Collaborative Combustion Research with BES

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FY2013 DOE Vehicle Technologies Program Annual Merit Review
Advanced Combustion Engine R&D / Combustion Research
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Program Manager: Gurpreet Singh

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Overview

Timeline

- Project provides fundamental research to support DOE/industry advanced engine projects
- Project directions and continuation are evaluated annually

Barriers

- Limited fundamental knowledge of combustion in advanced engine regimes
- Inability to predictively model IC engine combustion for design and engine control

Budget

- Project funded by DOE/VTP
  - → FY11 funding: $400 k
  - → FY12 funding: $315 k
  - → FY13 funding: $320 k

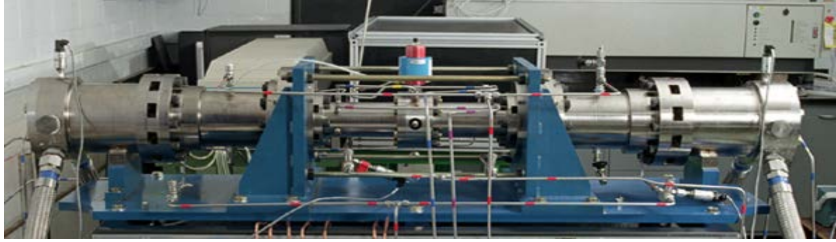
Partners

- ANL (CSE Division), LLNL
- U. of Akron, Marquette U., UW-ERC, NUI Galway, U. Lille, U. Leeds, KAUST, U. Michigan
- International RCM Workshop

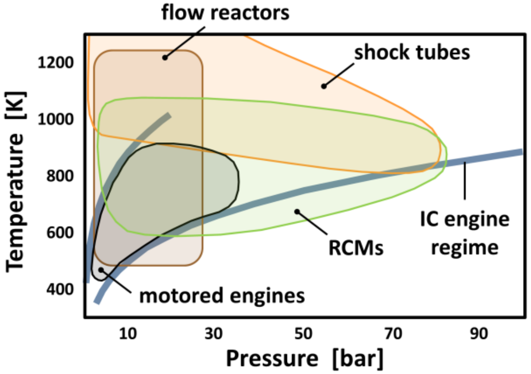
Objectives and Relevance to DOE

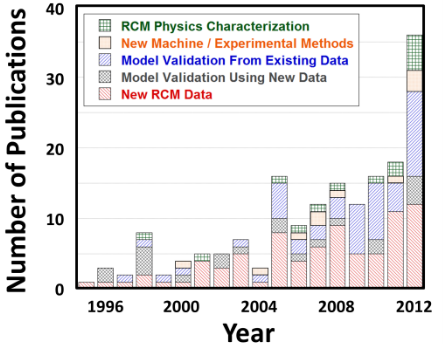
- **Acquire necessary data, and develop / validate / refine chemical kinetic and relevant models to achieve low uncertainty for transportation-relevant fuels (conventional and future gasolines, diesels and additives) at conditions representative of advanced combustion regimes, leveraging collaborations with BES-funded groups, and researchers across the broader community.**
- **Predictive simulations with these models could be utilized to overcome technical barriers to low temperature combustion (LTC) and achieve required gains in engine efficiency and pollutant reductions**

Project Approach
RAPID COMPRESSION MACHINE



- Utilize ANL's twin-piston RCM to acquire autoignition data
  - RCMs cover important regimes relevant to LTC, provide necessary data for model validation



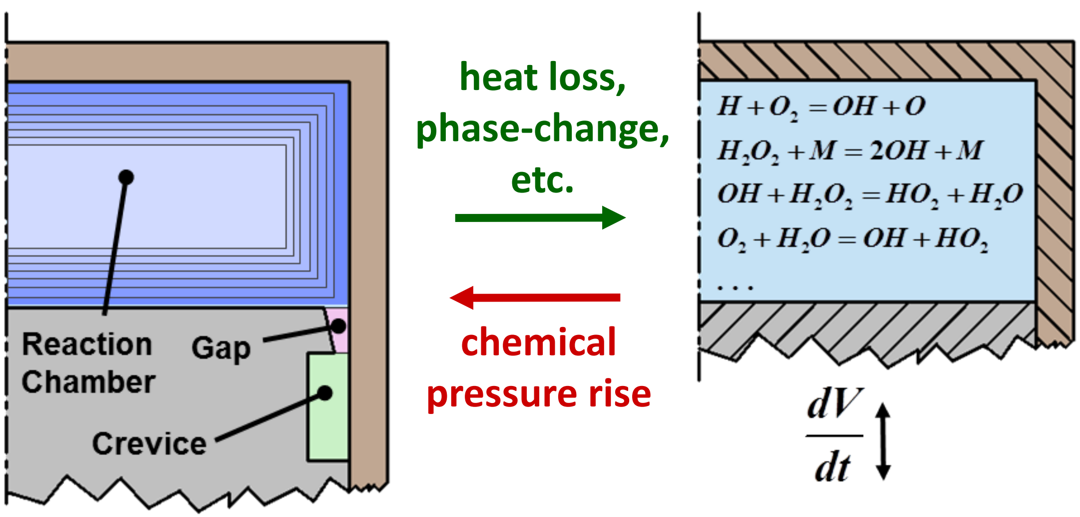


- Employ novel data analysis tools and advanced diagnostics
  - Physics-based, reduced-order system model
  - Developing time-resolved gas sampling and speciation
- Develop and synergistically refine models using advanced probing techniques (e.g., GSA) and detailed calculations of sensitive processes (e.g., individual reaction rates)
- Developing capability to utilize high MW fuels and blends within a new RCM

