Co-Optimization of Fuels & Engines

FOR TOMORROW'S ENERGY-EFFICIENT VEHICLES

Co-Optima Simulation Toolkit Team

June 9, 2016

Co-Optimization of Fuels and Engines (Co-Optima) – Simulation Toolkit Team

June 9th, 2016

M. McNenly,[1] S. Som,[2] D. Carrington,[3] K. D. Edwards,[4] R. Grout,[5] J. Kodavasal,[2] G. Lacaze,[6] J. Oefelein,[6] P. Pal,[2] V. Ram,[2] N. Van Dam,[2] J. Waters,[3] and R. Whitesides[1]

1. Lawrence Livermore National Laboratory
2. Argonne National Laboratory
3. Los Alamos National Laboratory
4. Oak Ridge National Laboratory
5. National Renewable Energy Laboratory
6. Sandia National Laboratories

Co-Optima DOE Management Team:
Kevin Stork and Gurpreet Singh (VTO)
Alicia Lindauer (BETO)

Part I: Relevance, Collaborations and Approach

1. Project Overview
2. Relevance
3. Team Approach
4. Task Approach and Relevance
5. Tracked Milestones
6. Reviewer Comments

Overview

Timeline

Project start date: FY16
Project end date: FY19*
Percent complete: 20%

Barriers and Challenges

Complexity: *Accurately modeling new fuels and their impact on engine performance requires analysis tools and expertise spanning more than a dozen software packages and several research groups.*

Timing: *Schedule for completing R&D and achieving market impact is extremely ambitious.*

Budget

Funding for FY16: $2.1M

- **VTO funding:** $2.1M
- **BETO funding:** $0

Partners

External Advisory Board:

- USCAR
- Advanced Biofuels Association
- EPA
- Dave Foster (U. Wisc)
- Truck & Engine Manufacturers Association
- API
- Fuels Institute
- CARB
- UL
- Joe Norbert (U.C. Riverside)

Stakeholders:

- 85 individuals representing 46 organizations

* End date for Thrust I (spark ignition R&D); Thrust II (advanced compression ignition) R&D will continue

Simulation Toolkit Team Relevance

Core tasks for the 18- month decision point:

1. Develop and test the Co-Optima Central Fuel Hypothesis
   - Extend the fuel & engine parameter space for conditions that can not be tested due to cost, time, or physical constraints
   - Test new fuel property combinations virtually using simulations
2. Identify and refine the coefficients in the Co-Optima Merit Function (a.k.a., the Miles Merit Function) that capture the impact on of fuel properties on engine performance
   - Compute sensitivity of coefficients with validated simulations using high-throughput HPC resources
3. Establish the constraints for the scenario analysis “optimizer”
   - Create the software to find optimized scenarios from the Co-Optima generated data and constraints

Approach: Assemble a highly skilled team of DOE VTO researchers

Argonne NATIONAL LABORATORY

S. Som

J. Kodavasal

P. Pal, V. Ram

N. Van Dam

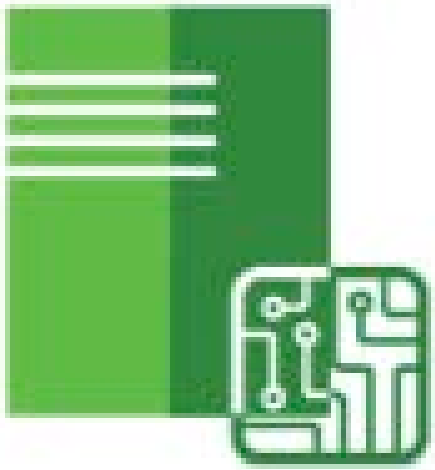
R. Grout

NREL

Lawrence Livermore National Laboratory

M. McNenly

R. Whitesides



OAK RIDGE National Laboratory

K. D. Edwards

Los Alamos NATIONAL LABORATORY EST. 1943

D. Carrington

J. Waters

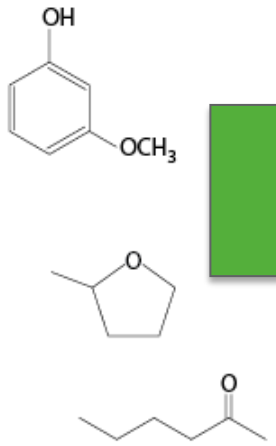
G. Lacaze

J. Oefelein

Sandia National Laboratories

Approach: Leverage existing VTO software and expertise spanning the simulation space

New Blendstock Candidates:



We have many simulation tools spanning the fuel-engine optimization analysis space:

- ConvergeCFD
- Kiva-hpFE
- RAPTOR
- GT-Power
- AVL Fire
- Chemkin PRO
- Zero-RK
- Autonomie

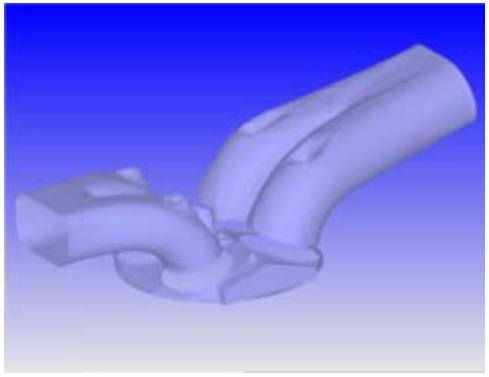
\+ many custom utilities

Approach: Build a shared community around computing and data to accelerate research

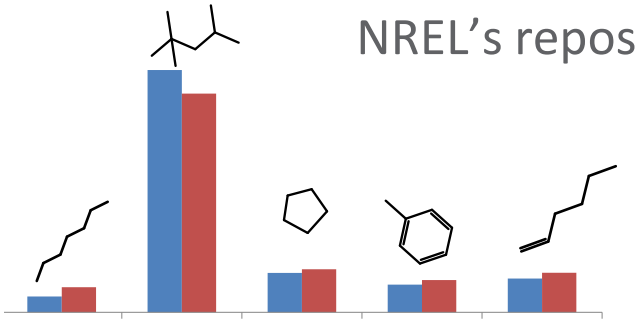
Shared Computing Resources:

- Peregrine at NREL
- 58K Intel Xeon CPUs
- 60M cpu-hour Co-Optima allocation for FY16
- Access for all Simulation Toolkit team members

Shared Data & Tools:



Engine Geometry



Fuel Models

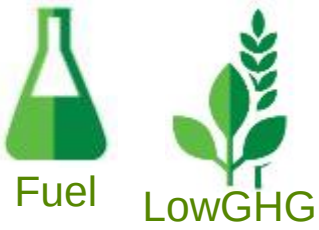
all tracked in NREL's repository

git

Zero-RK

Accelerated Solvers

Task approach and inter-team collaborations

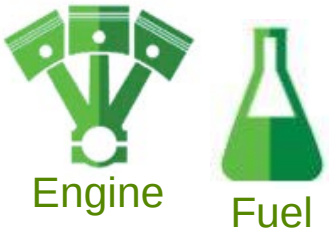


Task G.1. Fuel Property Simulations

Task G.1.1 – Blending model for simulation inputs

Task G.1.2 – Simulation support for small volume fuel testers

Task G.1.3 – Simulation support for kinetic mechanism development and canonical fuel experiments

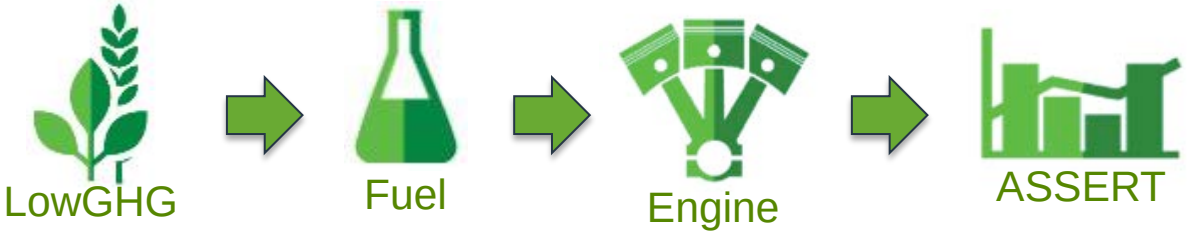


Task G.2. Advanced Engine Simulations

Task G.2.1 – Extreme mechanism reduction for advanced spark ignition engines (DISI)

Task G.3. Blendstock-to-Efficiency (B2E) Application

Create and validate a comprehensive workflow to simulate the impact of a new fuel composition on engine performance



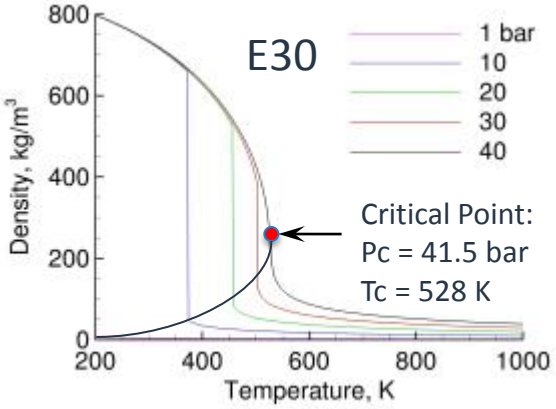
Task G.1.1 - Fuel Blending Model for Simulation Inputs

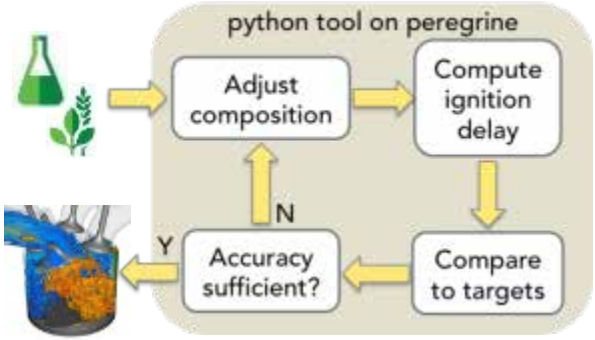
- **Goal:**

  Model any new and existing fuel blendstocks considered by Co-Optima in the suite of VTO software tools for combustion and engine analysis

- **Approach:**

  Create, test and validate thermophysical and chemical kinetic input estimation and generation techniques.





Adjust surrogate composition or key reaction rates to capture:

- Temperature
- Viscosity
- Surface Tension
- Enthalpy of Vapor.
- Vapor Pressure
- Thermal Conductivity
- Density
- Specific Heat
- AKI
- Sensitivity
- Distillation Curve
- H/C Ratio, PIONA
- RCM data
- IQT data
- μFIT data
- virtual CFR

Task G.1.1 - Fuel Blending Model for Simulation Inputs

- **New capabilities and analyses:**
  - Virtual tests to map changes in thermodynamic, transport, kinetic parameters to properties that characterize fuel performance or quality
  - Creation of virtual fuels with optimized properties
  - Simulation of Thrust I kinetic blending behavior experiments (e.g. IQT)
  - Use simulations to answer “what property range does an engines want?”

- **Co-Optima Impact:**
  - Creates the necessary tools to test and validate the Central Fuel Property hypothesis and the Co-Optima Merit Function sensitivity coefficients

Task G.1.2 - Support Small Volume Fuel Testing

- **Goal:**

  Reach the "game-changing" volume and throughput identified by B. Simmons (Co-Optima All Hands Mtg., Feb. 2016)

  – 20 μL samples at 100s of tests/mo

- **Approach:**

  – Develop new techniques to extract or infer kinetic data from experiments via sim

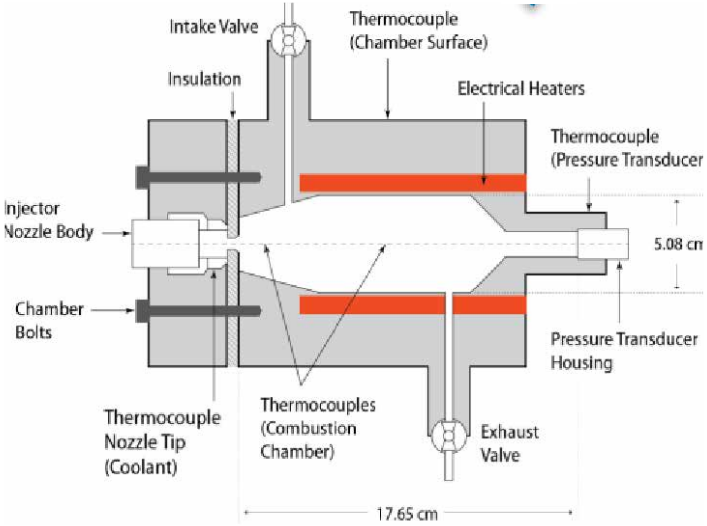
  – Simulate design improvements to increase sensitivity, reduce sample volume and increase throughput

- **Co-Optima Impact:**

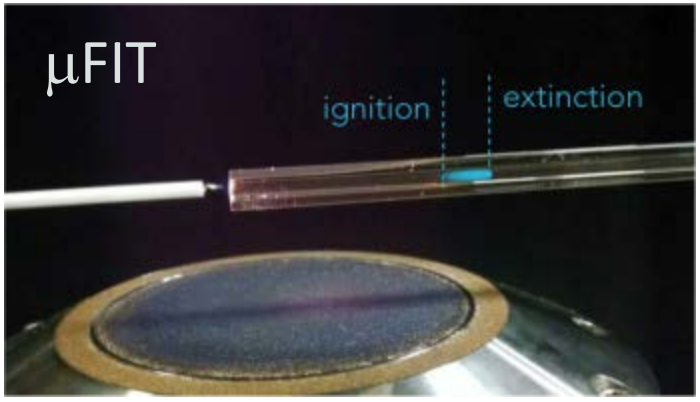
  – Dramatically lower the barrier to new fuel blendstock discovery

