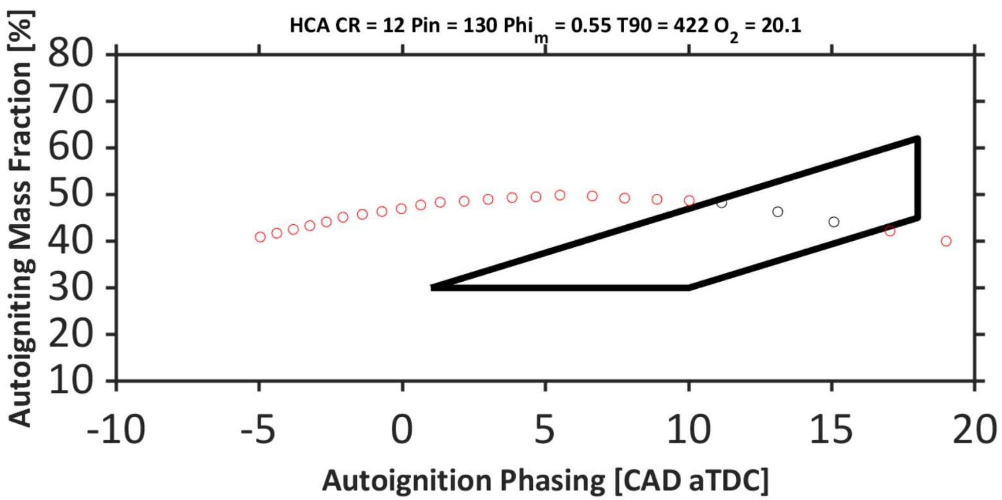




Managing Charge Reactivity for Operability

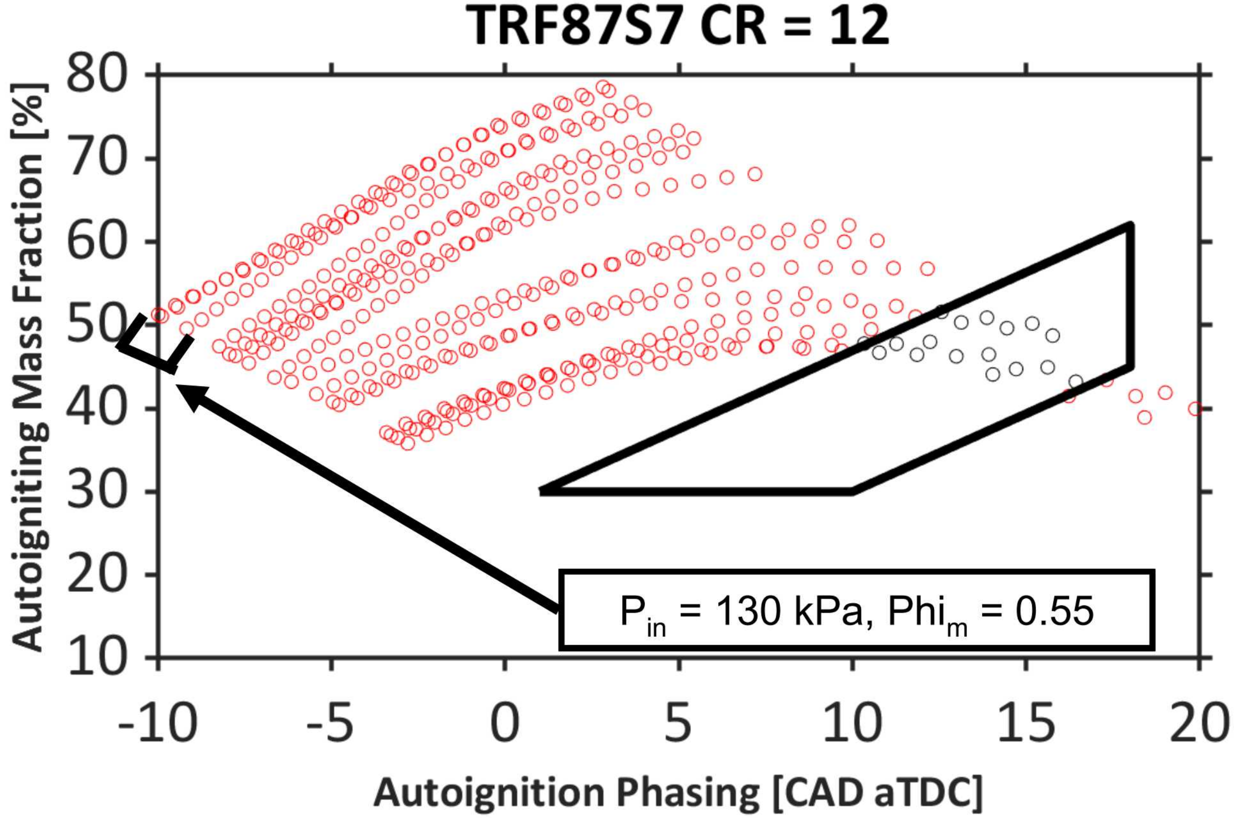
- Hold Constant: CR = 12, P_{in} = 100 kPa, ϕ_m = 0.45
- CA50 sweep intersects with range of operability
  - Predicted to not be knocking, not misfiring
- Increase trapped residual level
  - Effects charge temperature and oxygen concentration
  - Shifts autoignition phasing such that more mass is consumed by autoignition
- Increase ϕ_m
  - Increases compression heating by flame and raises end-gas reactivity
- Raise intake pressure
  - Raises reactivity such that later spark and autoignition phasings are required

