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

Co-Optimization of Fuels & Engines

FOR TOMORROW'S ENERGY-EFFICIENT VEHICLES

Simulation Tools

Co-Optimizer

In cylinder CFD

Small volume testing and inputs preparation

Summary

Simulation workflow includes developing detailed, validated in cylinder CFD from real geometry

Necessary inputs to CFD calculations (mechanisms, surrogate composition, initial conditions, liquid fuel properties, model validation…) generated with the aid of small volume test data, idealzied cacluations, synthetic experiements and sensitivity studies

Experimental engine ‘cloud of points’ will be augmented by simulation sensitivitities to refine engine merit function

Optimizer is client for data, but may drive workflow in the future

Framework for optimization

Multi-objective

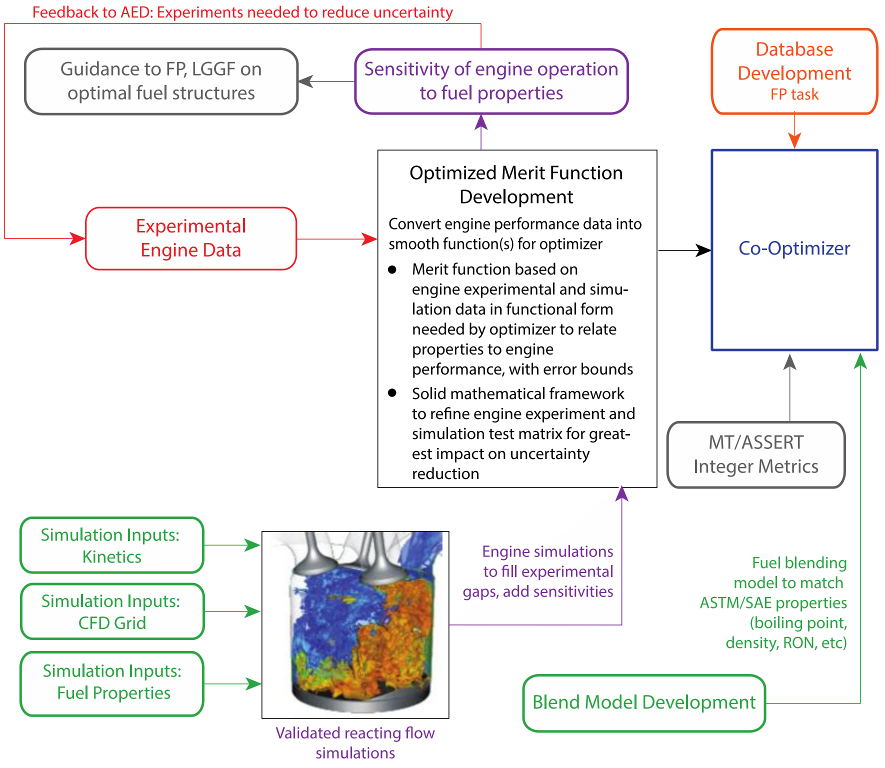
Goodness function non-linear function of composition (engine merit function) or integer valued (ASSERT/MT metrics)

Single point (no resource scheduling)

MINLP

Uncertainty in objective function

Uncertainty in contributions to objective function



$$
\begin{aligned}
Merit = {} & \frac{RON_{\text{mix}} - 92}{1.6} - K\frac{S_{\text{mix}} - 10}{1.6} \\
& + \frac{0.01(ON)(HoV_{\text{mix}} - 415)}{1.6} + \frac{HOV_{\text{mix}} - 415}{130} \\
& + \frac{S_{L,\text{mix}} - 46}{3} - LFV_{150} \\
& - H(PMI - 2)(0.67 + 0.5(PMI - 2))
\end{aligned}
$$

Non linear blending for properties

Framework built up on open source tools (PyOMO, IPOPT,…)

