Co-Optimization of Fuels & Engines

Co-Optima Boosted Spark-Ignition and Multi-Mode Combustion, Part 2

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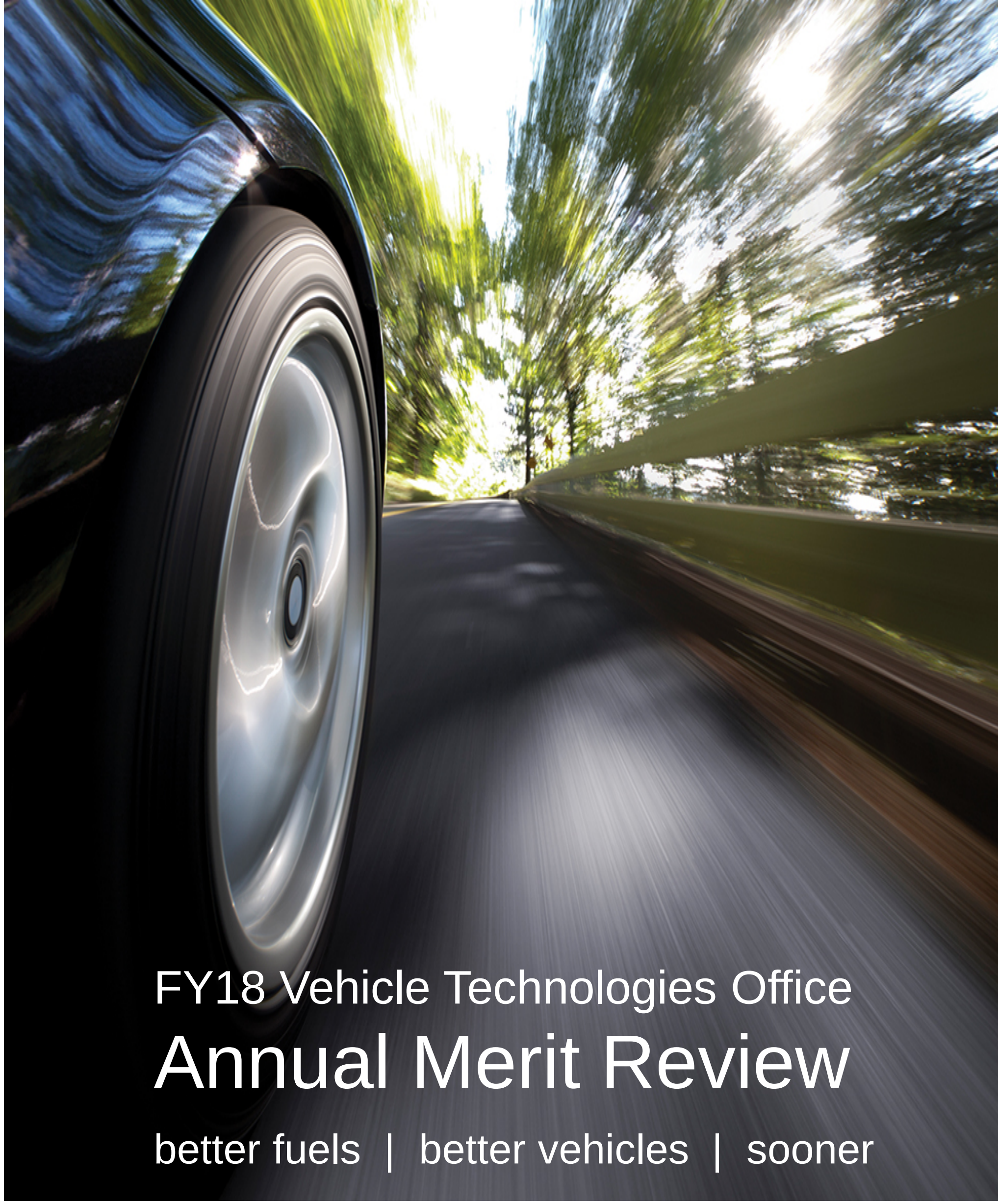
June 20, 2018

Project # FT054



FY18 Vehicle Technologies Office

Annual Merit Review

better fuels | better vehicles | sooner

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

VTO Program Managers: Gurpreet Singh, Kevin Stork, & Michael Weismiller

Overview

Timeline

- Project start date: 10/1/2015
- Project end date: *9/30/2018
- Percent complete: 88%

Budget

- Total project funding
  - DOE share: $855k
  - Contractor share:
- Funding in FY 2017: $1,300k
- Funding for FY 2018: $855k

*Start and end dates refer to three-year life cycle of DOE lab-call projects, Co-Optima is expected to extend past the end of FY18

Barriers

Lack of robust lean-burn and EGR-diluted combustion technology/controls

Inadequate fundamental knowledge base for clean diesel combustion and emissions processes

Determine factors limiting low temperature combustion (LTC) and develop methods to extend limits

Understanding impact of likely future fuels on LTC and whether LTC can be more fully enabled by fuel specifications different from gasoline and diesel fuel

Partners

Partners include nine national labs, 13 universities, external advisory board, and stakeholders (145 individuals from 86 organizations)

Overview

Boosted SI and Multimode SI/ACI Combustion, Part 2

Effects of fuel properties and property quantification on engine efficiency using engine experimental data to feed into the fuel and engine Co-Optimizer.

Project	PI
Fuel Properties Effects on Auto-Ignition in Internal Combustion Engines ($250k)	Kolodziej (ANL)
Virtual CFR engine based on CFD ($50k)	Som (ANL)
Co-Optimizer ($140k)	Grout (NREL), McNenly (LLNL)
Develop Co-Optimizer Inputs ($415k)	Grout (NREL), Mueller (LBNL) McNenly (LLNL)

Relevance

- Internal combustion engines will continue to dominate the fleet for decades and their efficiency can be increased significantly.
- Research into better integration of fuels and engines is critical to accelerating progress towards our economic development, energy security, and emissions goals.
- Improved understanding in several areas is critical for progress:
  - Fuel structure – property relationships
  - How to measure and predict key fuel properties
  - The impact of fuel properties on engine performance and emissions
- This presentation is focused on Boosted SI and SI/ACI multi-mode combustion. MD/HD diesel, and full-time ACI combustion strategies are addressed in other Co-Optima presentations.

ACI: advanced compression ignition
HD: heavy duty
LD: light duty
MD: medium duty
SI: spark ignition

Milestones

Month / Year	Description of Milestone or Go/No-Go Decision	Status
12/31/17	Baseline standard (N/A) ASTM RON test conditions to boosted CFR engine operation (ANL).	Completed
6/30/18	Release of Co-Optimizer as open source to external community (contingent on DOE assent) (NREL).	On track
9/30/18	Demonstrate ability of Co-Optimizer framework to incorporate synthetic data and optimize resulting merit function in one or more directions (LBNL).	On track
9/30/18	Measure the uncertainty quantification performance using a hierarchy of kinetic-based engine models at varying levels off chemical and fluid dynamic fidelity (LLNL).	On track

Approach

<u>Projects have contributed to Co-Optima in two ways:</u>

1 – Central Fuels Hypothesis

- If we <u>correctly identify the critical fuel properties that affect efficiency and emissions</u> performance for boosted SI and multi-mode engines, then fuels that have those properties will provide optimal engine performance.