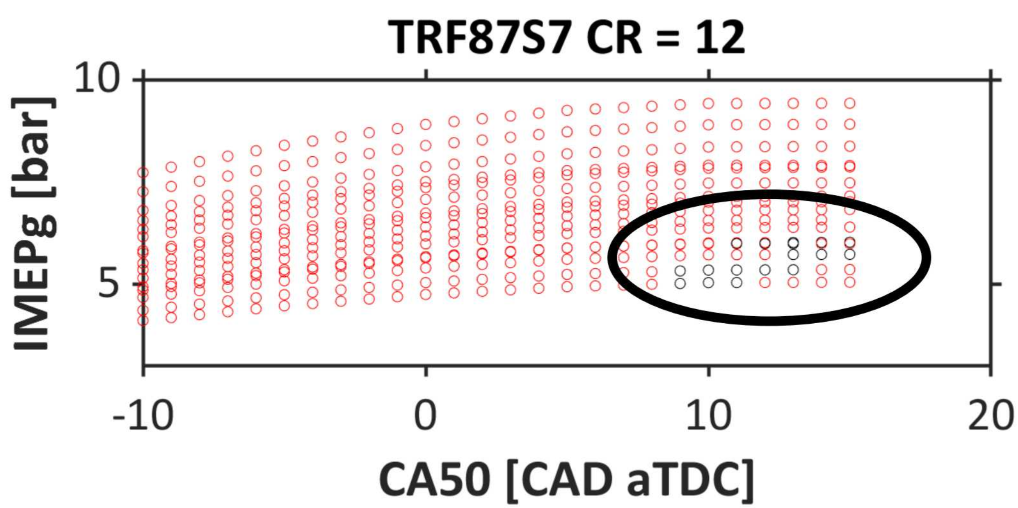




Assessing Operability of a Fuel

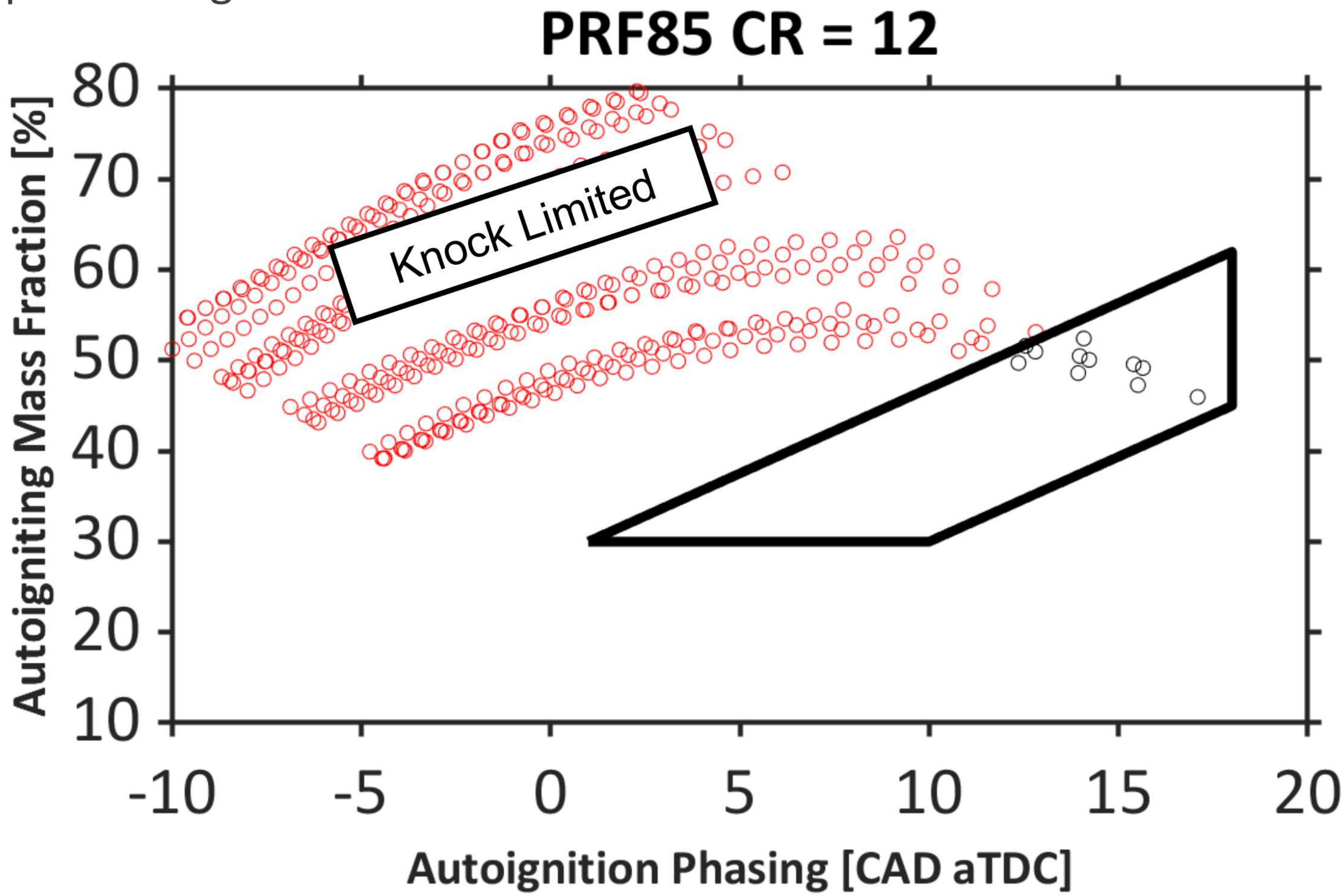
- Sweep CA50, trapped residuals, ϕ_m, and intake pressure
  - Determine intersection with knock and stability limits
- Fuel's reactivity and changes in reactivity with intake conditions determine intersection with operating space
- In this example, the fuel is too reactive to achieve high-load conditions
  - Only lower intake pressures and delayed combustion phasings allow operation without knock