Coefficients have uncertainty and subject to refinement

Unbounded

Maximize by inspection with

- High RON
- High S_L
- Low LFV150
- Low PMI

S, HOV, ON… it depends

Properties may be correlated

With a cost constraint, properties on cost basis determine solution

In Cylinder CFD

Sensitivities to Develop Merit Function

Engine experiments deliver a ‘point cloud’ of data mapping out property / performance relationships for a fixed engine design

Once validated, CFD can provide sensitivities to properties around operating conditions

Process has been to use a mixture of CAD and X-Ray data to build up geometry that is combined with thermo-physical and chemical inputs for simulation and compared to experiment for validation

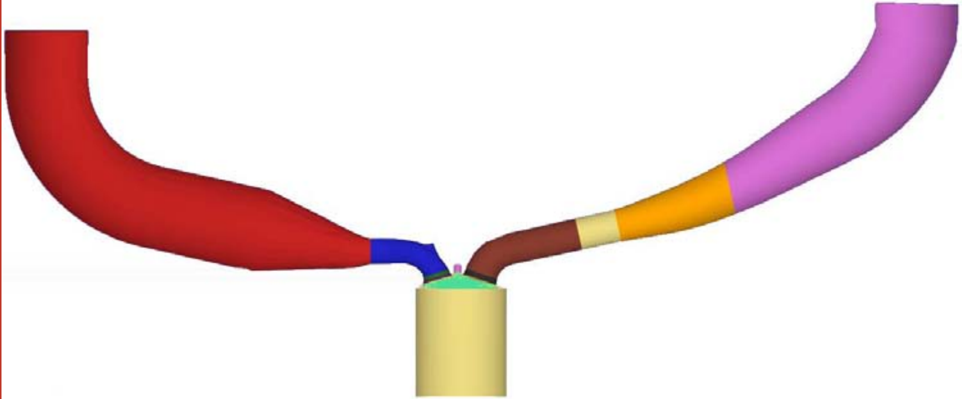
Validating the model set-up for DISI engine simulations, performed by ANL CFD team

- Compare against PIV and imaging data from Sandia DISI optical engine

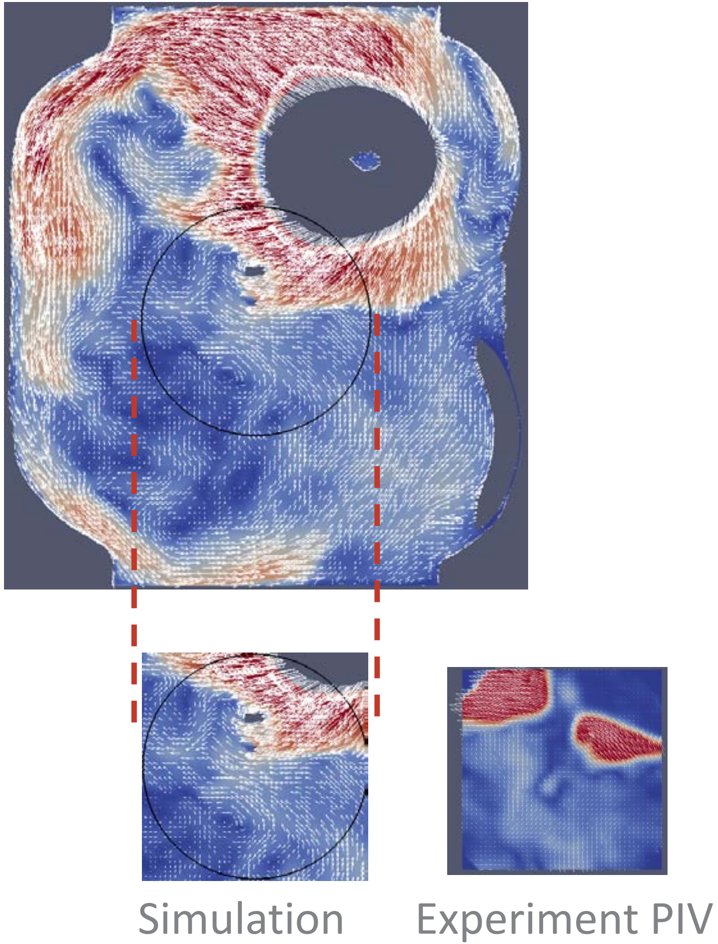
Simulating multiple engine cycles with LES