2 – Boosted SI Merit Function

RON & MON (S)

Measurement & Simulation

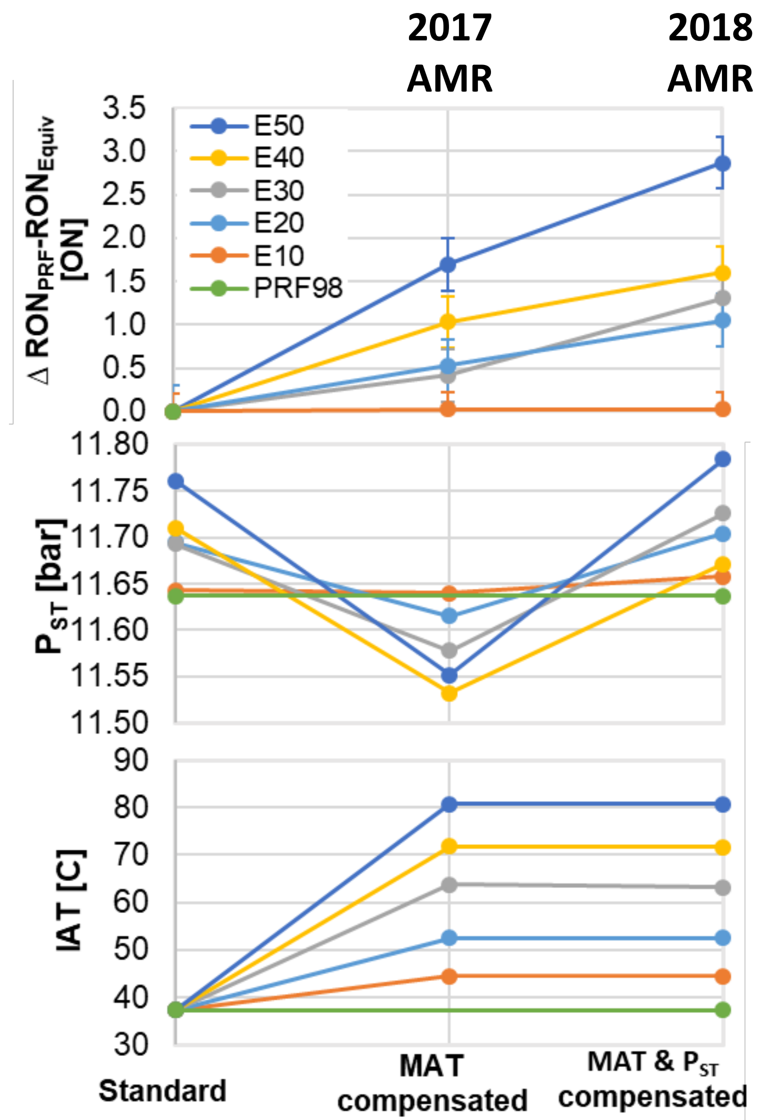
RON & HoV

$$Merit=\frac{(RON_{mix}-91)}{1.6}-K\frac{(S_{mix}-8)}{1.6}+\frac{0.085[ON/kJ/kg_{mix}]\cdot((HoV_{fuel}/(AFR_{stoich}+1))-(415[kJ/kg_{fuel}]/(14.3[-]+1)))}{1.6}$$
$$+\frac{((HoV_{fuel}/(AFR_{stoich}+1))-(415[kJ/kg_{fuel}]/(14.3[-]+1)))}{15.38}+\frac{(S_{L\,mix}-46[cm/s])}{5.4}$$
$$-H(PMI-1.6)[0.7+0.5(PMI-1.4)]+0.008^{\circ}C^{-1}(T_{c,90,conv}-T_{c,90,mix})$$

Co-Optimizer

Fuel Properties Effects on Auto-Ignition in Internal Combustion Engines

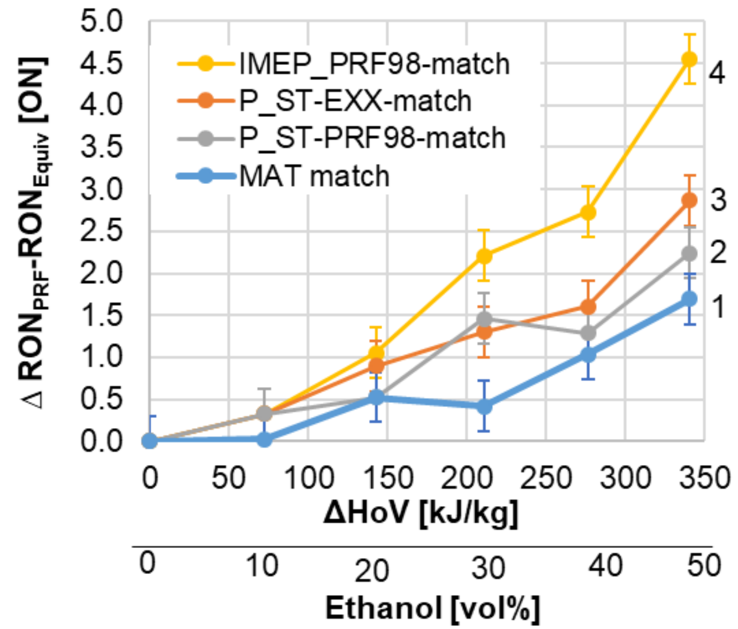
- **Objective**: Learn how fuel properties, such as heat of vaporization (HoV) or even RON itself affect a fuel's propensity for auto-ignition and knock intensity
- Last year, the HoV cooling effect on RON was compensated using intake air heating for constant RON 98 PRF-ethanol blends, expanding previous work by Foong et al.
- However increased intake air temperature (IAT) reduced cylinder pressure at spark timing (P_{ST})
- Using small amounts of intake pressure compensation, P_{ST} could be recovered at the same time as MAT with increased HoV
- Resulting test conditions were the same MAT as PRF and same P_{ST} that the high HoV fuel had under standard RON conditions