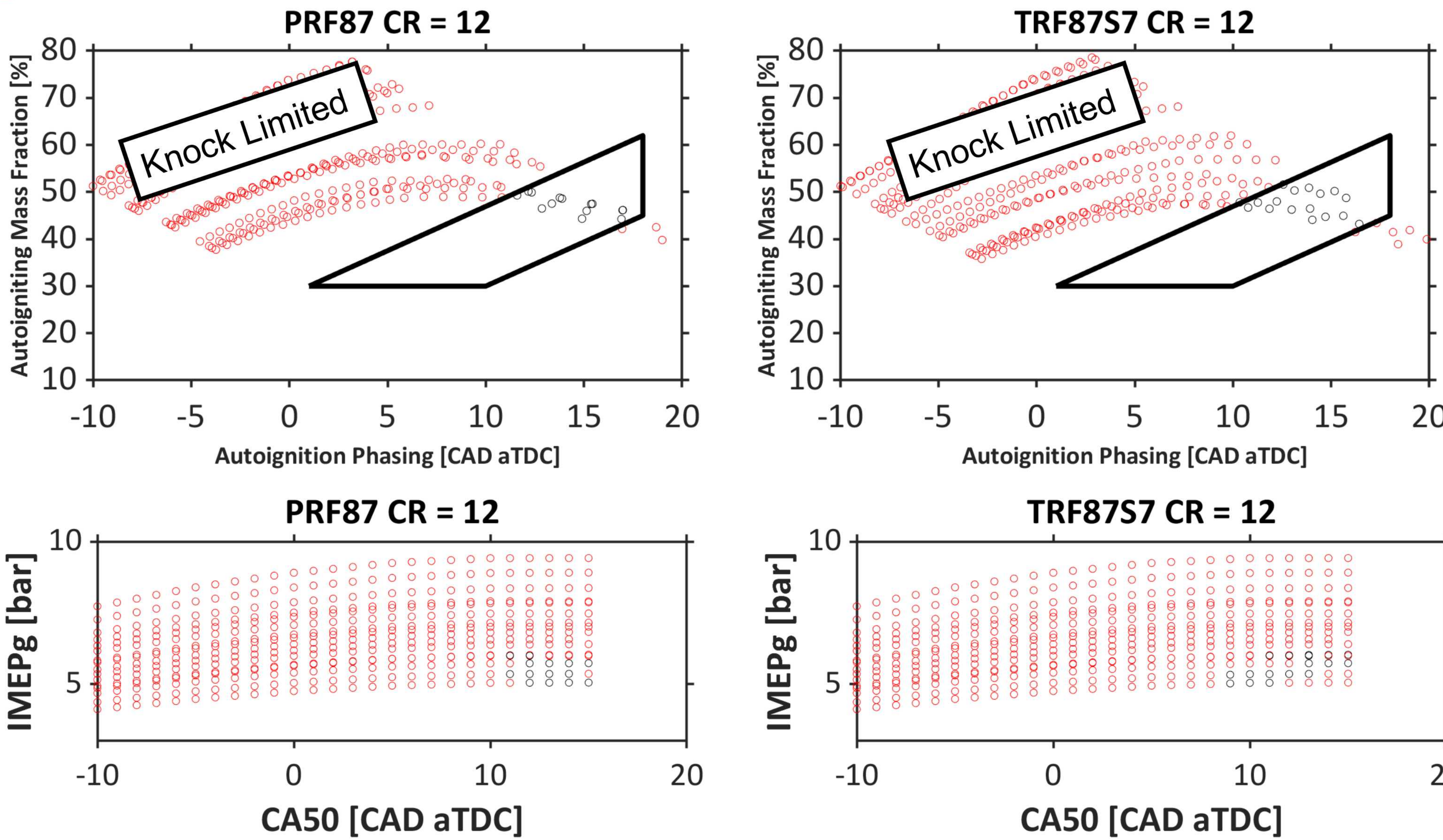
Effects of RON and Sensitivity

- Fuel RON sweep illustrates how more reactive fuels can diminish the operability range
  - Load range primarily determined by high-load limit
  - Low-load operation tested here achievable with trapped residuals and advanced spark timing



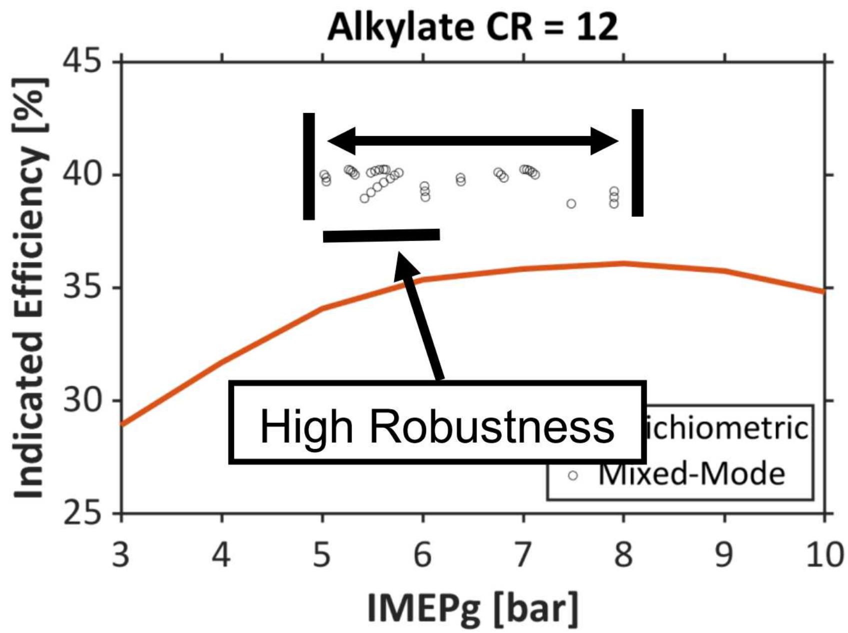
Effects of RON and Sensitivity

- Higher sensitivity fuels at same RON level show slightly lower reactivity
  - Permits higher-load operation