- Detailed geometry, including an x-ray scan of the head and valves
- Start with motored conditions including sprays to get correct composition and flow-field near the spark plug
- Move to combustion later
- Testing multiple mesh resolutions for accuracy/time trade-offs

Eventually Use the model set-up to perform Global Sensitivity Analysis to understand relative importance of different fuel properties for engine performance



In-cyl. Δ	P_{peak} (MPa)	Tot. KE ($kg\text{-}m^2/s^2$)
0.7 mm	2.630	0.01217
1.0 mm	2.652	0.01144
1.5 mm	2.673	0.01103
2.0 mm	2.697	0.01009
Exp	2.547	-



PIV data used to validate LES flow

- PIV limited in dynamic range
- Small view area

Only individual cycles completed for LES results

- Multi-cycle simulations in-progress
- General flow trends appear to be captured

After initial validation, further E30 operation at different operating conditions will be simulated by ANL CFD team

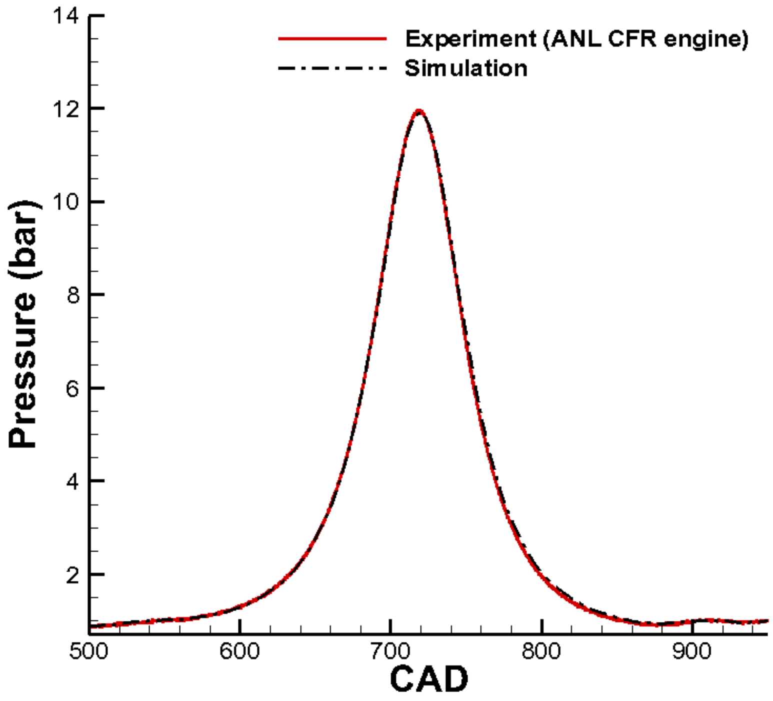
- Continue to expand the test matrix to fill an engine map

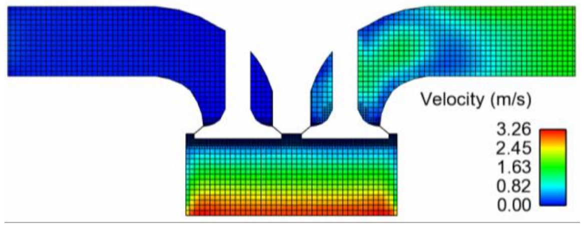
7

- Virtual CFR engine based on detailed CFD being developed and validated by ANL simulation team
- Objective: to evaluate the impact of biofuel composition and thermophysical properties on its ignition propensity
- 3D open cycle motoring simulations are performed and shown to match well with experiments