Fuel Properties Effects on Auto-Ignition in Internal Combustion Engines

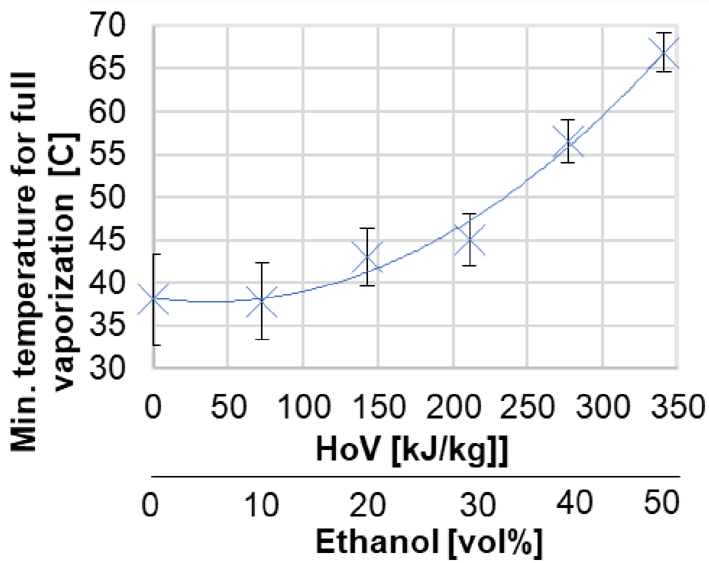
Levels of MAT and intake pressure compensation:

1. Heat IAT until MAT matches that of PRF
2. Increase intake pressure until P_{ST} of PRF fuel is matched from standard RON test
3. Increase intake pressure until P_{ST} of high HoV fuel is matched from standard RON test
4. Increase intake pressure until IMEPg is matched with that of the PRF (constant IMEPg fuel knock rating also compensated for MAT)



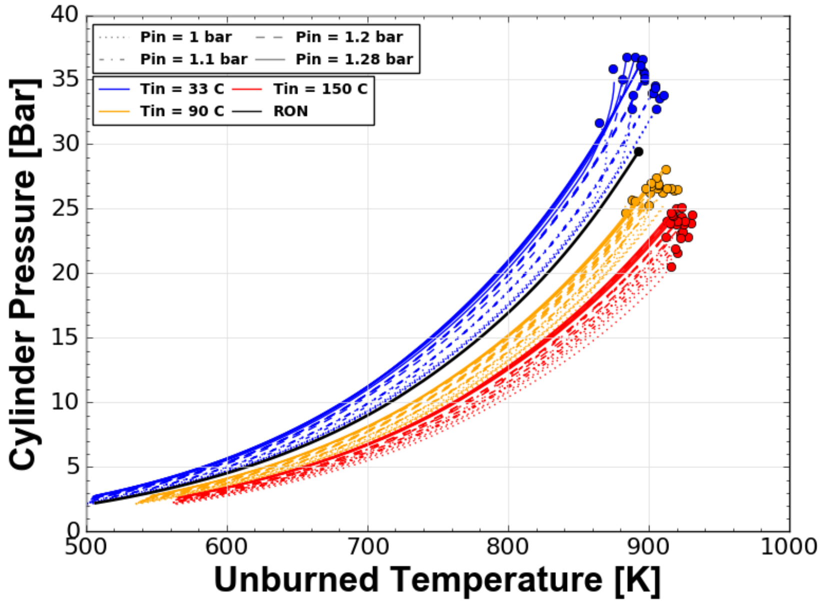
Evaluation of full fuel vaporization:

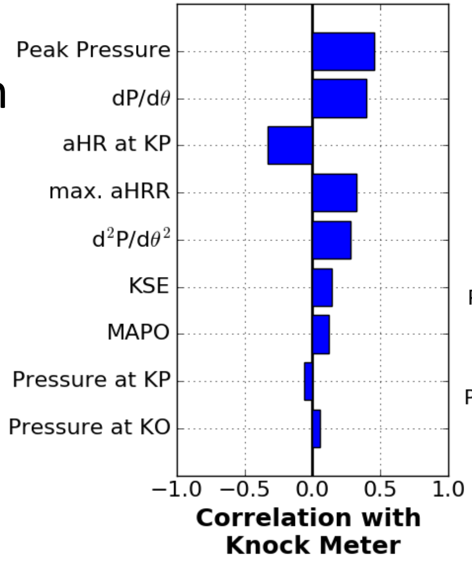
- Sweeps of IAT revealed the temperature where not all of the fuel was fully vaporized at the exit of the carburetor for each blend (technical backup slides)
- Compiling that data, a relationship between PRF-ethanol content and the minimum IAT necessary for full vaporization was made

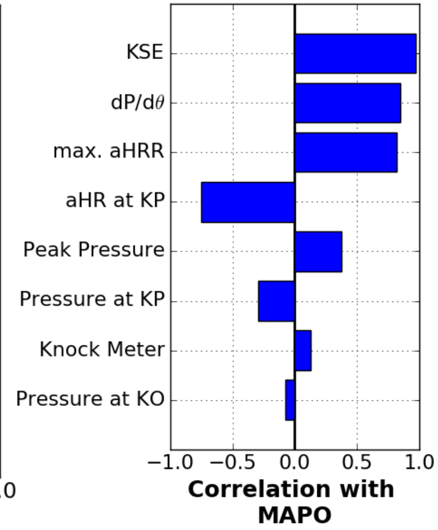


Fuel Properties Effects on Auto-Ignition in Internal Combustion Engines

- Studies of autoignition and various knock metrics with PRF 90 have been performed
- Octane is rated by CFR Knockmeter, whereas OEM knock calibration uses mean amplitude of pressure oscillations (MAPO)
- Cylinder conditions from near-MON to beyond RON examined
    - Intake P = 1.0 – 1.28 bar
    - Intake Port T = 33 – 150 °C
- Knock Metrics – Pearson Correlation
    - Overall weak correlations between CFR knockmeter to conventional knock metrics
    - Several pressure transducer-based metrics correlated to MAPO



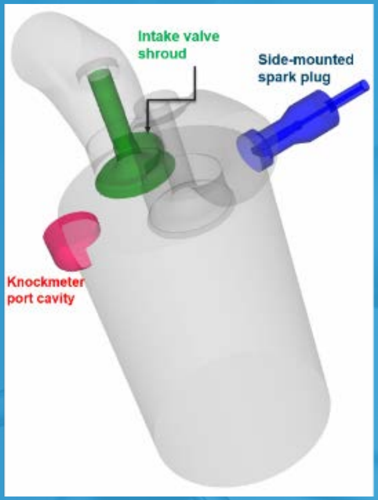




Virtual CFR Engine Based on CFD

Objective:

Develop a 3D CFD based CFR engine model to capture fuel effects on knock propensity



Approach:

Track turbulent flame front using level-set technique (with tabulated laminar flame speed) and predict end-gas autoignition using a multi-zone model

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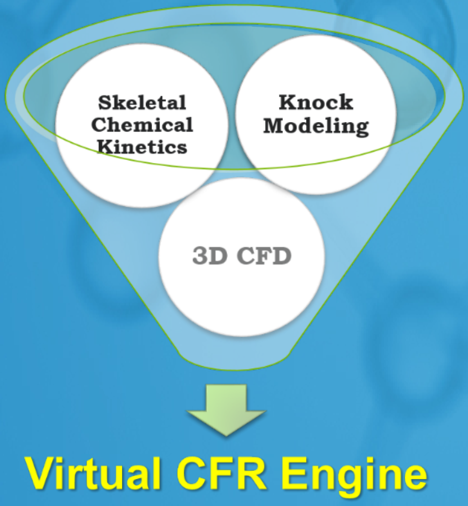