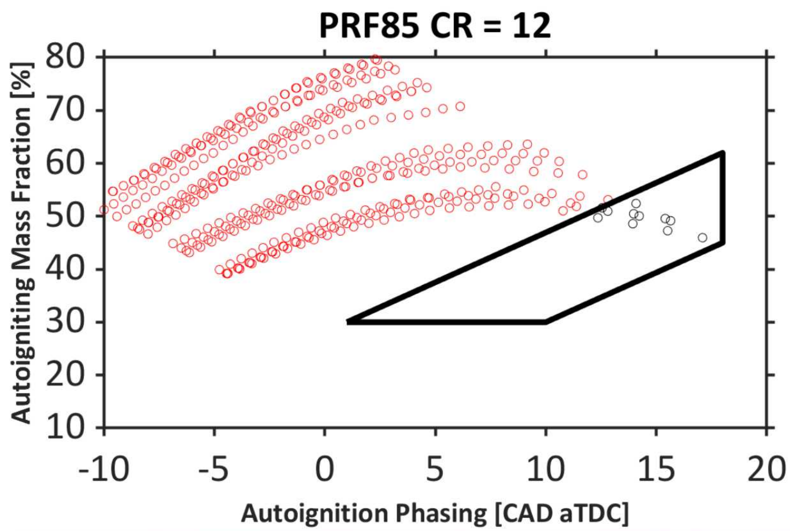


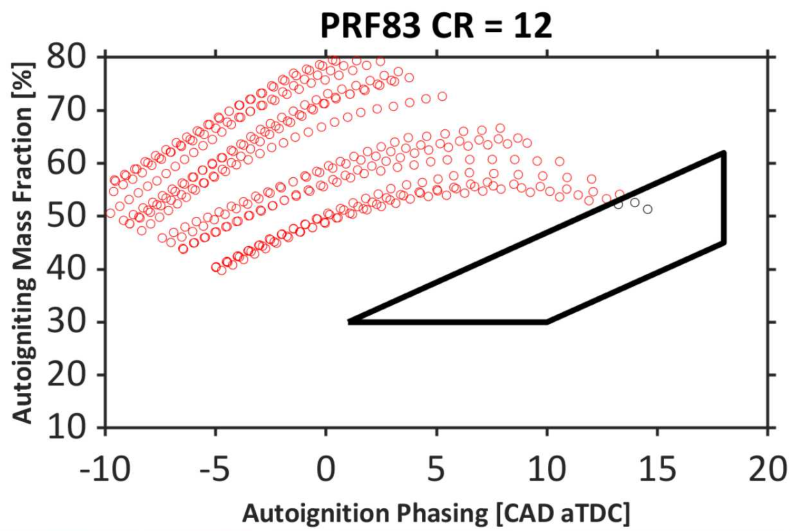
Assess Fuel Operability Range and Robustness

- Each fuel and CR assessed for load range and robustness
  - Range = difference between highest and lowest IMEP points
  - Robustness = # operating points / range
    - Robustness considers number of possibilities for achieving a given load; more possibilities allow for greater perturbation resistance



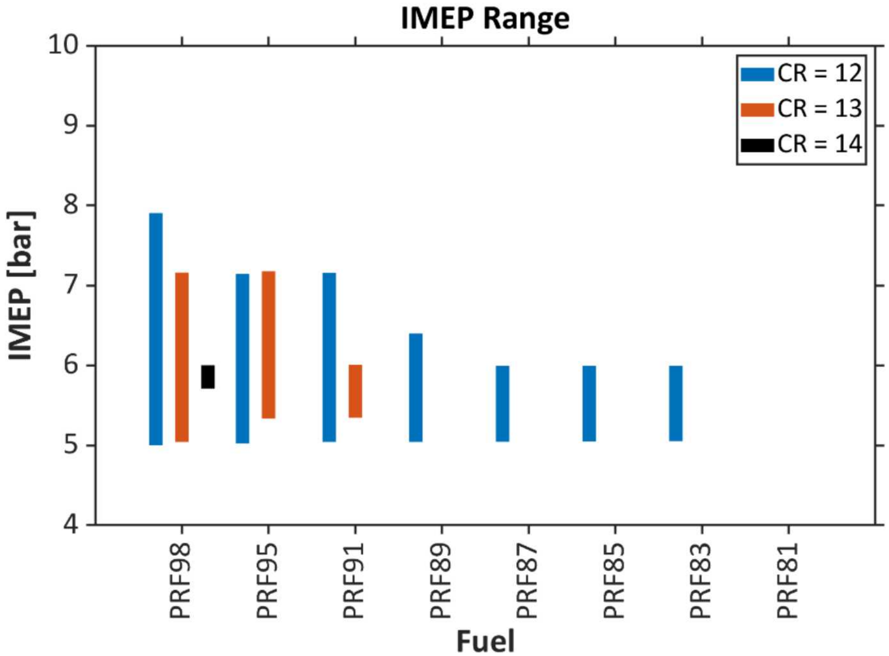
- PRF83/85 example highlights importance of robustness metric.
  - PRF 83 and 85 have nearly the same load range (~1 bar), but differ in robustness