Current CFR engine surface mesh provided by Dr. Ben Wolk (SNL) and Prof. J.Y. Chen (UCB)

CFR engine data provided by Dr. Thomas Wallner and Dr. Chris kolodziej at ANL



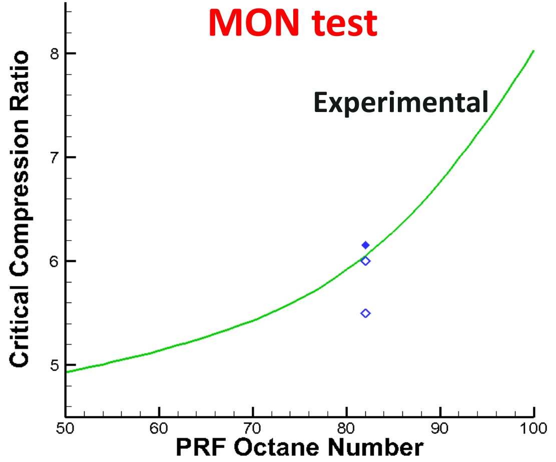


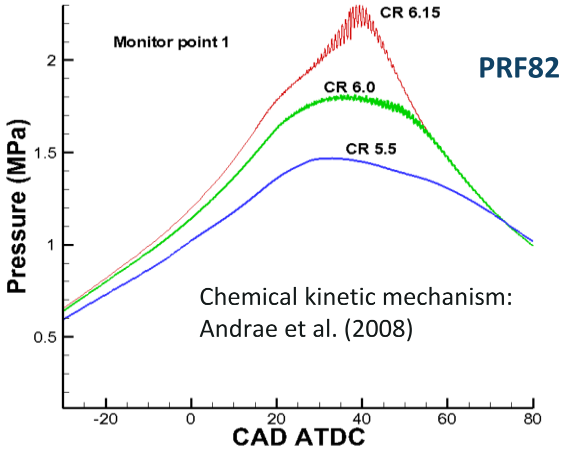
- 3D closed cycle simulations are performed at various compression ratios under typical RON/MON conditions for various PRFs

- Simulations are able to capture the onset of knock very well and are consistent with experimental data

- The CFD model can be used to predict which fuels are more susceptible to knock at a given compression ratio

- The end-gas pressure-temperature history from simulations are being used by the Fuel Property (FP) teams to identify relevant test conditions for RCM experiments





Small volume testers and CFD Inputs

SVTs provide rapid property screening for merit function inputs or other metrics

CFD requires tractable chemical mechanism and composition in terms of pure components

Simulations of SVTs aid in design, interpretation of results from SVTs as well as validation for simulations

SVTs also provide targets for determining surrogate composition as well as reduced mechanisms

Creation of fuel surrogates in chemical mechanisms done by matching targets for 0D simulations