Accomplishment:

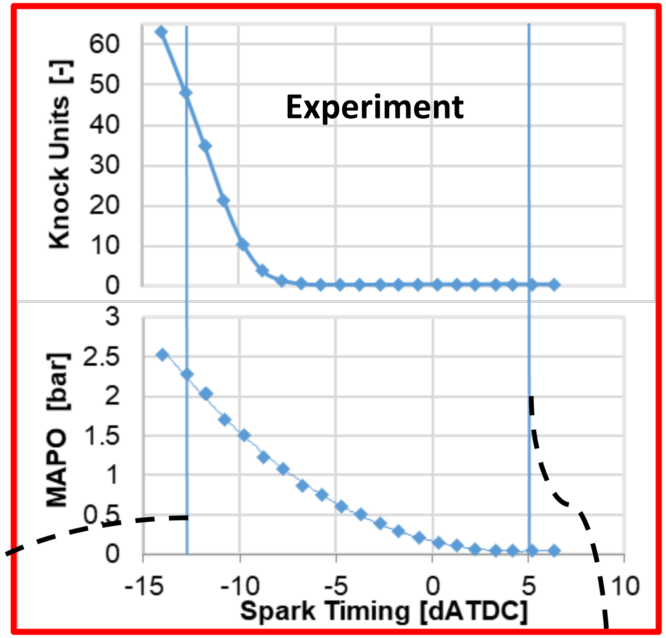
The model was validated against engine experiments and was demonstrated to be capable of predicting mean knock characteristics accurately for varying operating conditions and fuel composition

Virtual CFR Engine Based on CFD

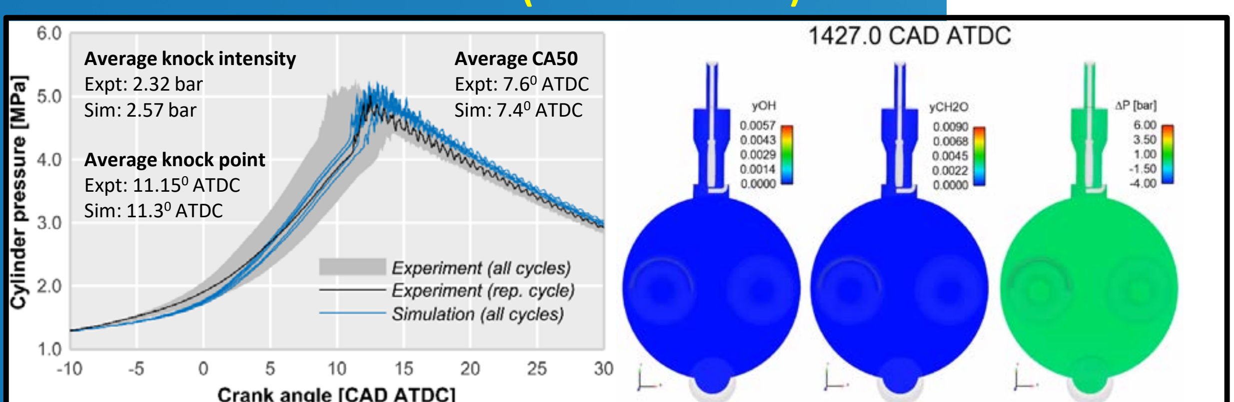
Model Validation:

- The CFD model was improved by incorporating realistic engine geometry
- Multi-cycle RANS simulations were performed for varying operating conditions and fuels, and were validated against engine experimental data
- The updated model captured local in-cylinder pressure evolution, mean knock characteristics (knock onset & knock intensity) and transition from non-knocking to knocking adequately

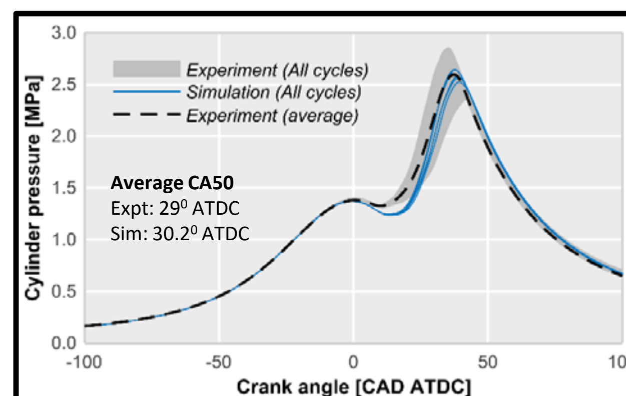
Iso-octane spark timing sweep (RON condition)



Knock (ST = -13^0 ATDC)



No knock (ST = 5^0 ATDC)

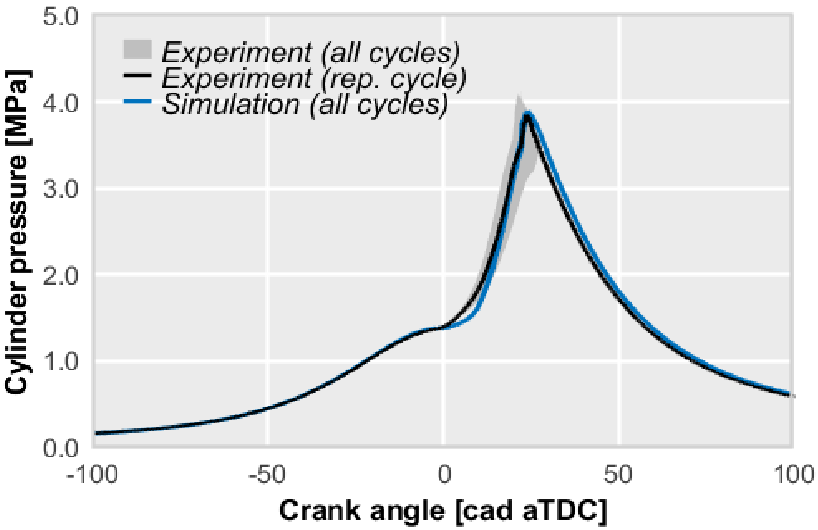


Virtual CFR Engine Based on CFD

KLSA prediction:

- The CFD model was evaluated for operating conditions near the boundary between knocking and normal SI combustion

KLSA for iso-octane ST sweep (ST = -4^0 ATDC)