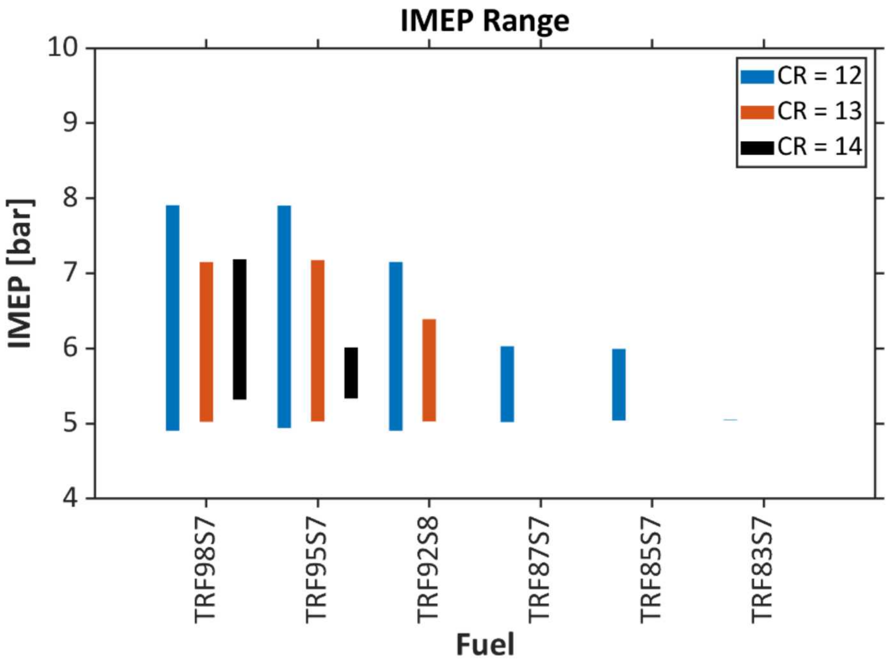




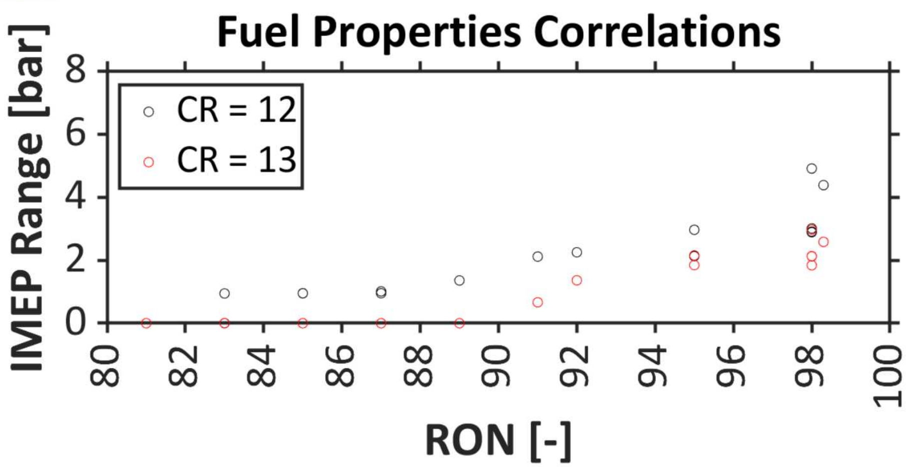
PRF & TRF Sweep: Minimum RON?

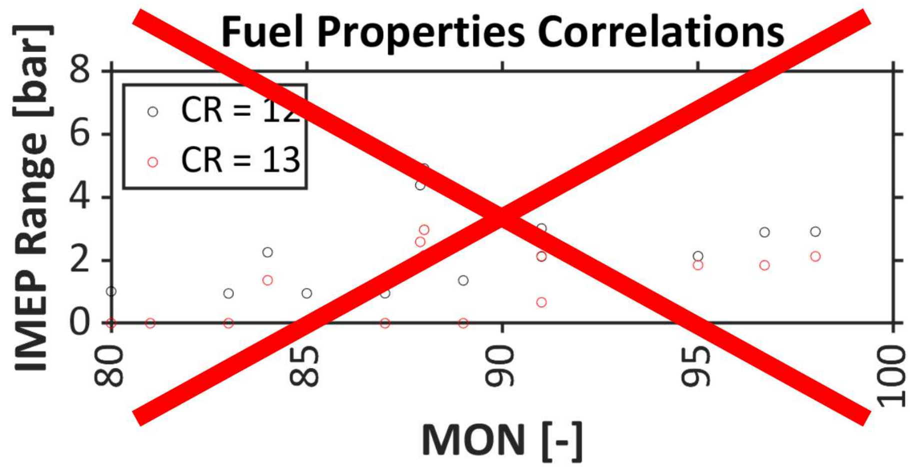
- Sweeps of reference fuels indicate a minimum autoignition resistance required under the chosen operating conditions
  - Shifts in engine speed, CR, or ϕ_m range would shift the minimum fuel autoignition resistance
- More autoignition-resistant fuels extend high-load range, but do not hinder low-load range
- Octane-sensitive fuels more tolerant of higher compression ratios