  – Create a rich set validation data for training new fuel chemistry models

Ignition Quality Tester (IQT)



μL Fuel Ignition Tester



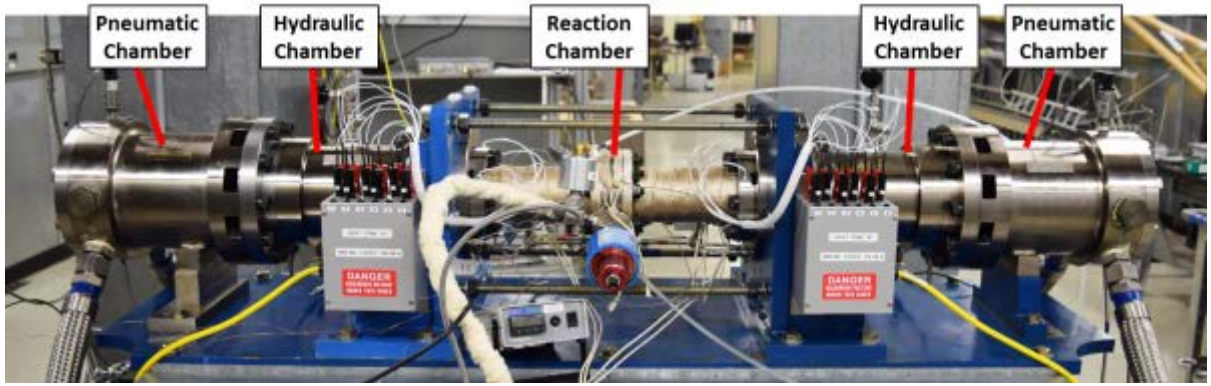
Task G.1.3 - Support Kinetic Mechanism Development

- **Goal:**

  Accelerate the development and use of new, detailed kinetic mechanisms for the Co-Optima program

- **Approach:**
  - Create any new or missing reaction classes to capture non-linear fuel blending interactions
  - Create new analysis tools using Zero-RK to more rapidly evaluate, validate or infer fuel kinetic information from canonical Co-Optima experiments (e.g., shock tubes, rapid compression machines, or flow reactors)

- **Co-Optima Impact:**
  - Delivers more accurate fuel chemistry in a shorter time to the Co-Optima analysis



Rapid Compression Machine (RCM) Goldsborough/ANL

Task G.2.1 - Extreme Mechanism Reduction for DISI

- **Goal:**
  - Improve time to result of the simulations
  - Improve accuracy of predictions

$$p(\lambda|d_{\mathbf{x}}) = \frac{p(d_{\mathbf{x}}|\lambda)\,p(\lambda)}{p(d_{\mathbf{x}})}$$

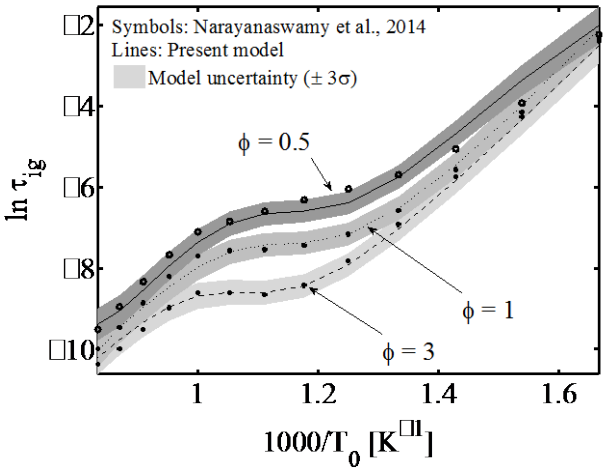
Likelihood Prior

Posterior

Evidence

- **Approach: Uncertainty Quantification (UQ)**

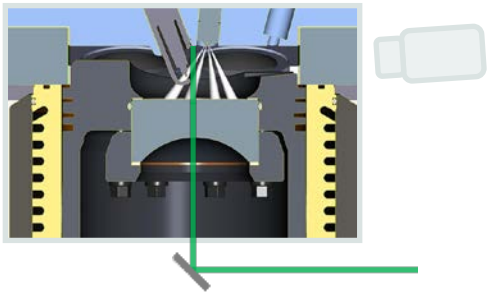
  Derive extremely reduced chemical mechanisms using Bayesian inference
  - Decrease CPU cost while capturing kinetic-dependent quantities of interest (ignition delay time, flame speed, heat release, *etc*.)
  - Produce quantified error bars



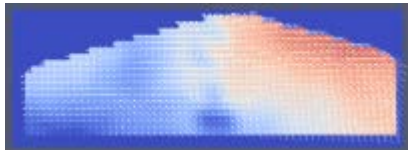
- **Co-Optima Impact:**
  - Quickly define chemical mechanisms based on new experimental measurements of biofuels (detailed mechanisms not needed)
  - Improve predictions and turn-around time of the Toolkit Team - simulations 100x faster

Task G.3 - Blendstock-to-Efficiency (B2E) Application

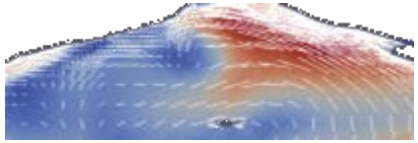
- **Goal:**
  - Create and validate a comprehensive and efficient workflow to simulate the impact of a new fuel composition on engine performance



- **Approach:**
  - Leverage simulation input generation from G.1.1
  - Conduct detailed single cylinder CFD calculations (ConvergeCFD & Kiva-hpFE) for advanced SI experiments to produce ethanol blending trends
  - Use single cylinder blending trends in multi-cylinder (GT-Power) analysis of multi-cylinder Thrust I experiments
  - Link multi-cylinder analysis to Autonomie model (funded by VSS185) for vehicle system efficiency



PIV- Experiment



CFD - Simualtion

- **Co-Optima Impact:**
  - Create a common language and workflow for faster analysis
  - Validate Co-Optima simulation tools
  - Measure and fix workflow bottlenecks
  - ID greatest sources of uncertainty

Tracked Milestones

Due	Type	Milestones	Status
9/30/2016	reg.	Provide a report to DOE and Co-Optima team on the performance of the simulation parameter generation techniques (owner NREL)	on schedule
9/30/2016	reg.	Provide a report to DOE and Co-Optima team on the current development status and potential for each of the three small volume fuel testing techniques (owner LLNL)	on schedule
9/30/2016	reg.	Provide a report to DOE and Co-Optima team on the ability to simulate the chemical kinetics and RCM for the new and existing fuels considered in FY16 (owner LLNL)	on schedule
9/30/2016	reg.	Provide a report to DOE and Co-Optima team on the performance of the extreme mechanism reduction for modeling advanced SI engines (owner SNL)	on schedule
9/30/2016	reg.	Provide a report to DOE and Co-Optima team on the ability to simulate the blendstock's engine impact for the Thrust 1 experiments using existing simulation capabilities for new and existing fuels (owner ANL)	on schedule

Reviewer Responses

Almost all of the Simulation Toolkit team's FY16 research is a new start. The following are responses to some of last year's VTO projects that are relevant to the Co-Optima program's goals.

1. [ACE012] "*there are a number of programs all funded in ACE which could be better integrated including, KIVA, high fidelity LES, computational speedup, to make sure that the technologies developed by DOE work together and feed into needed improvements*"

   The Simulation Toolkit team was designed from the start to go beyond the traditional organization of our research programs. All of our tasks require close collaboration across laboratories, simulation capabilities, and the other Co-Optima teams. To be successful, we have created a community of shared computing and tracked data repositories hosted by NREL. The team represents all the ACE simulation efforts and has made significant joint progress in the first six months of Co-Optima. Further, Task G.3 (Blendstock-to-Efficiency Application) is designed to integrate all the VTO and (eventual) University partners in a common framework. This will provide the Co-Optima program the following: tremendous time savings in human and CPU costs; more rigorous comparison of approaches; and

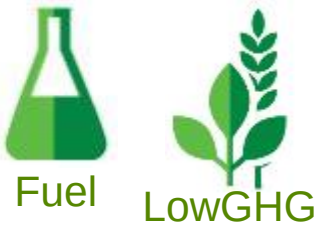
2. [ACE075] "*The portfolio of work should be adjusted so more gasoline sprays and combustion are being modeled if one hopes to impact petroleum consumption of the LD fleet.*"

   The Simulation Toolkit team selected the Advanced SI engine experiments with gasoline and bio-derived blendstocks for Task G.3 (Blendstock-to-Efficiency Application). This case was deliberately chosen to expand and validate our simulations using a challenging, but very relevant near-term application. Our research plan reflects a large increase in the VTO portfolio to include gasoline spray combustion modeling.

3. [FT026] "*Micro-FIT is an important breakthrough to experimental fuel volumes/cost.*"

   The Co-Optima program recognizes the enormous potential to accelerate new fuels research by developing small volume, high throughput kinetic measurements. Simulation is essential to increase the sensitivity and accuracy of new devices like micro-FIT and to extract kinetic data from the IQT and RCM. Simulation Toolkit tasks G.1.2 and G.1.3 directly supports these efforts.

Part II: Accomplishments & Future Work

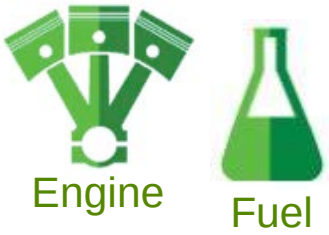


Task G.1. Fuel Property Simulations

Task G.1.1 – Blending model for simulation inputs

Task G.1.2 – Simulation support for small volume fuel testers

Task G.1.3 – Simulation support for mechanism development and canonical fuel experiments

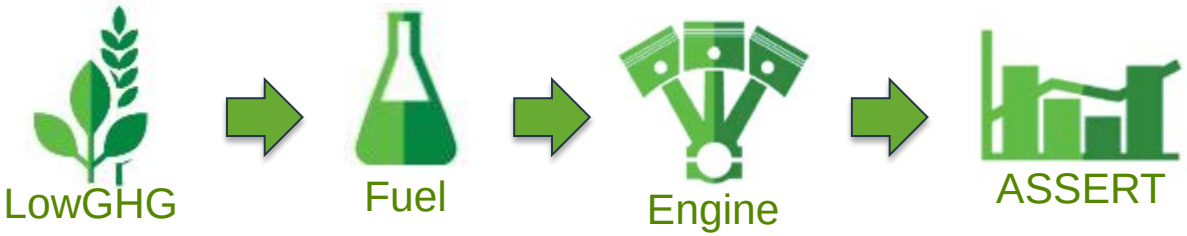


Task G.2. Advanced Engine Simulations

Task G.2.1 – Extreme mechanism reductions for advanced spark ignition engines (DISI)

Task G.3. Blendstock-to-Efficiency (B2E) Application

Create and validate a comprehensive workflow to simulate the impact of a new fuel composition on engine performance



Accomplishment: Task G.1.1 - Blending Model for Simulation

Surrogate Optimizer

Created an automated fuel surrogate optimizer to produce more realistic chemistry models for new blendstocks

Fuel specs from Co-Optima Teams

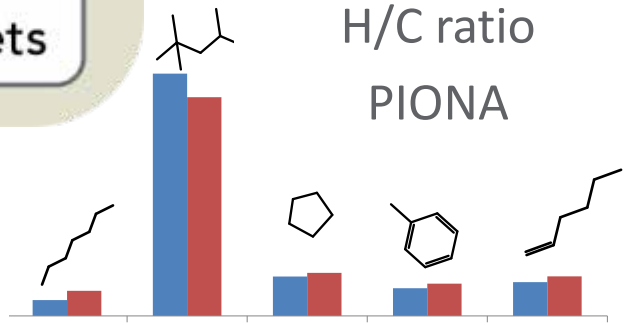
Fuel LowGHG

python tool on peregrine

Adjust composition → Compute ignition delay → Compare to targets → Accuracy sufficient? → Y: Ready for simulation; N: Adjust composition

Zero-RK

AKI
Sensitivity
Distillation Curve
H/C ratio
PIONA

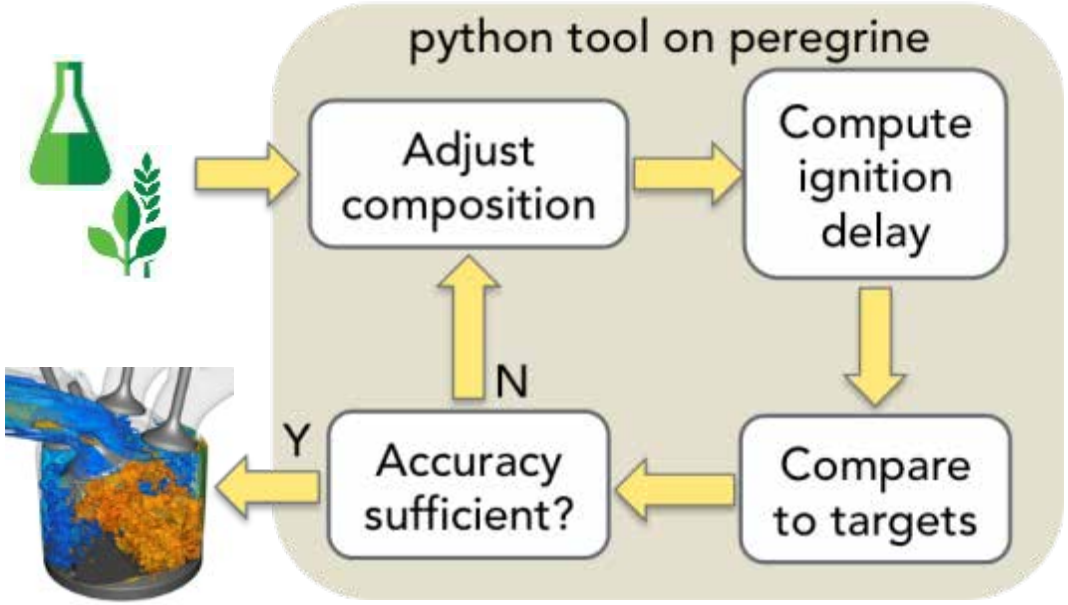


Accomplishment: Task G.1.1 - Blending Model for Simulation

Surrogate Optimizer

The surrogate optimizer offers a large time savings over the "hand-tuned" approach previously used by the Fuel Properties team.