AKI

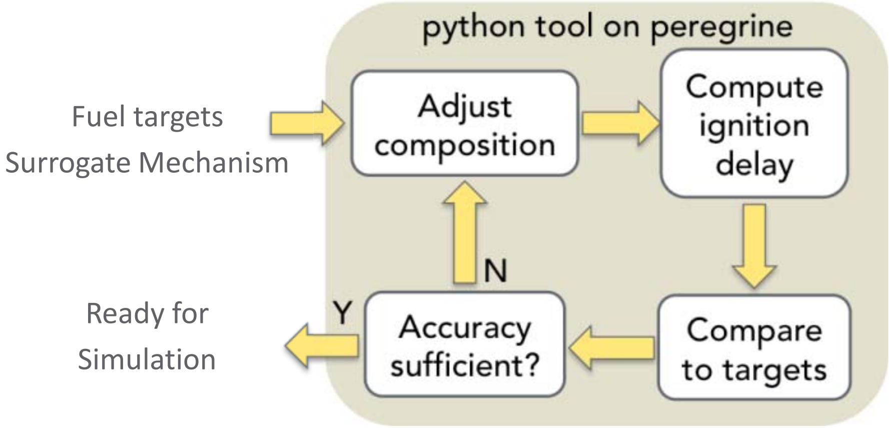
Sensitivity

Distillation Curve

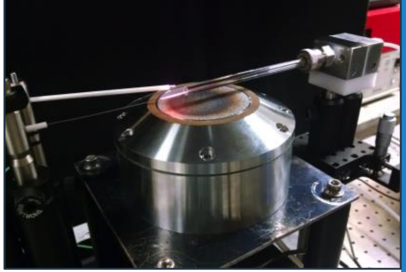
H/C ratio

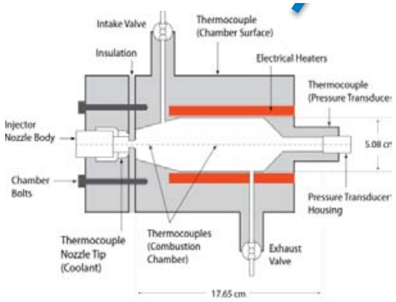
PIONA

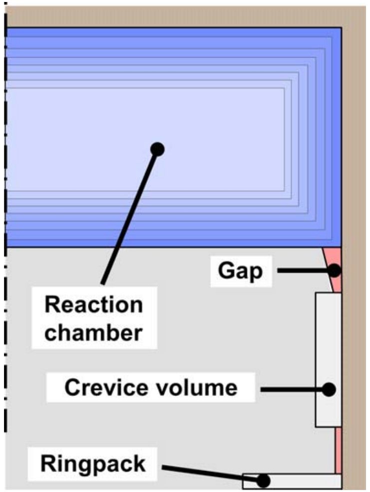
High throughput for optimization / search enabled by Zero-RK high performance chemical mechanism integrator



Zero-RK







Small volume testers used for rapid fuel screening

Simulations developed to aid design and understanding

Used as reduction targets along with traditional sources for chemical mechanisms and targets for surrogate generation

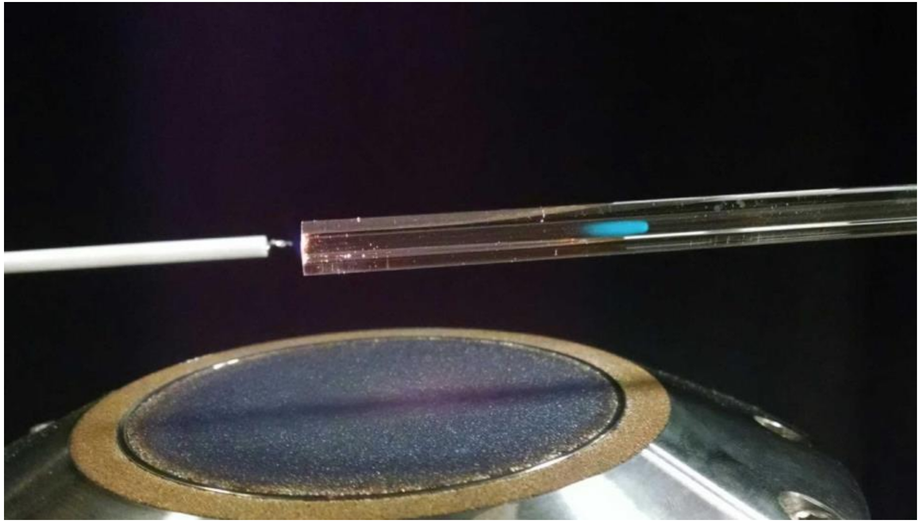
Under consideration: IQT, AFIDA, RCM, microFIT, micro flow reactor, virtual CFR engine