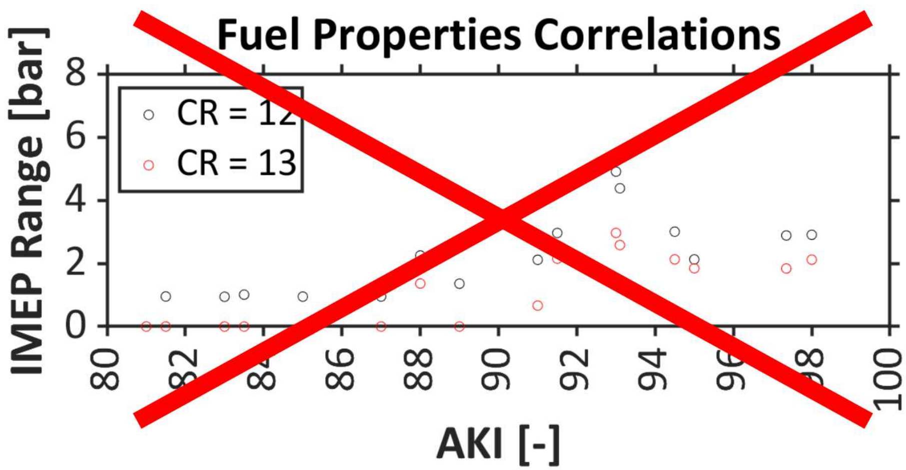


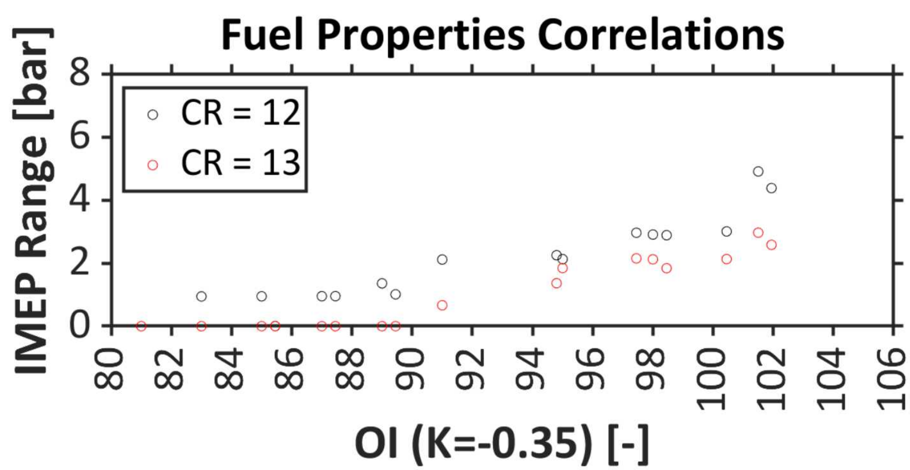


RON and MON as Predictors of Load Range



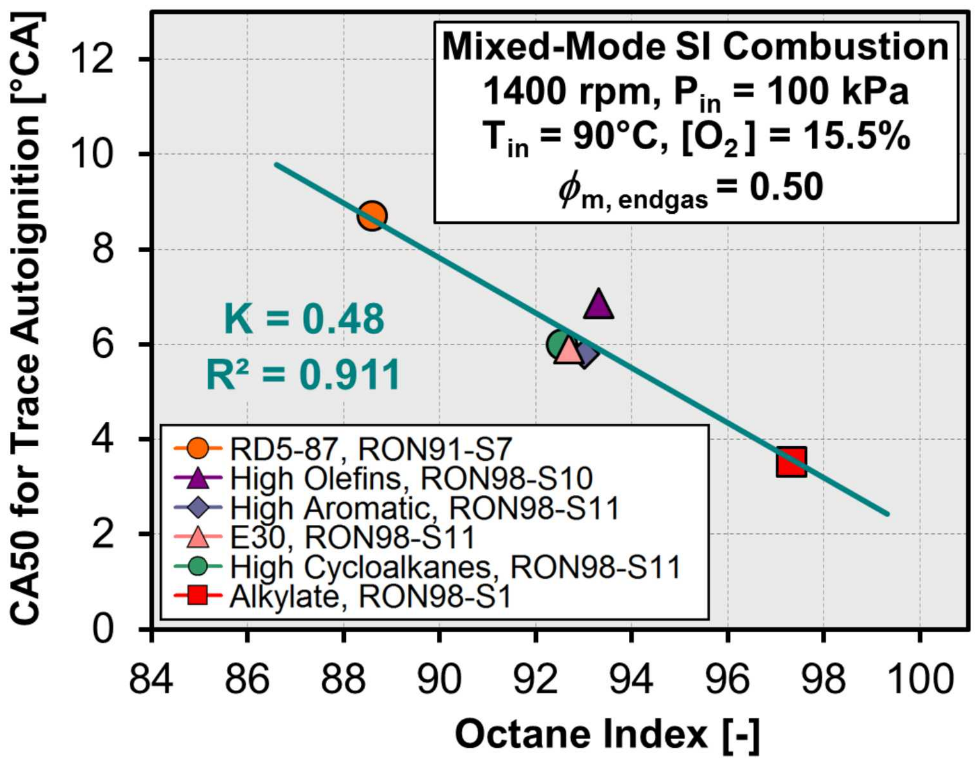






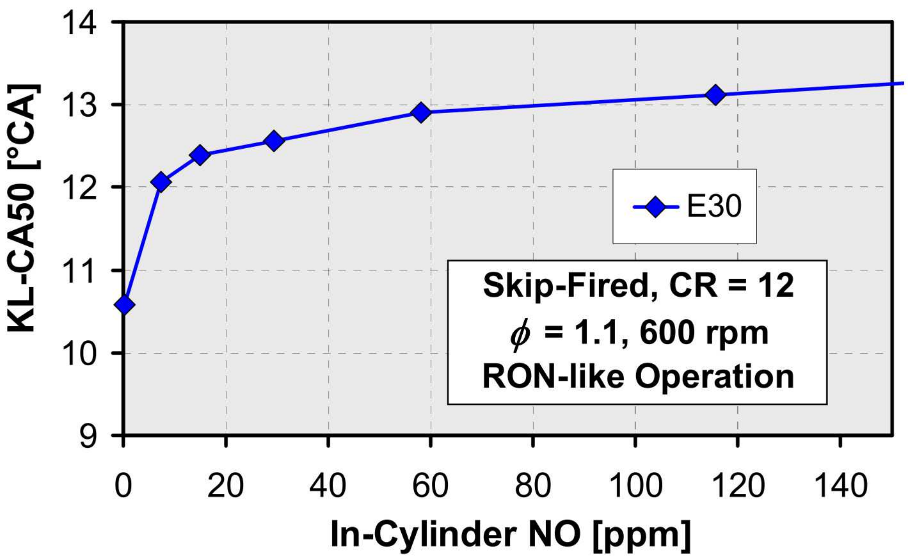
Octane Index vs. Autoignition

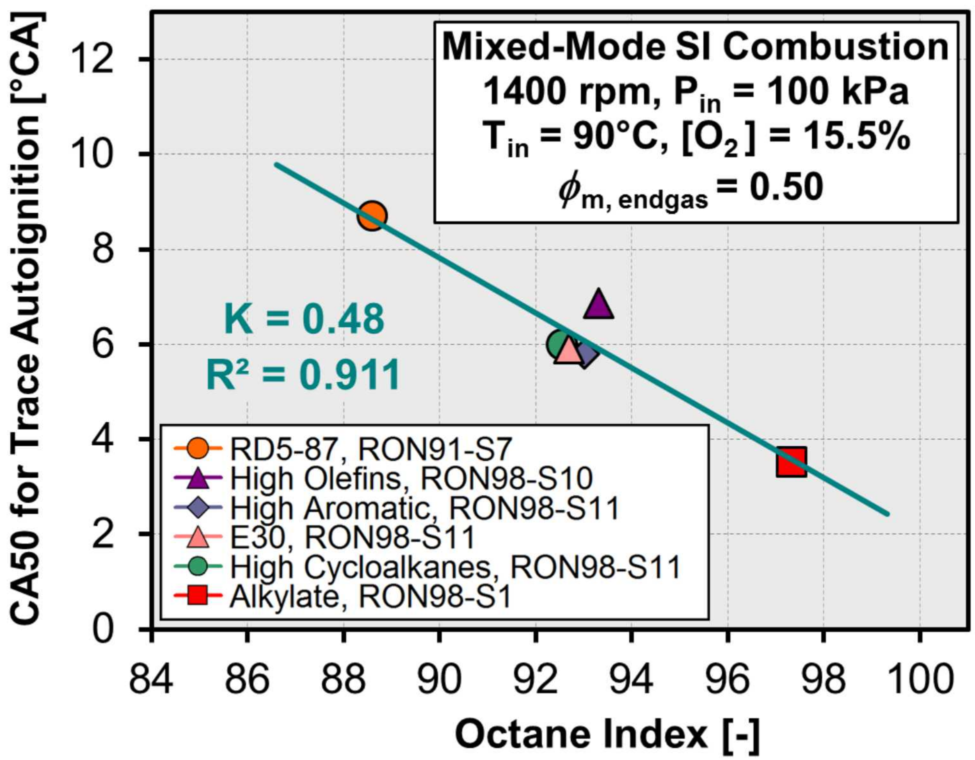
- Six fuels have been tested experimentally in this combustion mode.
- For those operating conditions that allow meaningful application of Octane Index, the correlation has generally been OK.
- Yesterday, Dario Lopez-Pintor examined several factors that can cause poor correlation between autoignition and OI.