- Efficiently computes large mechanisms (+2000 species)
- Each calculation 10-15x faster than commercial solvers
- Available now on peregrine for all Co-Optima teams
- Targets captured more accurately than hand-tuned methods



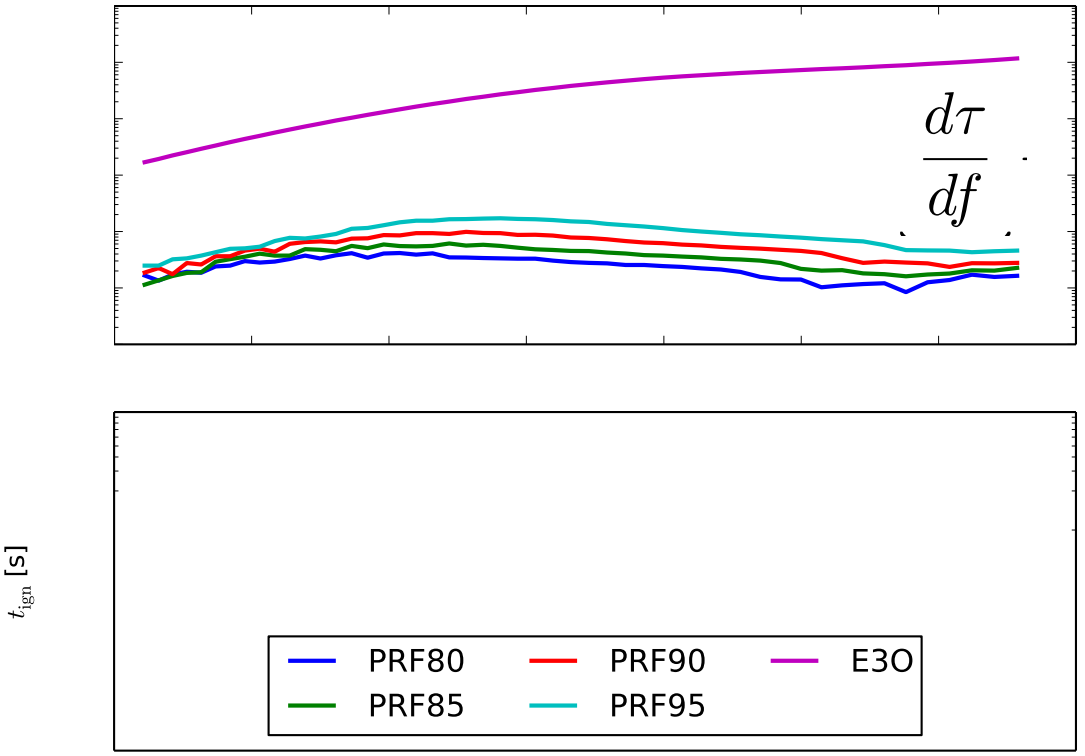
Future Work:

- Add RCM experimental data
- Add distribution of carbon bond types
- Update AKI/Sensitivity correlations with virtual RON & MON tests

Accomplishment: Task G.1.1 - Blending Model for Simulation

Sensitivity of ignition delay time to fuel composition

- 0D ignition delay (with Cantera) calculations performed for different PRFs and E30 compositions
- Sensitivity of ignition delay time to composition for PRF and E30 blends
- This forms part of the overall relation between performance and blend composition
- For E30 changes in iso-octane fraction have much more impact
  - Could impact dominant term

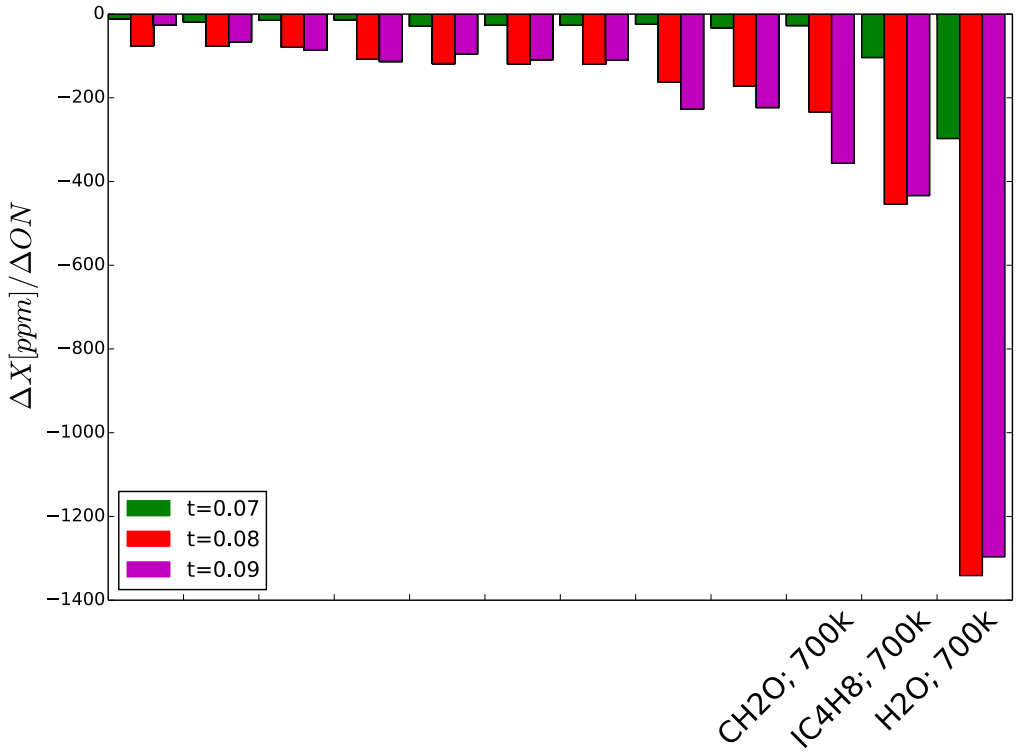


$$\frac{\partial \mathrm{IMEP}}{\partial f} = \underbrace{\frac{\partial \mathrm{IMEP}}{\partial \mathrm{RON}}}_{\mathrm{CFD}} \overbrace{\frac{d\mathrm{RON}}{d\tau}}^{\mathrm{Virt.CFR}} \underbrace{\frac{d\tau}{df}}_{\mathrm{0D}} + \frac{\partial \mathrm{IMEP}}{\partial \ldots}$$

Accomplishment: Task G.1.1 - Blending Model for Simulation

Identification of flow reactor targets to improve accuracy

- Sensitivity study to changing PRF composition (ΔON)
  - Detailed mechanism (LLNL supplied)
  - 1 atm, 700-900k, constant P reactor
  - Variety of times up to 0.1ms
  - Species sorted by sensitivity to ON based on PRF composition
- Highest sensitivity at lower temperatures for same time (earlier in ignition process)



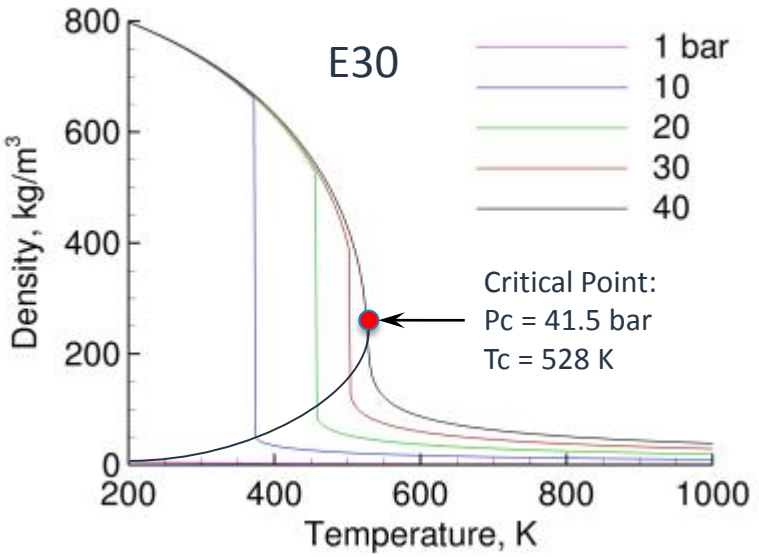
Needs to be repeated with more complicated fuels, in conjunction with virtual CFR models to map kinetics/composition to properties

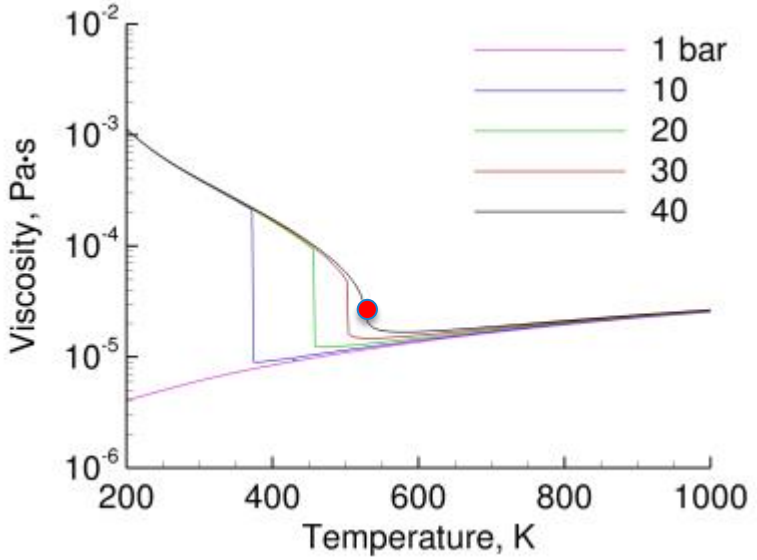
Accomplishment: Task G.1.1 - Blending Model for Simulation

Blending model for biofuel thermophysical properties

Detailed treatment of thermodynamics and transport properties for multicomponent fuels:

- Real-fluid mixture properties obtained using Extended Corresponding States model
- Multicomponent formulation using cubic (PR/SRK) or BWR equations of state
- Generalized to treat wide range of biofuel blendstocks (Fuel/Oxidizer/Products)





Provides Tabulated Input for Project Codes (e.g., CONVERGE):

- Temperature
- Viscosity
- Surface Tension
- Enthalpy of Vaporization
- Vapor Pressure
- Thermal Conductivity
- Density
- Specific Heat

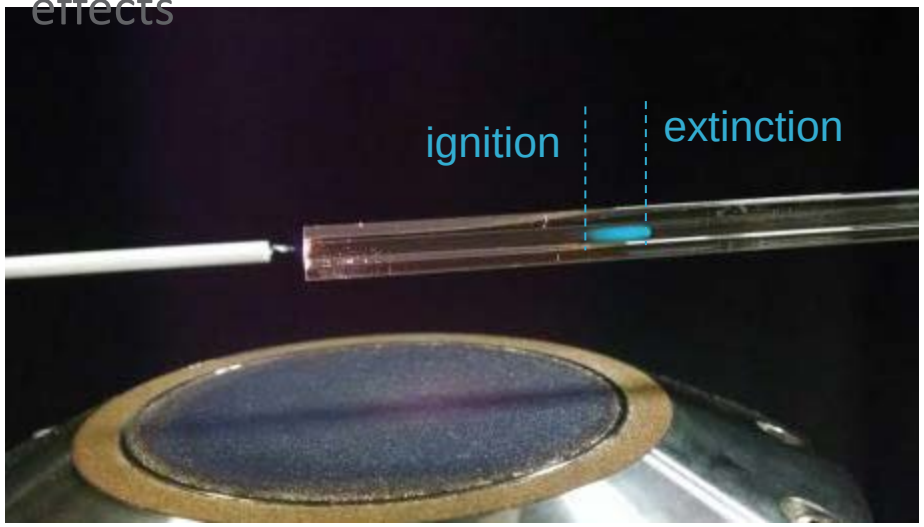
e.g., Variation in liquid-gas density and viscosity for E30 as function of pressure and temperature shown on right