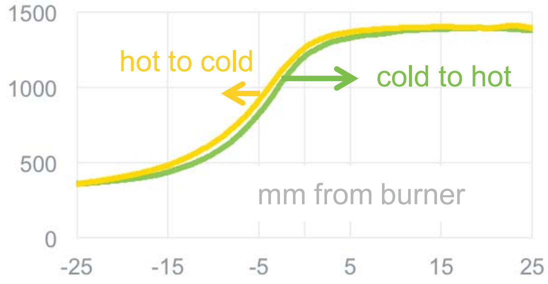
The micro-liter fuel ignition tester uses an unsteady flame in a mm-scale channel to measure fuel chemistry effects

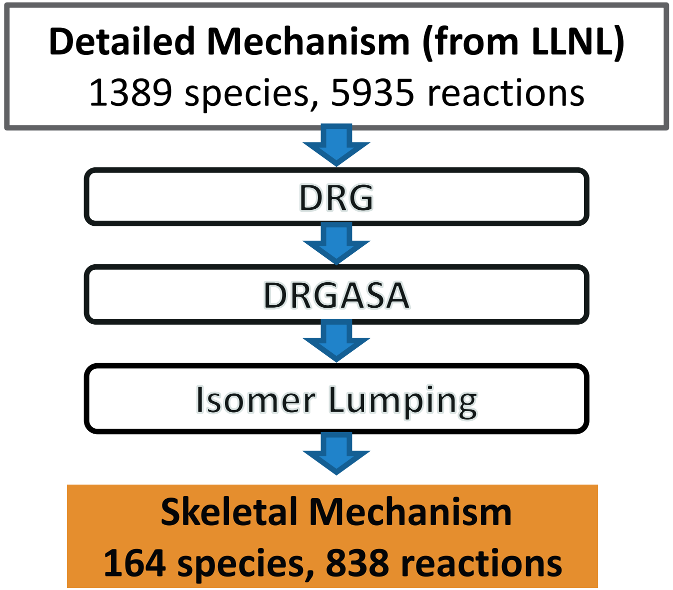
A detailed thermal model was created of the temperature difference between the thermocouple and wall

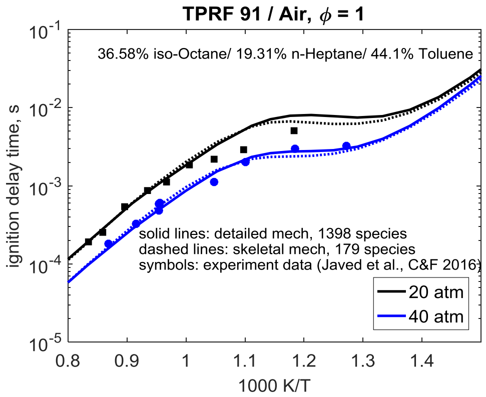
Modeling showed the thermocouple holder and translation speed affected the measured temperature, resulting in a 30K error corrected on redesign

Thermal model for microFIT improves measurement accuracy









- Development of more robust and predictive reduced chemical kinetic mechanisms underway
- Mechanism reduction is performed with a focus on gasoline surrogates (PRFs/TPRFs) and gasoline/ethanol blends
- Starting point: LLNL detailed (1389 species) gasoline surrogate mechanism
- Reduction performed by Y. Wu and Prof. T. Lu at UConn

Range of validity:

- ✓ Pressure: 1-100 atm
- ✓ Equivalence ratio: 0.5-1.3
- ✓ Initial temperature: 750 – 1800 K

Summary

Simulation workflow includes developing detailed, validated in cylinder CFD from real geometry

Necessary inputs to CFD calculations (mechanisms, surrogate composition, initial conditions, liquid fuel properties, model validation…) generated with the aid of small volume test data, idealzied cacluations, synthetic experiements and sensitivity studies

Experimental engine ‘cloud of points’ will be augmented by simulation sensitivitities to refine engine merit function

Optimizer is client for data, but may drive workflow in the future