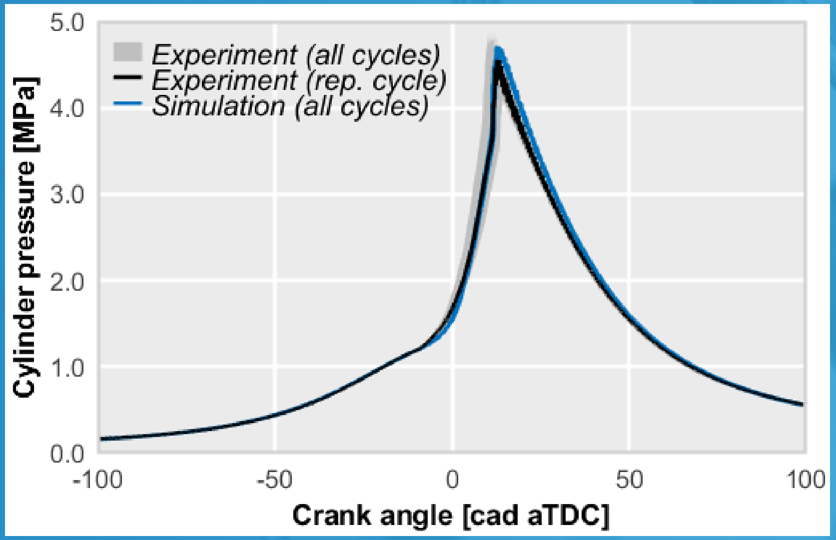


Knock characteristic	Experiment	Simulation
Average knock intensity	0.51 bar	0.66 bar
Average knock point	22.82^0 ATDC	22.44^0 ATDC
Average CA50	17.7^0 ATDC	18.8^0 ATDC

Sensitivity to Fuel composition:

- Knock propensity was captured reasonably well for multi-component blends

PRF96.9 RON condition (ST = -13^0 ATDC)



Knock characteristic	Experiment	Simulation
Average knock intensity	2.1 bar	2.4 bar
Average knock point	10.9^0 ATDC	11.59^0 ATDC
Average CA50	8.3^0 ATDC	9.5^0 ATDC

Co-Optimizer

Multi-objective optimization approach:

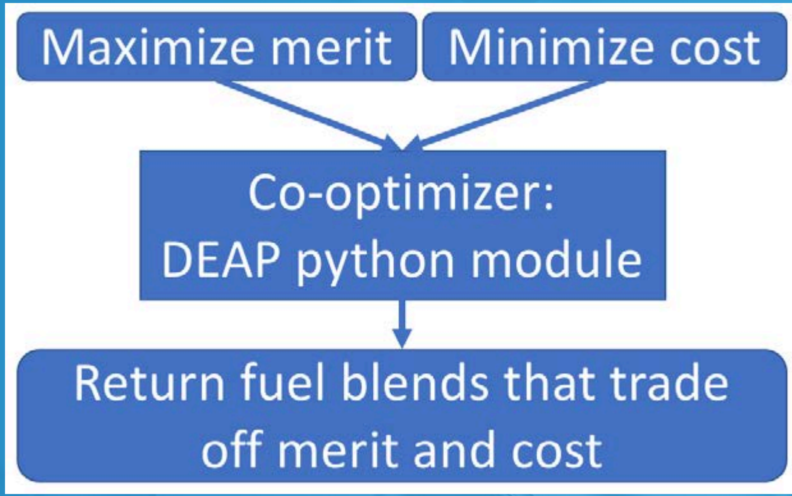
Optimize several conflicting objectives simultaneously, e.g.,

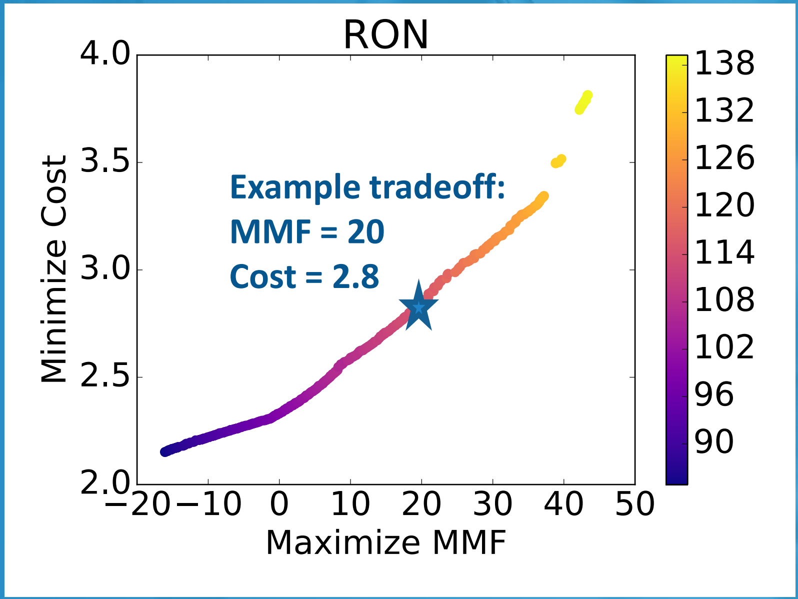
1. Maximize engine efficiency (merit, SI MF) and minimize fuel costs
2. Maximize predicted engine performance (NMEP) and minimize uncertainty (using Gaussian process models trained on experimental data)

→ The co-optimizer is agnostic as to what the objectives are.

Uses the python package DEAP (evolutionary algorithm), suitable for fast-to-compute objective functions. Tradeoff (Pareto) curves inform about:

1. The cost to be expected for a desired efficiency value and vice-versa (see figure)
2. The predicted reachable performance and the associated uncertainty, which indicate fuel property ranges for future experiments

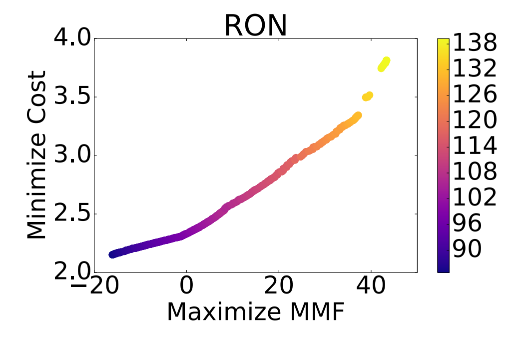




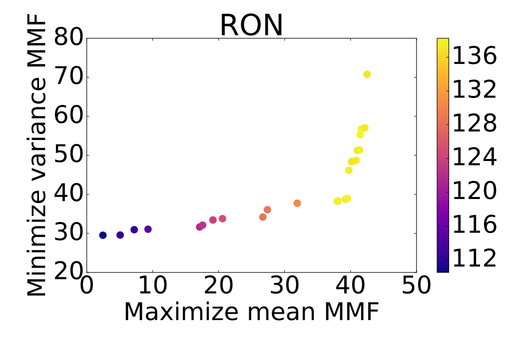
Co-Optimizer

Numerical Experiments:

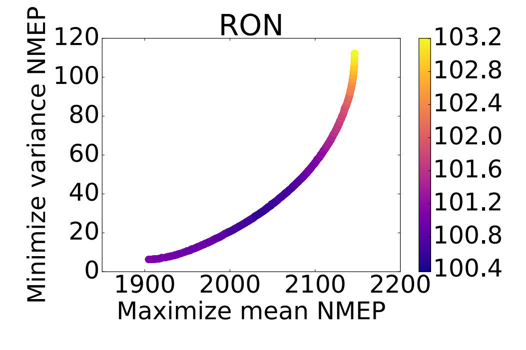
1. *Deterministic optimization*: maximize SI MF and minimize fuel cost (using 22 fuel components, linear blending model)



2. *Optimization under uncertainty:* assume uncertainty in all coefficients of the SI MF (different distributions, 100 random samples); maximize the means SI MF and minimize the variance of SI MF



3. *Optimization under uncertainty using emulation of experimental data:* maximize predicted NMEP and minimize uncertainty of the prediction using Gaussian Process model



Take-home: co-optimizer is agnostic to what your objective functions are

Co-Optimizer

Decision Support:

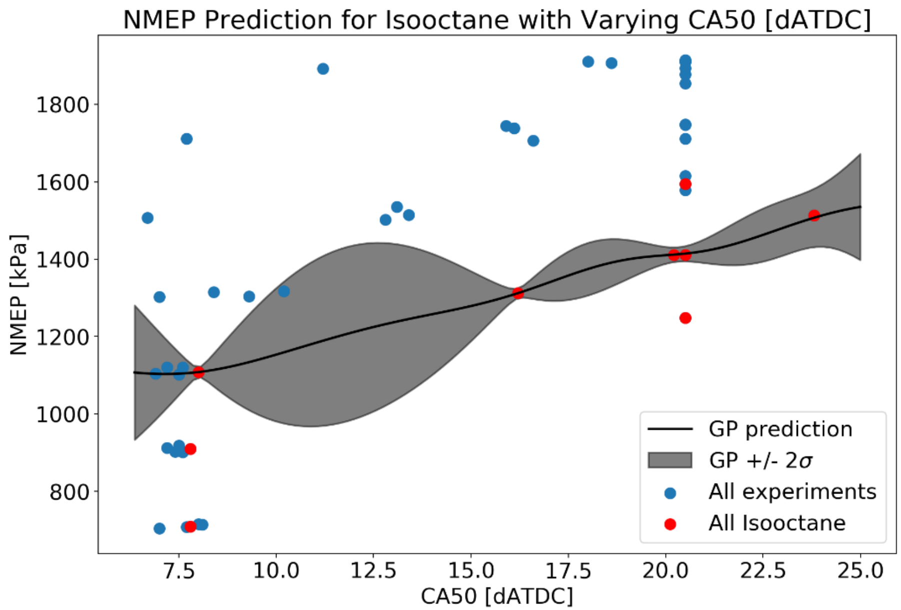
What we can do so far:

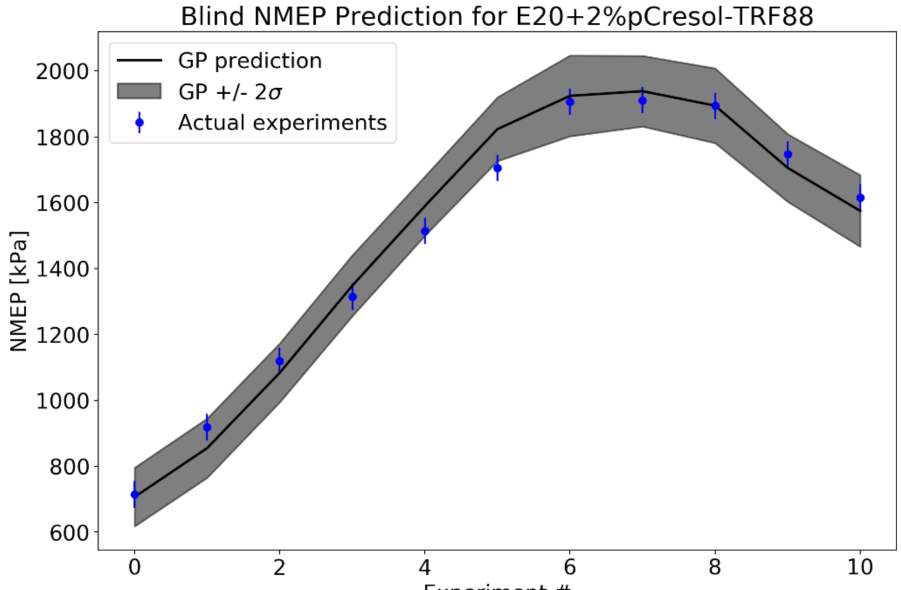
- Tradeoff curves allow *insights into relationships between different optimization goals* (e.g., what range of SI MF value can I achieve given cost X)
- Tradeoff curves enable experimentalists to *identify promising future experiments* (e.g., fuel properties and engine operation conditions that are predicted to yield high NMEP)
- UQ tools allow to study the *sensitivity of the tradeoff curves to different (random) conditions* (e.g., changes in fuel costs, deviations in fuel composition) and to derive robust fuel properties and operating conditions

What we still have to do:

- “Collect” more data for more accurate approximation models (need support from experimentalists)
- A ”true” co-optimization of fuels and engines by bi-level optimization:
  - At the high level: select fuel
  - At low level: optimize corresponding engine operation for max performance
  - Alternate between high and low level
- Software release with current capabilities, possibly with GUI

Develop Co-Optimizer Inputs





Data-driven Gaussian Process Surrogate Modeling:

- Gaussian processes perform Bayesian inference to learn the distribution of possible functions.
- Provides closed form expression for prediction mean and variance.
- Successfully interpolates experiments and predicts the performance of unseen fuels.

$$f\left(\boldsymbol{\theta}\right) \sim \mathcal{GP}\left(\mu\left(\boldsymbol{\theta}\right), k\left(\boldsymbol{\theta}, \boldsymbol{\theta}'\right)\right)$$

$$k_{f|\mathcal{D}}\left(\boldsymbol{\theta}^*, \boldsymbol{\theta}\right) = k\left(\boldsymbol{\theta}^*, \boldsymbol{\theta}^*\right) - \mathbf{k}_*^\mathsf{T}\mathbf{K}^{-1}\mathbf{k}_*$$

$$\mu_{f|\mathcal{D}}\left(\boldsymbol{\theta}^*\right) = \mathbf{k}_*^\mathsf{T}\mathbf{K}^{-1}\mathbf{y}$$

Develop Co-Optimizer Inputs

Nonlinear octane model created for Co-Optimizer inputs:

- Co-Optimizer previously limited to linear blending model for RON/MON (ignores synergistic/antagonistic effects)
- For surrogate blends, correlations based on zero-dimensional ignition simulations provide better estimates for RON/MON but fail in some cases (max abs. error ~10 ON, r.m.s. error ~2 ON)
- A new prediction method was created with artificial neural networks (ANN) using ignition simulations and other readily available fuel mixture properties
- Superior to linear blending models

$$\mathrm{RON}_{pred} = \sum_{i=0}^{nsp} x_i \mathrm{RON}_{i,measured}$$

$$\mathrm{RON}_{pred} = f(\tau_{ign})$$

$$\mathrm{RON}_{pred} = f(\tau_{ign}, \mathrm{HOV}, \mathrm{structure}, \ldots)$$

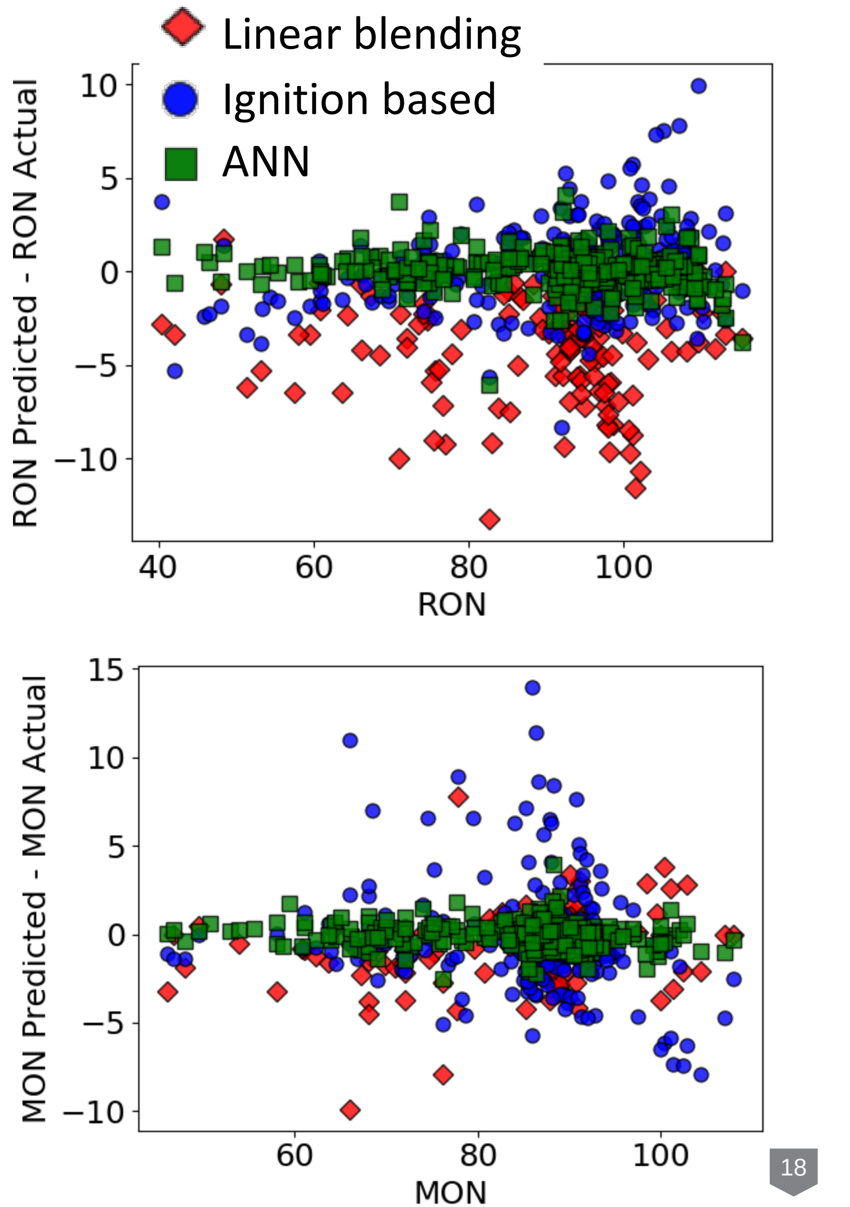
Surrogate fuel blends can be any combination of the 31 hydrocarbon and 25 high performance blendstocks from the Co-Optima gasoline surrogate.

Develop Co-Optimizer Inputs

ANN octane model trained & tested on >700 RON/MON published experiments:

- New approach gave three times more accurate prediction of RON and MON than linear blending
- Can be used in the high level fuel comparison process of Co-Optimizer
- Easy to build virtual surrogate fuels to test blending effects

Method	RON MAE	RON RMSE	MON MAE	MON RMSE
Linear	13.2	4.8	9.9	2.3
Ignition	9.9	2.3	14.0	3.2
ANN	6.0	1.0	4.0	0.7



Responses to 2017 AMR Reviewer Comments

- *"…the project is well conceived, plays an important role in Co-Optima, and addresses critical technical barriers."*
  - Reviewers had very positive feedback on the approach, accomplishments and collaborations
- *"RON and HoV effects, and development of the virtual CFR engine, address downsized boosted engines, which are very pertinent for light-duty OEMs." "…using engine experiments and simulations to provide information regarding how fuel properties affect engine efficiency, is excellent…"*
- *"the modeling capability with the virtual CFR engine results was impressive"*
  - Further progress has been made at understanding how fuel properties and engine cylinder conditions affect the RON measurement, and better understanding its use and limitations
  - Tighter collaboration between Virtual CFR simulations and experiments have been important
  - Three-prong attack on RON/MON measurements, 3D CFD simulations, and ANN predictions
- *"only small concern at this point is that collaborations could be expanded to include others with CFR engines and/or modified CFR engines"*
  - New collaboration this year on CFR research with Prof. Bengt Johansson from KAUST
- *"The reviewer liked the fact that uncertainty is captured in the Co-Optimizer tool, and added that it is important that the output is capable of producing distributions and space plots rather single curves."*
  - Improvements have been made to further reduce uncertainty

Collaborations

Co-Optimization of Fuels and Engines

- Collaboration across nine national laboratories and two DOE offices
- Eight university teams joined in FY17
- Industry FOA issued April, 2018
- 145 stakeholders from 86 organizations
  - External advisory board
  - Monthly telecons with technical and programmatic updates
  - One-on-one meetings and conference presentations

Fuel Properties Effects on Auto-Ignition in ICEs

- CFR Engines, Inc. – Hardware support and technical guidance
- Marathon Petroleum – Hardware support and technical guidance
- KAUST – Ongoing discussions with Bengt Johansson and hosted PhD student

Virtual CFR Engine Based on CFD

- Convergent Science – CFD code guidance
- Univ. of Connecticut – Mechanism reduction

Co-Optimizer

- NREL (Grout, King), LBNL (Mueller), LLNL (McNenly)

Inputs to the Optimizer

- LLNL (Pitz, Wagnon), ANL (Som, Pal)