Accomplishment: Task G.1.2 - Small Volume Fuel Testers

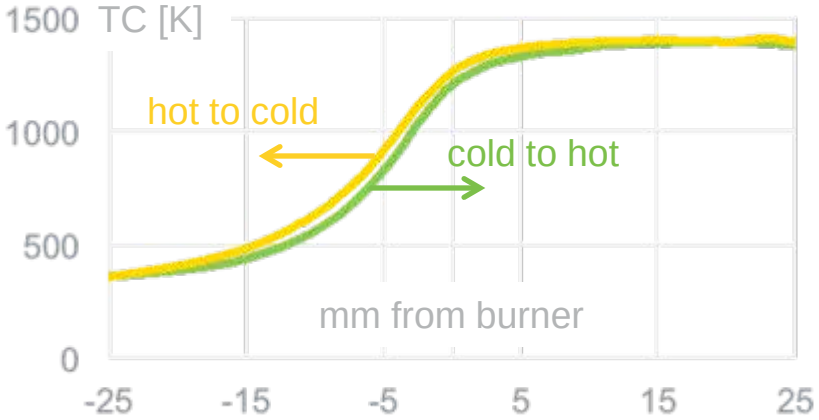
Thermal model for μFIT improves measurement accuracy

Created a detailed thermal model to quantify the temperature difference between the thermocouple and the wall conditions

The micro-liter Fuel Ignition Tester (μFIT) uses an unsteady flame in a mm-scale channel to measure fuel chemistry effects



μFIT prototype operating at LSU by Schoegl under the Co-Optima Fuel Properties team (propane shown)



Detailed modeling uncovered:

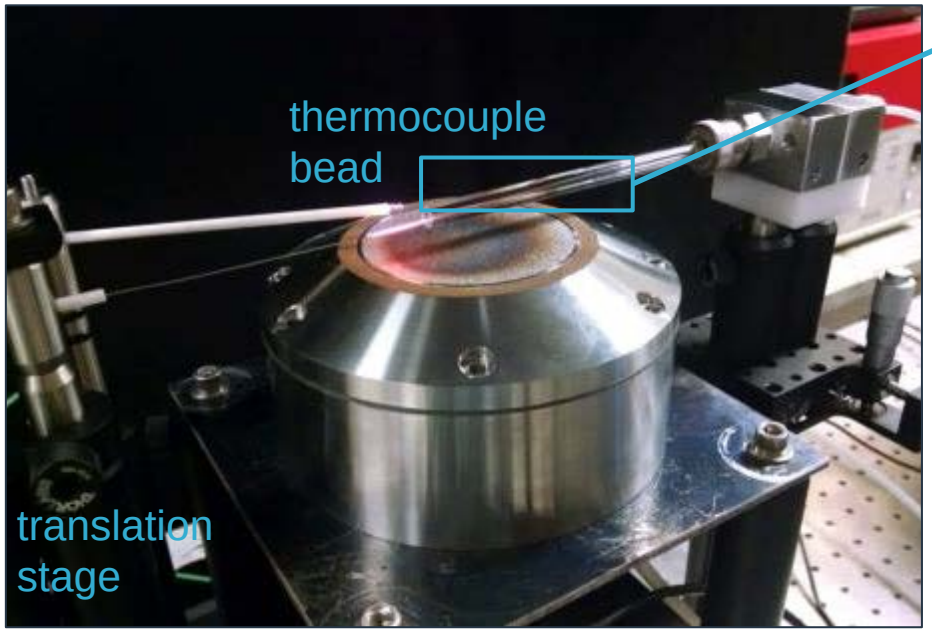
- thermocouple holder affects the measured temperature in the tube
- thermocouple translation speed originally too fast
- +30K measurement error corrected in less than a week

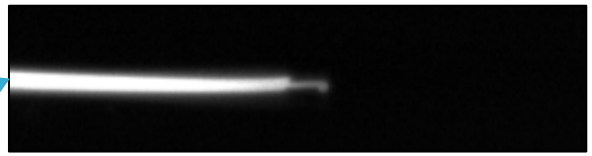
Future Work: Task G.1.2 - Small Volume Fuel Testers

Use simulations to extend μFIT applicability

Accurate wall temperature measurements are critical to enable the extraction of kinetic information μFIT from using simulation

Wall temperature measurement in action





CH*
filter

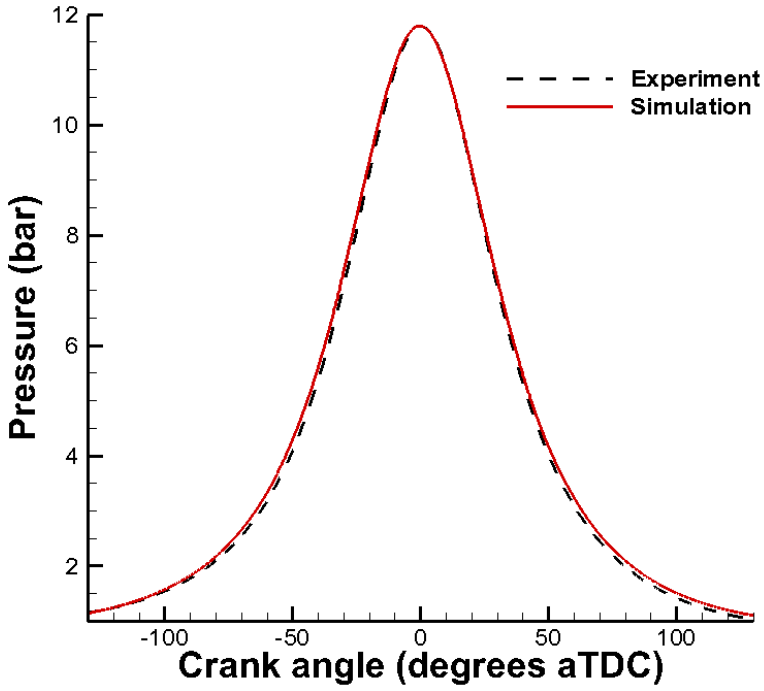
Future Work:

- quantify the model sensitivity and uncertainty resolving the wall temperature profile
- redesign (with LSU) the external heating profile to increase the measurement sensitivity for low temperature heat release
- determine the flow and heating conditions needed to operate μFIT at pressures greater than 30 bar

Accomplishment: Task G.1.2 - Small Volume Fuel Testers

Virtual CFR Engine* based on CFD to estimate RON and MON

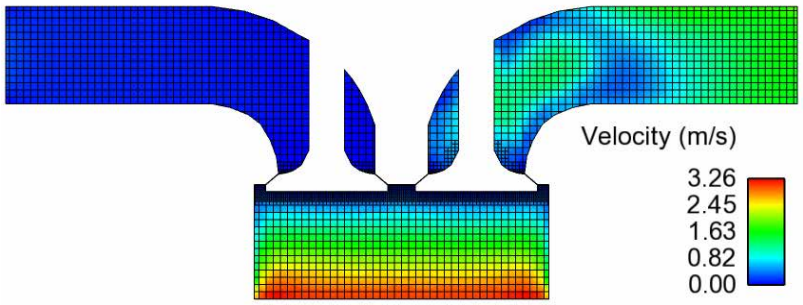
- Bore = 8.265 cm, stroke = 11.43 cm, connecting rod = 25.4 cm, swept volume = 613.25 cc, CR = 7
- T_{IVC} = 54.5^0 C, P_{IVC} = 1.145 bar, cylinder jacket temperature = 81^0 C, engine speed = 900 RPM
- 3D Closed cycle RANS motoring simulations from IVC to EVO are performed and shown to match well with experiments



Future Work

- Full cycle RANS and LES of CFR engine incorporating gas exchange processes, at fired conditions
- Knock capturing with CONVERGE using adaptive mesh refinement
- **Virtual RON/MON simulation tests for gasoline-ethanol blends, validation against experimental data from CFR engines and development of novel theoretical correlations to rapidly determine octane numbers**
- New CFR engine at ANL to provide experimental data in future

Base grid size = 2 mm
Min. grid size = 0.5 mm



* Current CFR engine surface mesh provided by Dr. Ben Wolk (SNL) and Prof. J.Y. Chen (UCB)
* CFR engine data provided by Dr. Vi Rapp at LBNL

Future Work: Task G.1.2 - Small Volume Fuel Testers

Ignition Quality Tester experiments and simulations

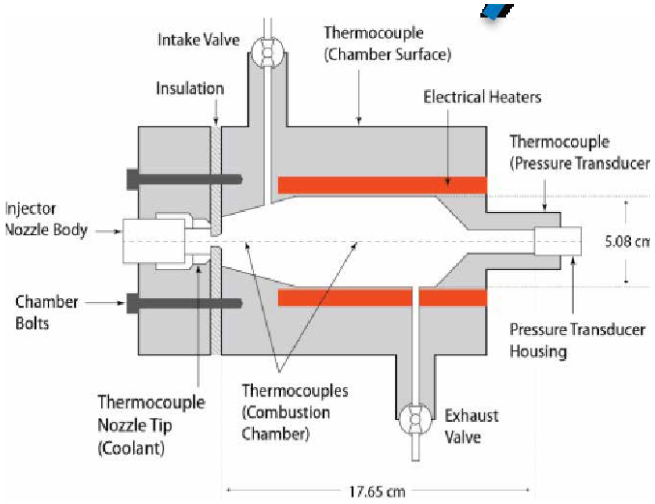
Objective is to study **ability of surrogate mechanism to capture sensitivity to surrogate fuel compositions** in a multi-physics environment

- Prof. G. Bogin (CSM) will conduct CONVERGE simulations of IQT experiments for ethanol & iso-octane blends
- Iso-octane baseline established, binary and reference blends being simulated now
- Online mechanism reduction (DRG) included to establish appropriate level of reduction in mechanism for capturing realistic ignition process

Future Work:

- Capturing sensitivities to kinetics dependent properties requires simulations that can propagate kinetics sensitivity through CFD calculation, including turbulence-flame interaction

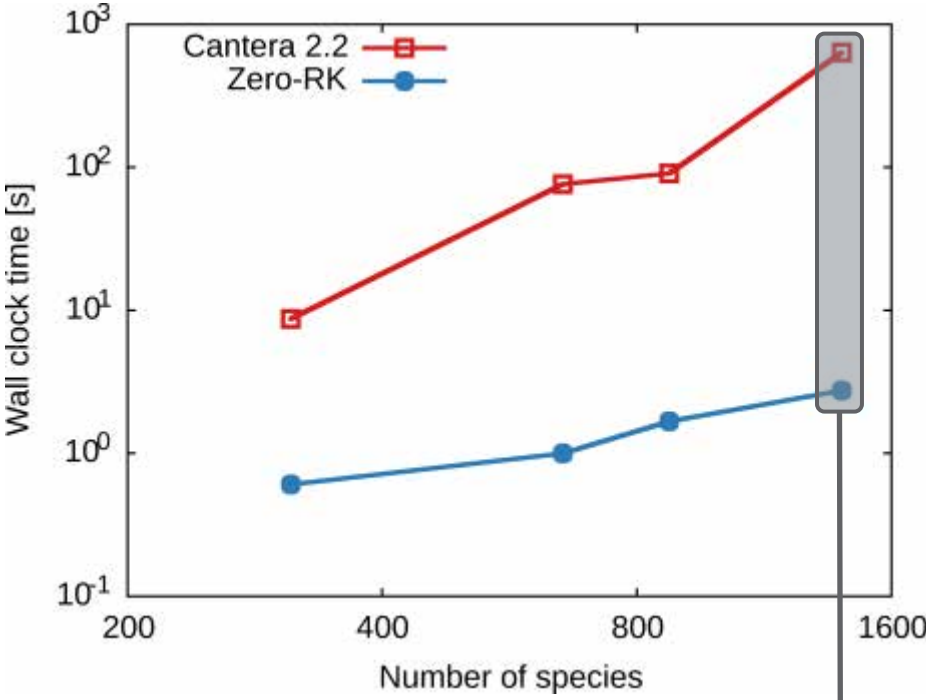
Ignition Quality Tester (IQT)

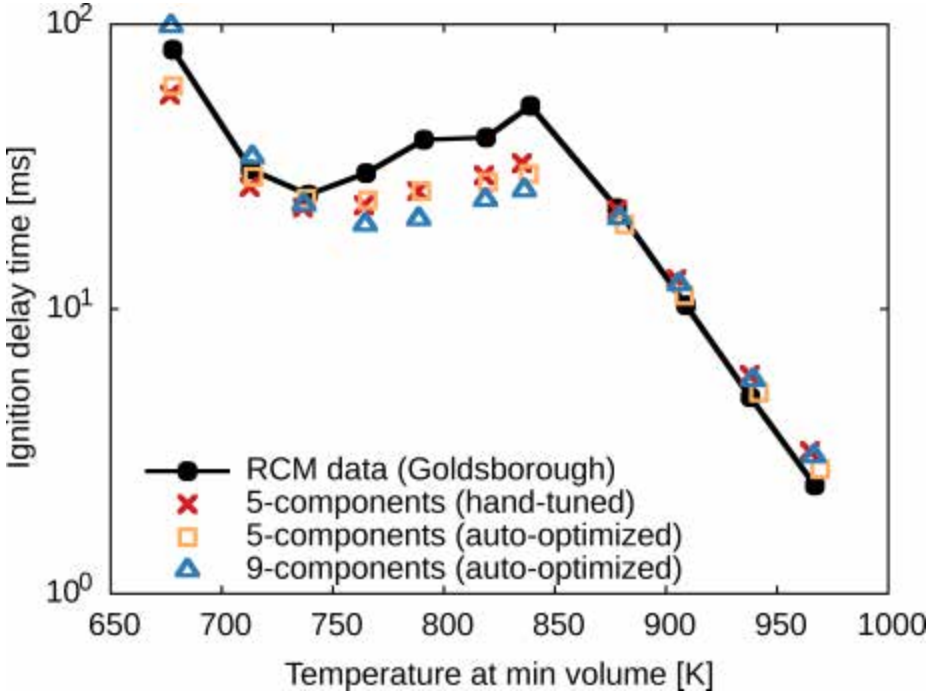


Accomplishment: Task G.1.3 - Kinetic Mechanism Support

Created two new Zero-RK tools to analyze experiments

Developed new tools for high throughput modeling of the constant pressure flow reactor experiments (NREL) & RCM experiments (ANL)