  - Engine speed.
  - Lower ϕ.
  - Lack of deflagration-based pressure rise in HCCI mode.
- Another factor may be absence of residual NO_x for pure HCCI mode.



Role of NO_x for Autoignition and OI

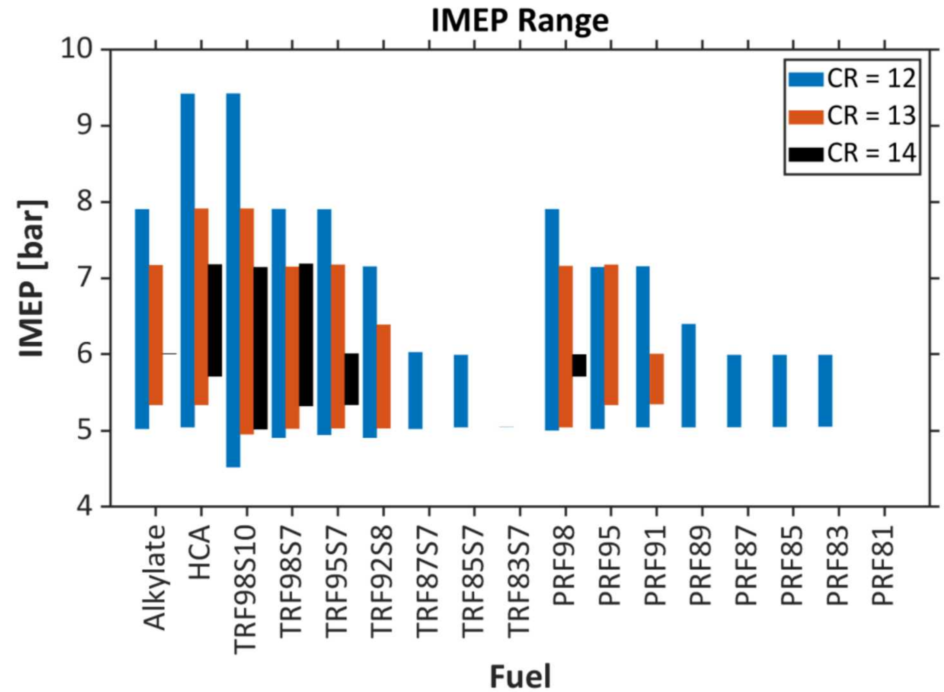
- Another factor may be absence of residual NO_x for pure HCCI mode.
- RON and MON tests are "tainted" by residual NO_x.
- Sensitivity to NO_x is likely to differ between fuels.
  - As well as between combustion modes and operation conditions.