Remaining Challenges and Barriers

- Formally complete boosted SI work; ensure results inform external debate on new fuels/engines
- Developing fundamental autoignition understanding for blendstocks of diverse composition under full boosted SI operating pressure range
- Developing combined experimental/ modeling approach to identifying fuel property/engine parameter impacts for wide array of ACI approaches
- Developing high-fidelity, computationally efficient kinetic and fluid dynamic models and high quality experimental data to validate
- Developing improved analysis tools that assess process economics, refinery integration of new blendstocks, technology readiness, sustainability, and infrastructure compatibility to guide R&D efforts

Future Work

Fuel Properties Effects on Auto-Ignition in ICEs (Kolodziej-ANL)

- Test autoignition and knock characteristics of Co-Optima RON 98 core fuels in beyond RON and beyond MON pressure-temperature conditions

Virtual CFR Engine Based on CFD (Som-ANL)

- Numerical interrogation of fuel-engine interactions at beyond RON/MON conditions for Co-Optima core fuels as well as their blends with Tier 3 biofuel blendstocks
- Incorporate improved models for wall heat transfer and conjugate heat transfer

Develop Co-Optimizer Inputs and Co-Optimizer (Grout-NREL, Mueller-LBNL, McNenly-LLNL)

- Development of a bi-level optimization tool that at the upper level optimizes the fuel and at the lower level optimizes the engine configuration
- Investigate the space of a possible data-derived multi-mode merit function
- Validate octane prediction performance for new BOBs
- Test other fuel properties as inputs for Neural Network

Any proposed future work is subject to change based on funding level

Summary

Relevance:

- Better integration of fuels and engines research critical to accelerating progress towards economic development, energy security, and emissions goals

Approach:

- Engine experiments and simulations provide detailed analysis on how fuel properties affect engine efficiency and help to refine the SI Merit Function, which feeds into the overall Co-Optimizer function for engine efficiency and fuel blend cost

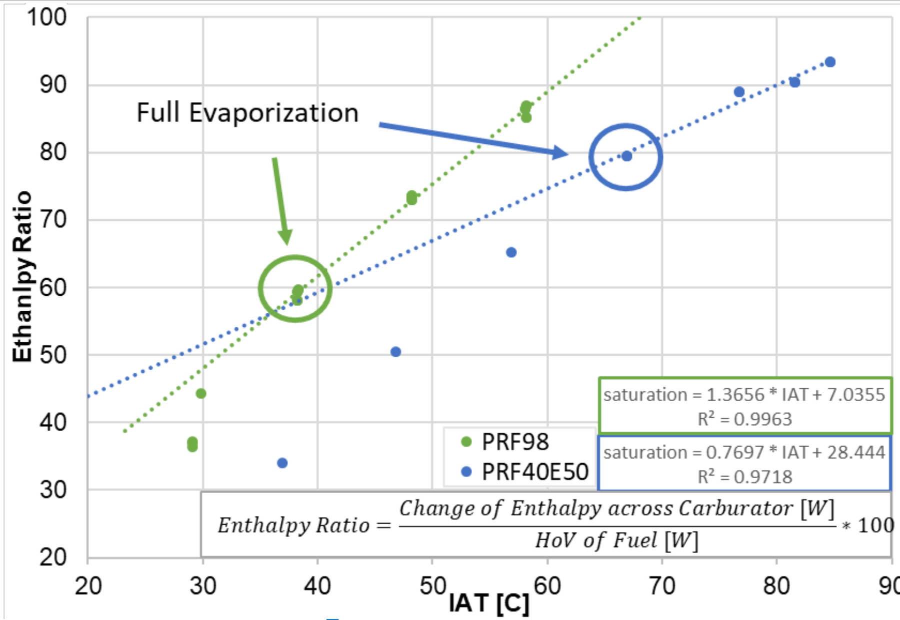
Accomplishments:

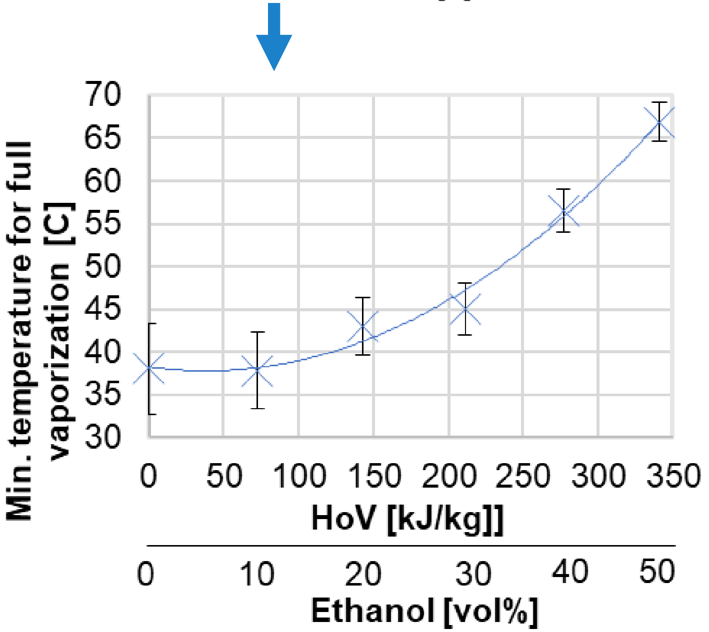
- Performed deeper evaluation of the effects of fuel HoV on RON testinng, including temperature of full vaporization and compensating for cylinder pressure in addition to mixture air temperature up to 50% ethanol content
- Found inconsistencies between CFR knockmeter response to intake pressure, temperature, and compression ratio compared to several cylinder pressure transducer based knock metrics
- The Virtual CFR CFD model was validated against engine experiments and was capable of predicting mean knock characteristics accurately for varying operating conditions and fuel composition
- Used Co-Optimizer to examine experimental engine data and tradeoffs between engine performance, fuel cost, and uncertainty, as well as to guide future experiments for improvements in these three areas
- Created new tool for predicting octane numbers of surrogate fuels with ~1 ON accuracy

Technical Back-Up Slides

Fuel Properties Effects on Auto-Ignition in Internal Combustion Engines

- IAT sweeps were performed with each PRF-ethanol blend
- At high enough IAT, each fuel had a linear "enthalpy ratio" response
- At lower IAT where super-saturation occurred, actual enthalpy change across carburetor would drop below linear trend seen at higher IAT when fully evaporated
- From the vapor fraction analysis, the minimum IAT required for full fuel evaporation at the outlet of the carburetor can be estimated
- Unclear if liquid droplets entering the engine have an important effect on knock or RON rating





Develop Co-Optimizer Inputs

ANN Approach

- Supervised learning
  - Define neural network architecture (inputs/outputs/hidden layer(s))
  - Stochastic gradient descent
- Large “labeled” database
  - RON/MON measurements
  - >700 surrogate measurements collected from literature
- Use cross-validation to prevent over-fitting
- Inputs include ignition data, HoV, molecular formula, and liquid density