- Simple Zero-RK interface created on peregrine to couple with existing NREL python tools
- +200x speedup over Cantera for the target Thrust 1 mechanism

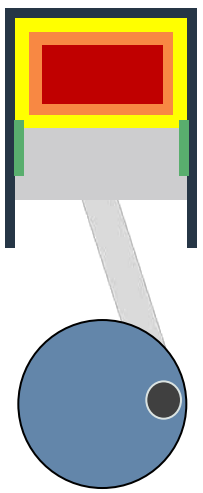
- Batch processing of RCM simulations has high throughput for automated optimization of new fuel surrogates
- New Zero-RK tool avoids large human setup cost (and errors)

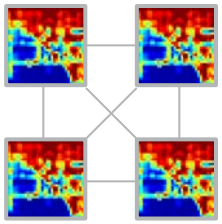
Future Work: Task G.1.3 - Kinetic Mechanism Support

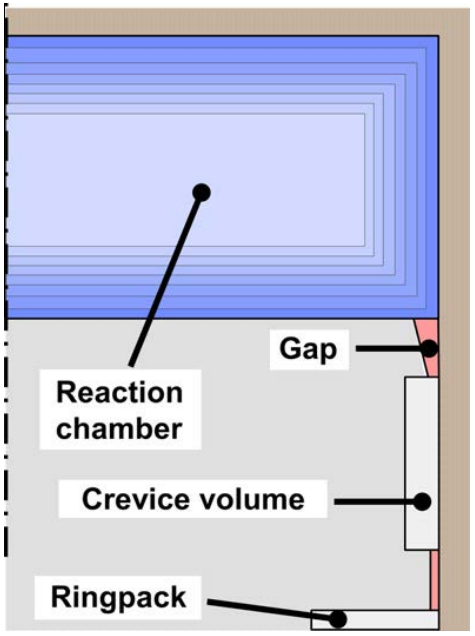
Create Zero-RK multizone models of experiments

Increase the accuracy of the high-throughput, chemical kinetics tools to test the Co-Optima central fuel hypothesis, and rapidly evaluate the sensitivity of the merit function coefficients.

Quasi-Dimensional Multizone





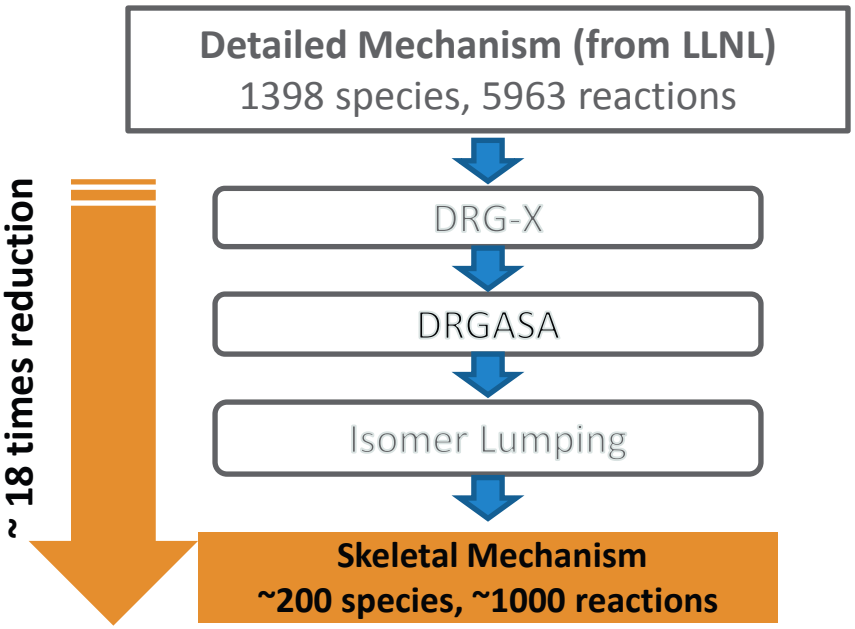


- Develop a multizone model for virtual RON and MON experiments
- Test virtual RON and MON models in the surrogate optimization loop

- Accelerate the RCM model of Goldsborough (CNF 2012) to capture crevice effects with Zero-RK

Accomplishment: Task G.1.3 - Kinetic Mechanism Development

Thrust 1 mechanism reduction



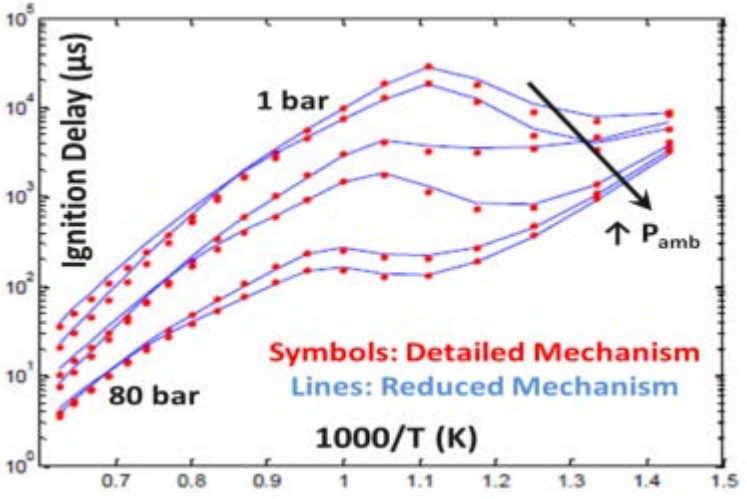
Computational time scales:

- with N^2 ~ N^3 of number of species
- linearly with number of reactions

Range of operation:

- ✓ Pressure: 1-100 atm
- ✓ Equivalence ratio: 0.5-2.0
- ✓ Initial temperature: 700 – 1800 K

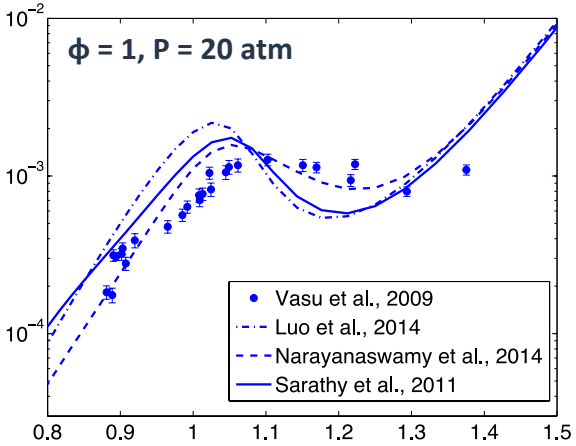
- Surrogate mixture identified through the surrogate blend optimizer developed under Co-optima (for different blends of gasoline with alcohols)
- Detailed mechanism developed at LLNL and validated against RCM data at ANL
- Mechanism reduction performed in collaboration with **Prof. Tianfeng Lu at University of Connecticut** (was being done under NSF-DOE collaboration between UConn and ANL)
- Expected accuracy of the reduced mechanism is shown below. This reduction was performed for n-dodecane molecule

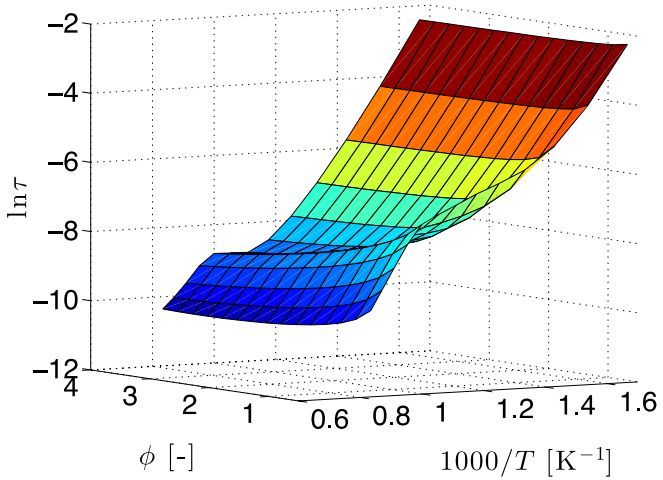


Accomplishment: Task G.2.1 - Extreme Mechanism Reduction

Optimized reduced mechanisms with <5 species

Objective: Capture auto-ignition delay time for any molecule at engine conditions





Form of the optimized mechanism for n-$C_{12}H_{26}$/Air:

$$C_{12}H_{26} + 12.5O_2 \rightarrow 12CO + 13H_2O$$

$$CO + 0.5O_2 = CO_2$$

$$k_1 = A \exp(-E_a/RT)[C_{12}H_{26}]^{0.25}[O_2]^{1.5}$$

$$k_2 = 3.98 \times 10^{14} \exp(-40/RT)[CO]^1[H_2O]^{0.5}[O_2]^{0.25}$$

$$k_{-2} = 5.00 \times 10^8 \exp(-40/RT)[CO_2]^1$$

} Coefficient from Westbrook CST 1981

The parameter **A** is actually a complex function (found by least-square fitting) of T_0 and ϕ to capture non-linear behavior of ignition delay:

$$E_a = \eta_0$$

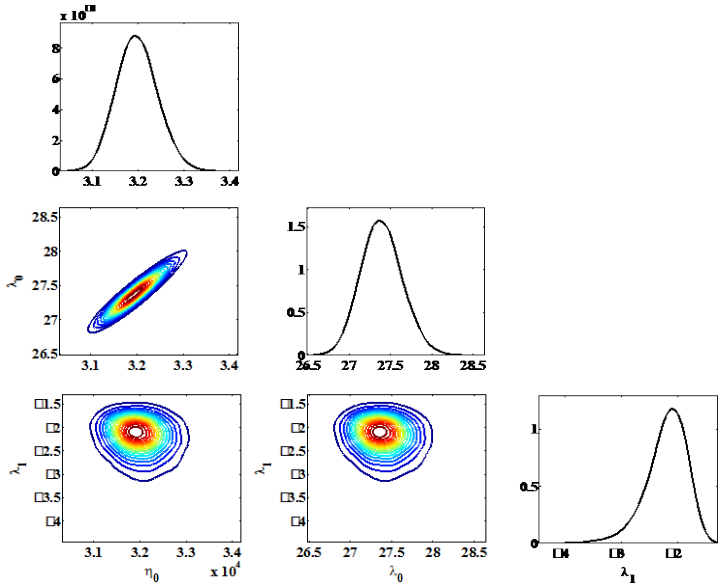
$$\ln A = \lambda_0 + \lambda_1 \lambda_2^{\phi} + \lambda_3 \tanh(\lambda_4 + \lambda_5 \phi) T_0 + \lambda_6$$

Those are the parameters to infer

Accomplishment: Task G.2.1 - Extreme Mechanism Reduction

Optimized reduced mechanisms with <5 species

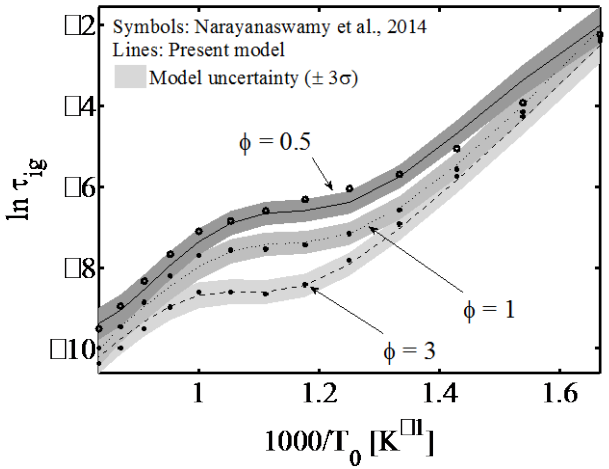
- Build surrogate and use Bayes' rule to find parameters (pdf)

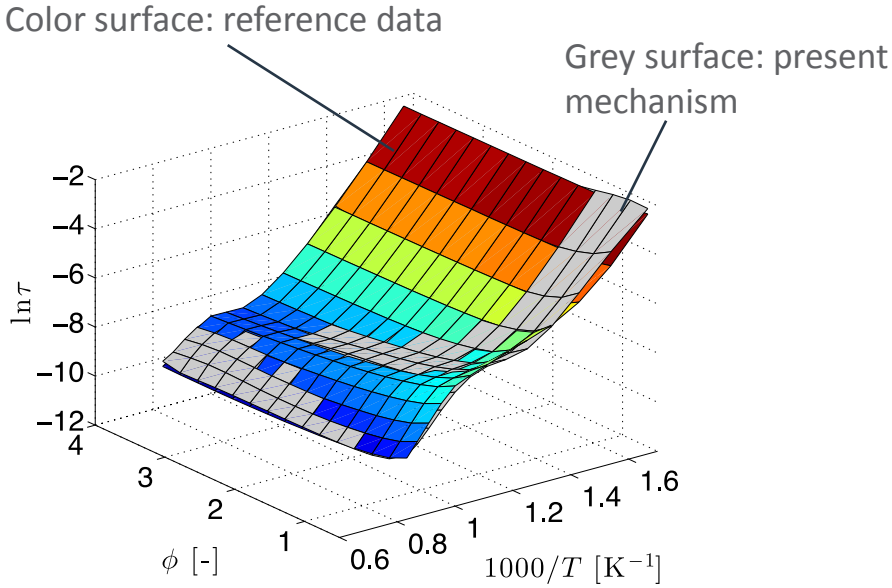


Sampling performed using Metropolis Markov Chain Monte Carlo (MCMC):