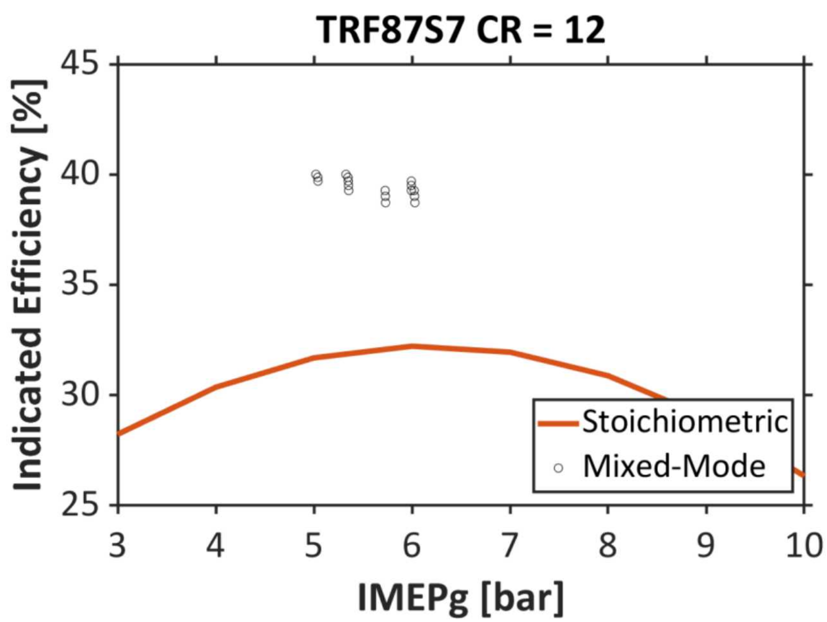


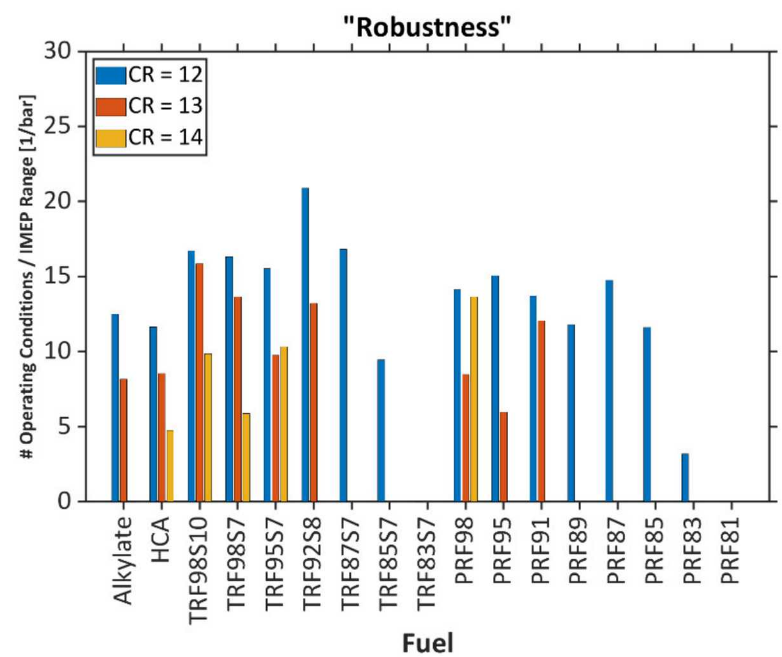


Future Work: Extending Study to Drive Cycle

- Range of operating conditions will be expanded to consider engine speeds from 1000 – 2000 rpm.
- Results will be used to assess benefit over drive cycle using a time-weighted approach.
  - Lower-RON fuels may see larger relative benefit (due to more-severe stoichiometric knock limits) but offer less load range and robustness.



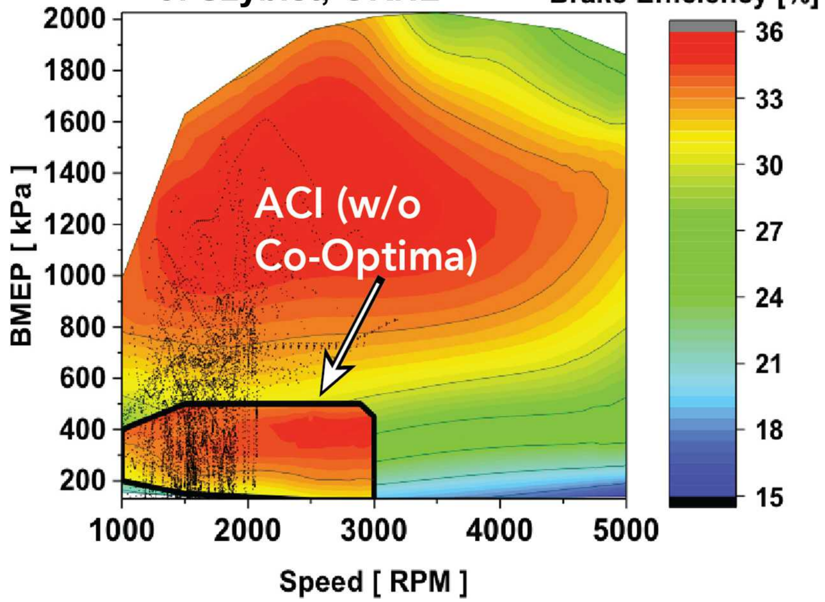


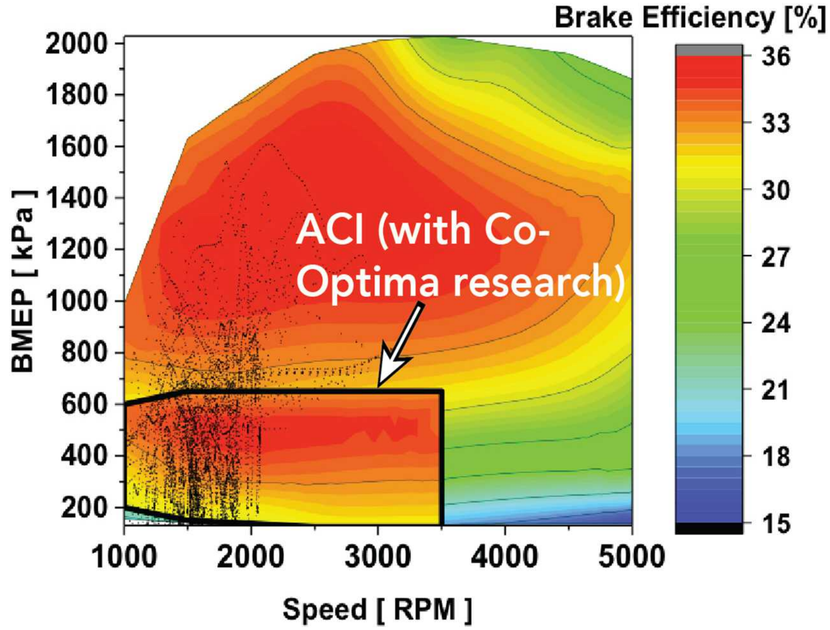


Future Work: Identify Fuel Properties

- The promise of Co-Optima is to identify the optimal combination of fuel and engine combustion.
- Need to perform extensive search for better fuels.
- What fuel property metrics are best at capturing the observed FE gains of mixed-mode combustion?
- Large data sets will be available for "data mining".

Figure credit:
J. Szybist, ORNL





Summary

1. **What is lean end-gas autoignition?** A 50-50 deflagration-autoignition combustion mode for efficient, lean, controllable combustion.

2. **Can we model fuel effects leading to efficiency benefits?** Yes, with appropriate validation we can construct models which reproduce trends observed experimentally, and translate this to anticipated efficiency gains.

3. **What have the models taught us?** The fuel requirement synergies between stoichiometric SI and mixed-mode combustion are surprisingly strong. Both modes require autoignition resistant fuels to achieve "High Loads." Fuels with high Octane Sensitivity show less sensitivity to intake boosting, thereby extending load range.

4. **Future Work:** Extend study to broader engine speed range, assess benefit over drive cycle. Conduct experimental validation on predicted limits. Make data available for "data mining".

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