- High-dimensional complex (non-Gaussian) using Monte Carlo
- Contains adaptation and rejection rules
- 200 000 samples required to get parameters

- Mechanism performance:



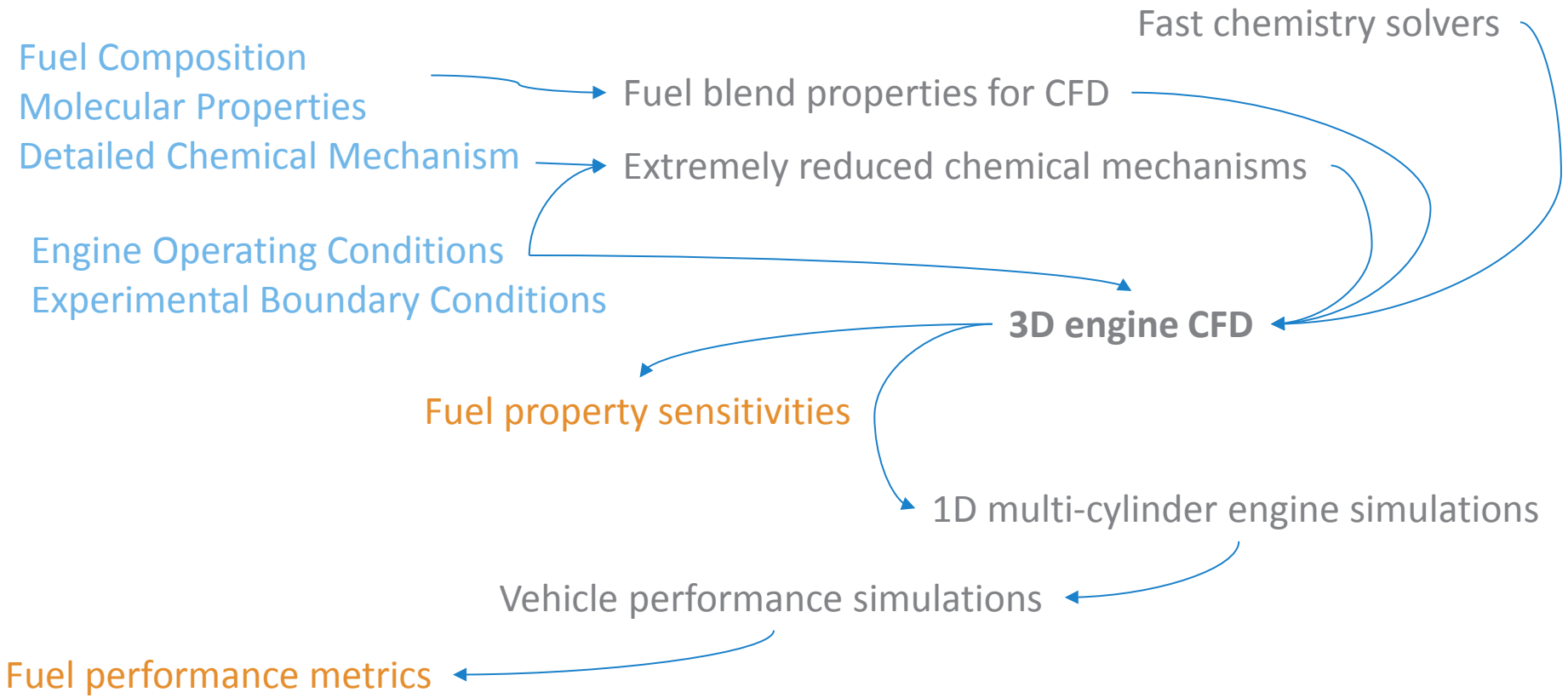


Future work will focus on Thrust I Ethanol-gasoline blends and bio-diesels

Task G.3 - Blendstock-to-Efficiency (B2E) Application

Accomplishment: Workflow development

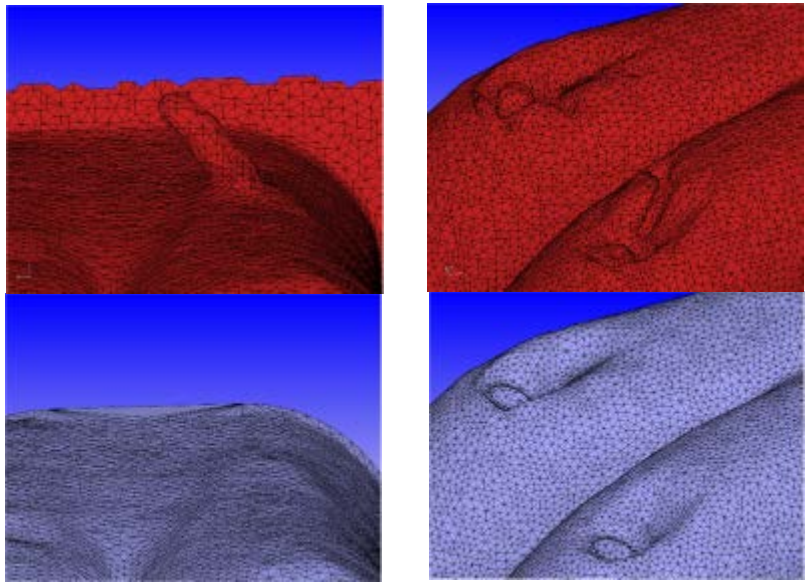
- Unify multiple simulation components into a single toolchain
- Analyze candidate fuels from composition and basic properties through whole-vehicle analysis



Accomplishment: Task G.3 - Blendstock-to-Efficiency Application

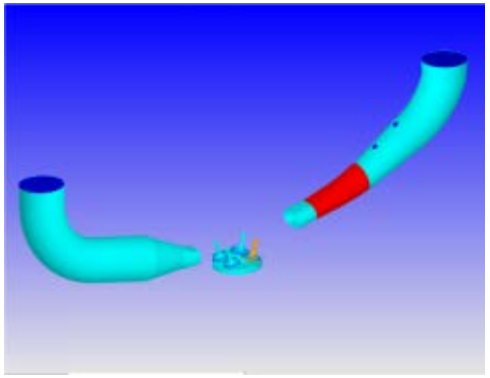
High-fidelity DISI engine geometry creation

- Head geometry previously unknown
- An X-ray scan of the head was combined with known piston, intake and exhaust geometries
  - CAD and X-ray data courtesy of Sjöberg at Sandia
- The X-ray scanned geometry needed to be cleaned and merged with the known CAD geometry
  - Done jointly with Scarcelli at Argonne
- Full geometry now available to all Co-optima groups



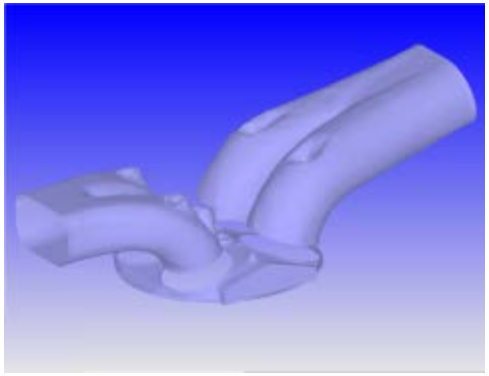
Sample X-ray feature needing correction

Available CAD Geometry



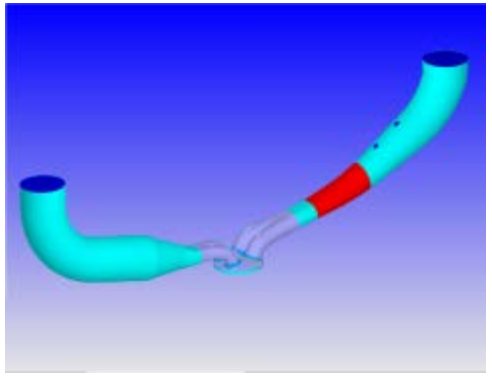
+

Clean X-ray Head Scan



=

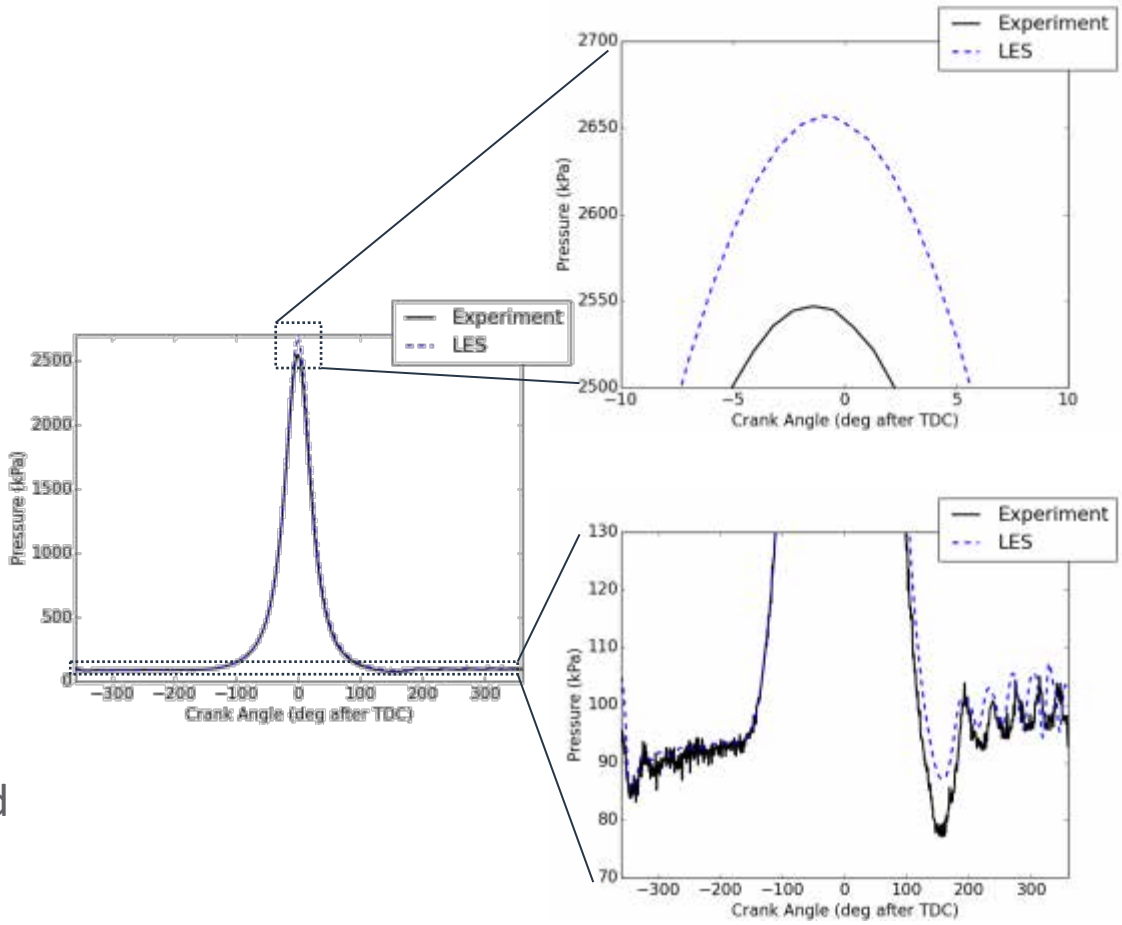
Open-cycle CFD Geometry



Accomplishment: Task G.3 - Blendstock-to-Efficiency Application

DISI Engine Simulations

- High-swirl motored engine case
  - One valve deactivated
  - No fuel injection
- Nominal compression ratio: 12:1
- Typical timing: fuel injection -30° aTDC, spark -25° aTDC
- Intake Pressure: 94 kPa
- Intake Temperature: 31° C
- CFD simulations performed with CONVERGE software
  - Large-eddy Simulations (LES) with Dynamic Structure turbulence model
- Crank-angle resolved pressure and temperature boundaries
- Wall boundary temperatures estimated from measured coolant temperatures
- Need to verify wall boundary temps



- Measured pressures not precisely aligned with CFD domain boundaries, need to account for phase shifting
- Engine compression ratio needs to be verified

Accomplishment: Task G.3 - Blendstock-to-Efficiency Application

Velocity contour predictions vs. experimental data

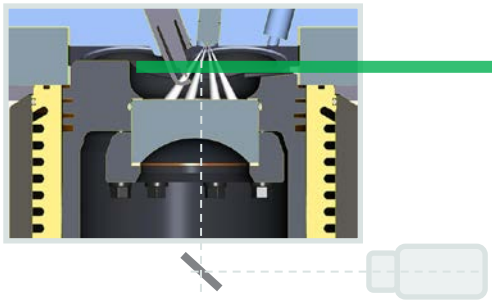
- Particle Image Velocimetry (PIV) measurements in swirl and tumble planes from Sandia
- Data from -30° aTDC, near nominal injection timing
- Simulation data from 2nd LES cycle (i.e., not ensemble averaged)

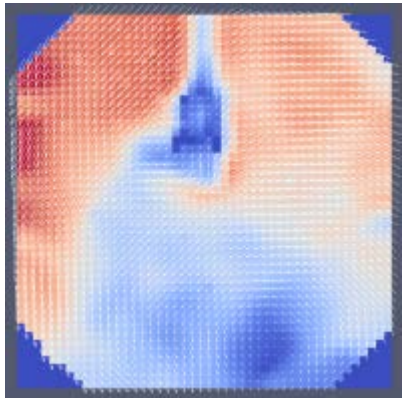
Cutting Plane Schematic

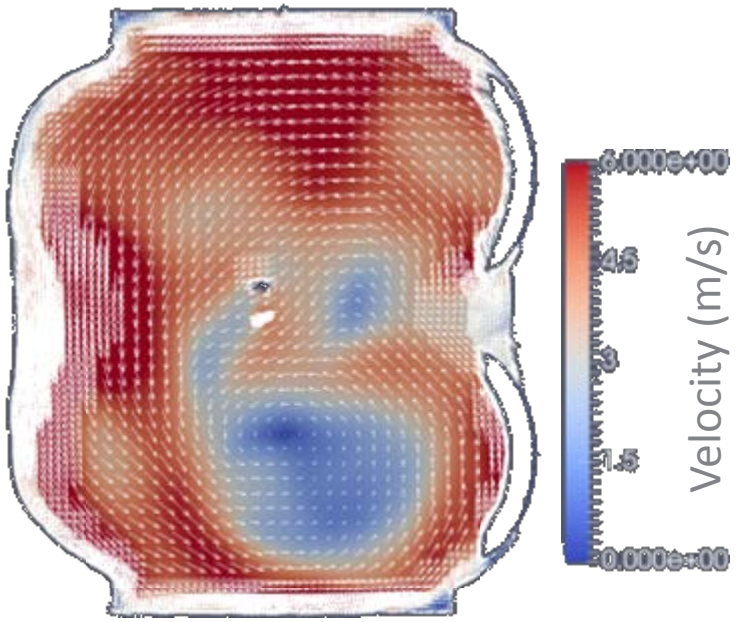
Experiment PIV

LES Simulation

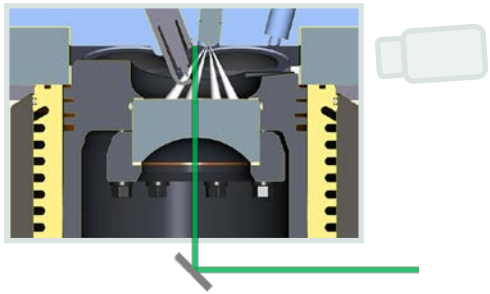
Swirl

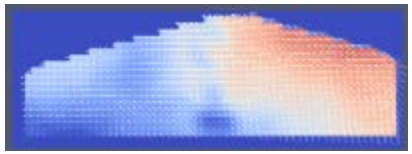


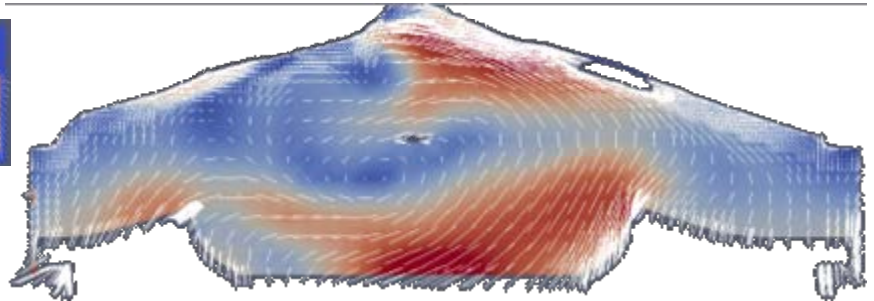




Tumble







Accomplishment: Task G.3 - Blendstock-to-Efficiency Application

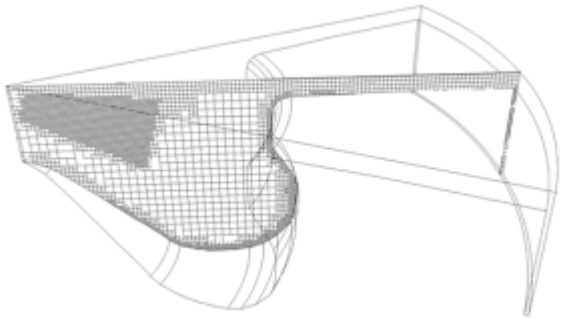
Effect of Fuel properties on engine performance (setup)

- production GM 1.9 L diesel engine run on gasoline compression ignition mode (GCI)
- CFD used to optimize combustion using CONVERGE code
- Global Sensitivity Analysis (GSA) on fuel properties

128 cases run in 5 days on Mira

5 fuel-related inputs perturbed

400K cells

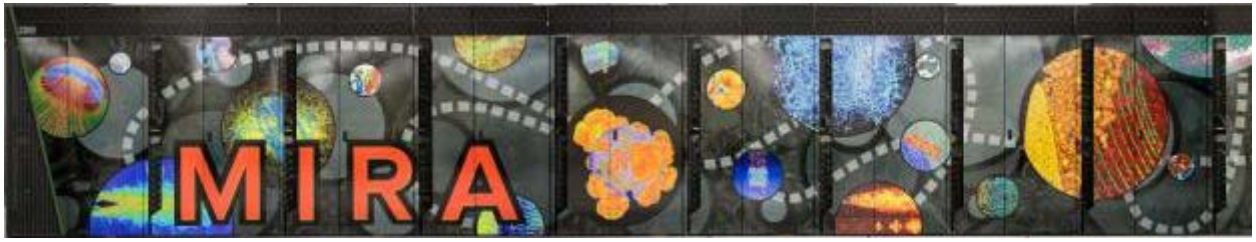


128 simulations

8000 cores

50 sp, 150 rxn (Liu)

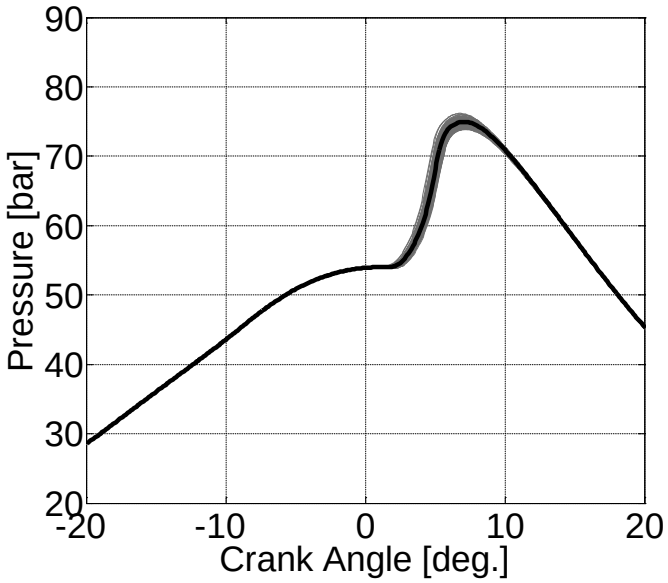
CONVERGE v2.1

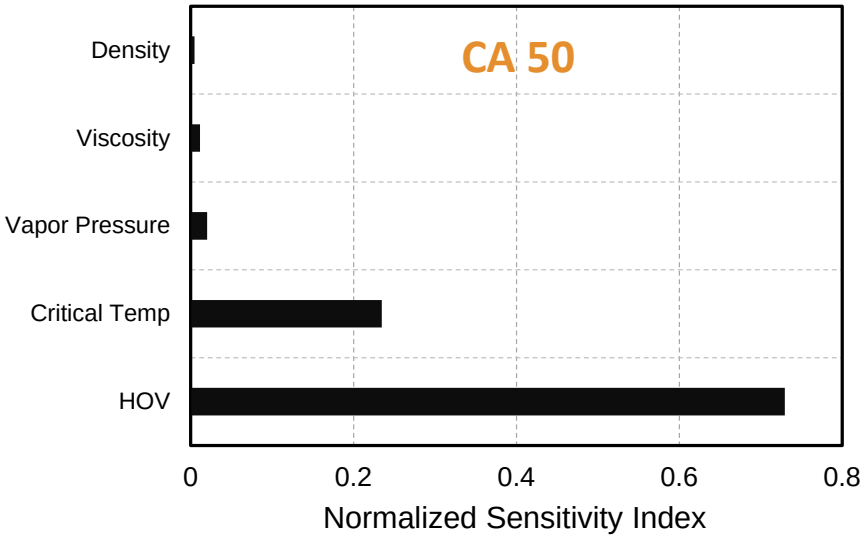


Accomplishment: Task G.3 - Blendstock-to-Efficiency Application

Effect of Fuel properties on engine performance

variable	description	baseline	min	max
$T_{(f,crit)}$	fuel critical temperature	540 k	530 k	550 k
Density	fuel density	1.00	0.95	1.05
HOV	fuel heat of vaporization	1.0	0.9	1.1
VP	fuel vapor pressure	1.0	0.9	1.1
Viscosity	fuel viscosity	1.0	0.7	1.3





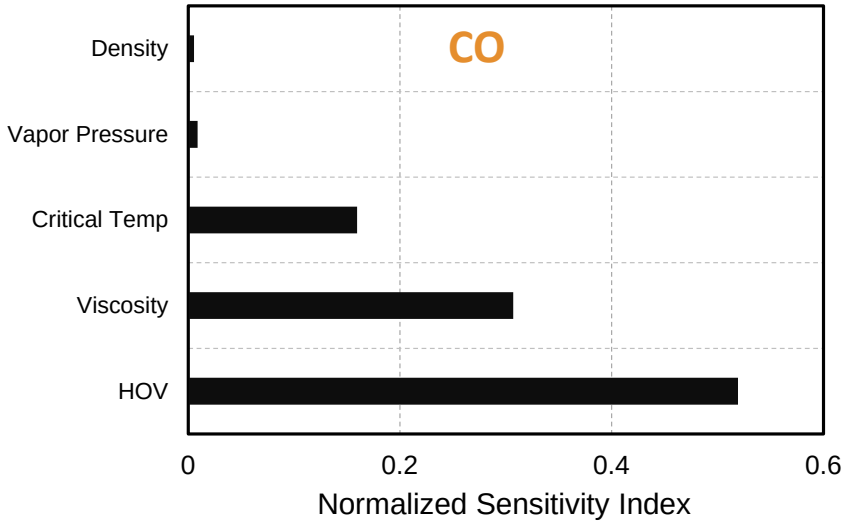
- Fuel properties varied (in Monte Carlo fashion) to demonstrate the capability of GSA tool
- Fuel property variations (in this range) have a significant influence on CA50
  - Fuel HOV and critical temperature seem to influence CA50

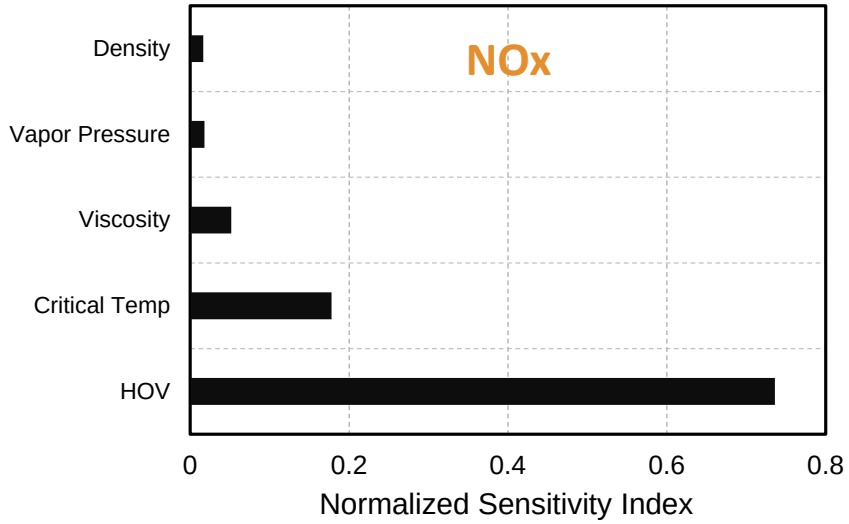
Future Work: Task G.3 - Blendstock-to-Efficiency Application

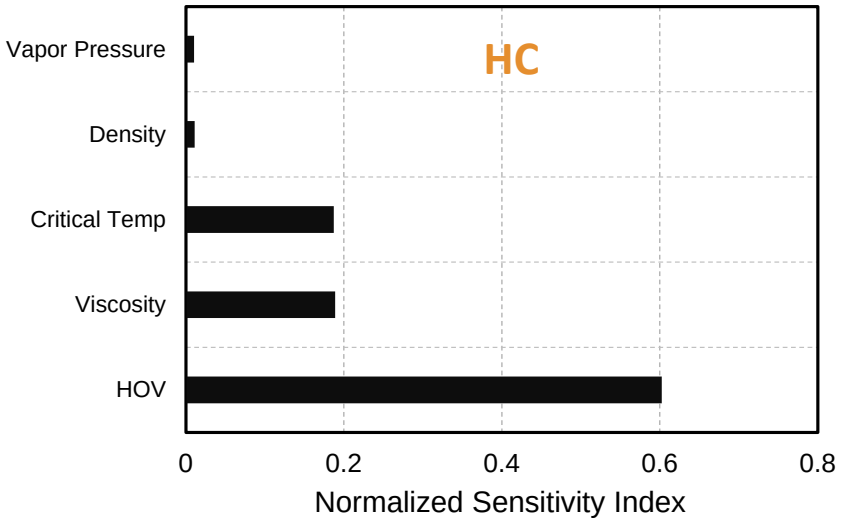
Effect of Fuel properties on DISI engine performance

Sandia DISI Engine

- Validate gas-exchange flow and combustion
- Simulate multiple engine operating conditions
  - Both those measured experimentally and those not
- Perform GSA for fuel property effects similar to the one done for GCI analysis



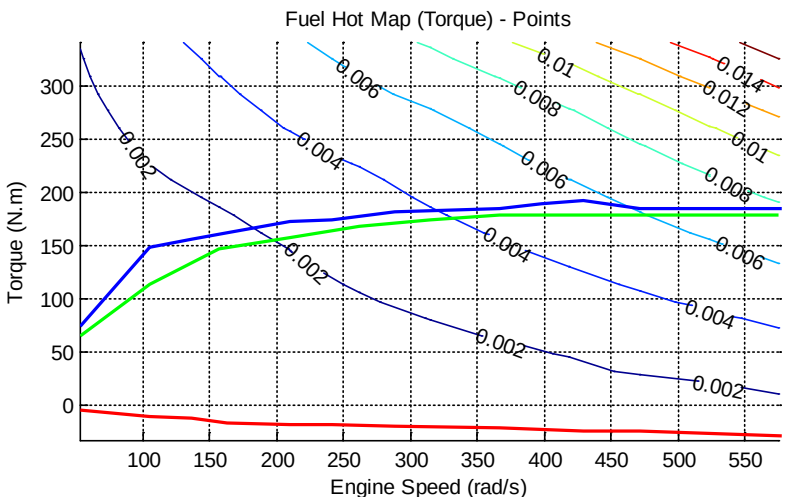




Future Work: Task G.3 - Blendstock-to-Efficiency Application

Linking engine simulations to efficiency

Fuel maps from engine simulations



- Proof-of-concept for the whole workflow exists (AMR2016_Project ID # VS185). Several portions need automation:
  - engine simulation maps => Autonomie
- The workflow allows us to compute fuel saving potential of engine & fuel choices

Transportation surveys

Vehicle Miles Travelled

Autonomie

Fuel economy in Regulatory & Real World Conditions

Analysis

Gasoline Savings attributable to new technology

Market Penetration Estimates

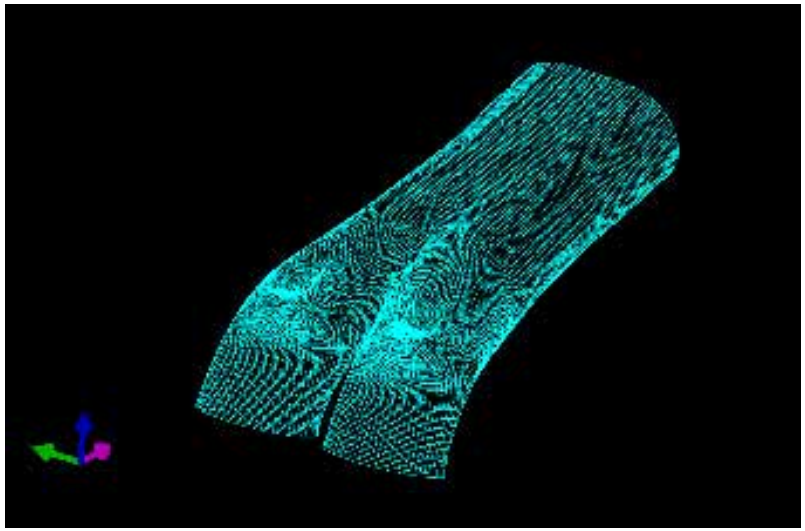
AUTONOMIE

ASSERT

Future Work: Task G.3 - Blendstock-to-Efficiency Application

Single cylinder engine modeling with KIVA-hpFE

- **Fielding KIVA-hpFE to model engine performance w/new fuels**
  1. Grid developed for Thrust I DISI engine (Sjoberg, SNL) and other chosen engines (ongoing)



GridPro mesh for Intake Manifold of Sandia DISI engine taken from X-ray generated faceted surface

  1. Chemkin chemistry solver functionality in KIVA-hpFE (ongoing)
     - collaborating with ANSYS's Reaction Design group
  2. Incorporate realistic thermophysical properties for liquid fuel blendstocks
  3. Perform full engine simulation for Thrust I engine and fuels

Future Work: Task G.3 - Blendstock-to-Efficiency Application

Multi-cylinder engine performance modeling

Multi-cylinder simulation studies at Oak Ridge National Laboratory

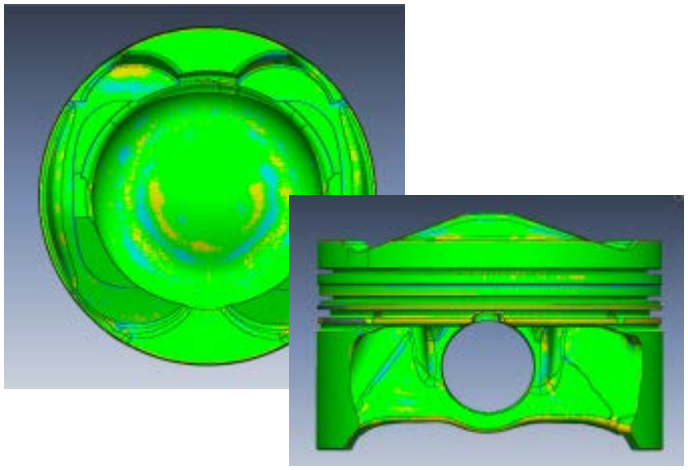
- Full-engine GT-Suite simulations of 1.6-L Ford GDI engine
- Supports experimental, high-octane fuel studies (Sluder/ORNL)

Efforts will expand upon experimental capabilities to further explore potential benefits of high-octane fuel blends

- Explore enhanced boosting strategies to enable additional engine down-sizing
- Coupled GT-Power/CONVERGE simulations in collaboration with ANL to explore fuel-vaporization and knock onset
- Provide engine maps to ANL for fuel-economy simulations with Autonomie

1.6-L Ford GDI engine installed in dynamometer cell at ORNL

Hardware scans and engine measurements necessary for constructing the 1-D and CFD geometry models are underway



Future Work: New FY17 Task

Create tool to search for optimized scenarios w/Co-Optima data

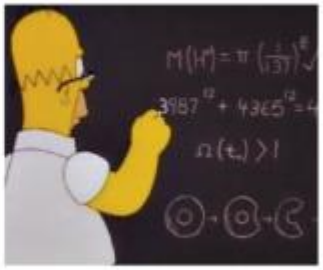
Database: fuel properties, sustainability, affordability, scalability, infrastructure, and retail attributes

ΔGHG	=	*a*
H_2O consumption	=	*b*
Viable routes	>	*c*
Feedstock cost	<	*d*
Pipeline compatibility	=	*e*
Tech Readiness Level	>	*f*
Energy density	>	*g*
Biodegradability	>	*h*

Scenario constraints

"Optimizer"

Engine/vehicle merit function



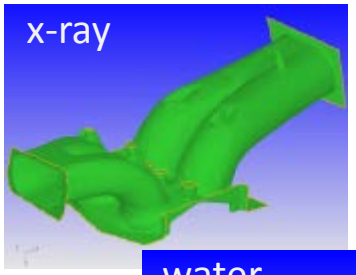
Optimal fuel blend formulations

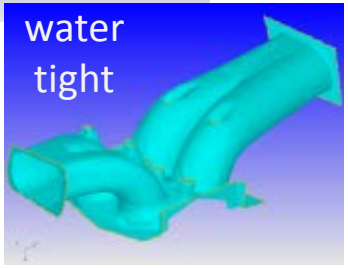
Important to account for uncertainty

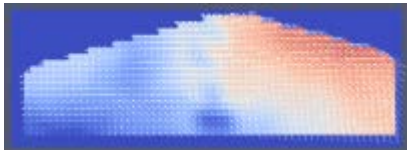
Summary of FY16 Accomplishments

shared data & resources

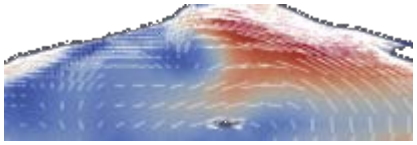
real geometry CFD validation





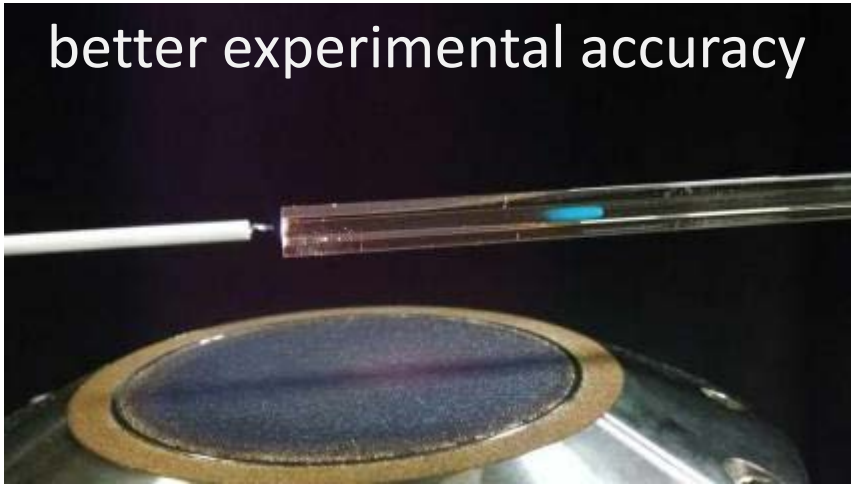


PIV- Experiment

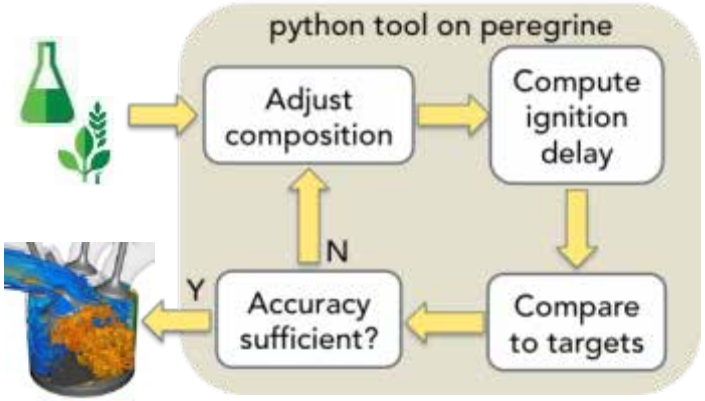


CFD - Simulation

better experimental accuracy



faster setup time for new fuels



Technical Backup Slides

Approach/Strategy: Six Integrated Teams

Low Greenhouse Gas Fuels

Identify promising bio-derived blendstocks, develop selection criteria for fuel molecules, and identify viable production pathways

Fuel Properties

Identify critical properties and allowable ranges, systematically catalogue properties, and predict fuel blending behavior

Advanced Engine Development

Quantify interactions between fuel properties and engine design and operating strategies – enable optimal design of efficient, emission-compliant engines

Modeling and Simulation Toolkit

Extend the range, confidence and applicability of engine experiments by leveraging high-fidelity simulation capabilities

Analysis of Sustainability, Scale, Economics, Risk, and Trade

Analyze energy, economic, and environmental benefits at US economy-level and examine routes to feedstock production at scale through existing biomass markets

Market Transformation

Identify and mitigate challenges of moving new fuels and engines to markets and engage with full range of stakeholders

Task G.2.1 – Details on extreme mechanism reduction

1. Get **experimental data on new fuels** from other Co-Optima teams (i.e. ignition delay time) over ranges of interest (P, T, phi)
2. Define the **"form" of the optimized chemical mechanism** (2, 4, 6 steps, and the uncertain chemical parameters). The approach helps finding the unknown chemical parameters
3. Build **surrogate (Polynomial Chaos Expansion)** of the chemical model: homogenous reactor simulations used to find the surface response of the mechanism in parameter space.
4. Use **Bayes' Rule and PCE to find chemical parameters** of optimized mechanism
5. Propagate parameters' uncertainties to get error bars on prediction

Bayes formula gives the joint PDFs on parameters of interest (called posterior):

$$\underbrace{p(\lambda|d_{\mathbf{x}})}_{\text{Posterior}} = \frac{\overbrace{p(d_{\mathbf{x}}|\lambda)}^{\text{Likelihood}}\ \overbrace{p(\lambda)}^{\text{Prior}}}{\underbrace{p(d_{\mathbf{x}})}_{\text{Evidence}}}$$

- Prior: knowledge on the parameters (ranges, …)
- Likelihood: obtained by sampling the PCE in parameter space
- Evidence: normalizing constant in the present context