Project Approach

RCM System Model

- Physics-based, reduced-order model coupled with chemical kinetics software – accounting for physical-chemical interactions during experiments (e.g., LTHR + crevice flows)
  - Computationally-efficient approach improves simulation fidelity
  - Facilitates utilization of additional metrics for mechanism validation / refinement (e.g., ROHR (1st, 2nd stages))



derive from physical model

$$-\frac{V^{\gamma+1}}{\gamma}\left[\frac{\ln V}{V^{\gamma}}\frac{d\gamma}{dt}+\frac{1}{C}\frac{dP}{dt}\right]=\frac{dV}{dt}$$

supply to kinetics software

doi:10.1016/j.combustflame.2012.07.010

Improved adiabatic core, Homogeneous Reactor Model

Project Milestones

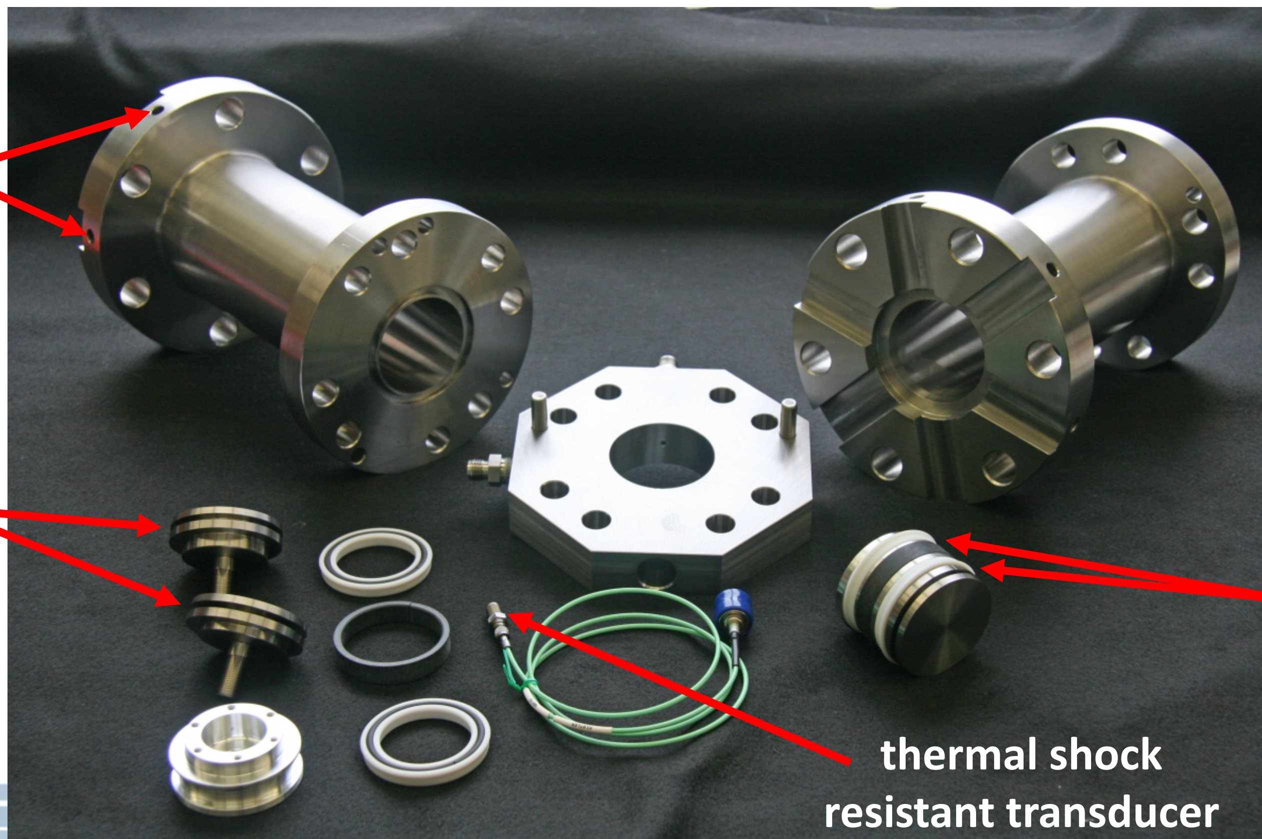
FY2013 Budget – $320k

Subtask	Milestone	Date
1	Upgrade RCM components / systems including reaction chamber, pistons, heating system and mixture preparation tank.	Dec ’12
2	Refine reduced-order, physical models for accurate simulation of RCM experiments, including piston crevice sub-models. Integrate a multi-zone reactor model to account for inhomogeneous ignition in the RCM, especially for NTC conditions.	Jul ’12
3	Acquire ignition delay measurements for gasoline surrogate fuels + reactivity modifiers. Use 2 to 5 component surrogates + blends of 2-ethyl-hexyl nitrate ($C_8H_{17}NO_3$), di-tert-butyl-peroxide ($C_8H_{18}O_2$). Develop, validate chemical kinetic models.	Jul ’13
4	Acquire ignition delay measurements of FACE gasoline fuels + reactivity modifiers.	Sep ’13
5	Develop reduced-order, control-oriented ignition model covering wide range of fuel reactivity (e.g., octane number, ON sensitivity) and charge dilution.	Sep ’13

Technical Accomplishments

System Modifications

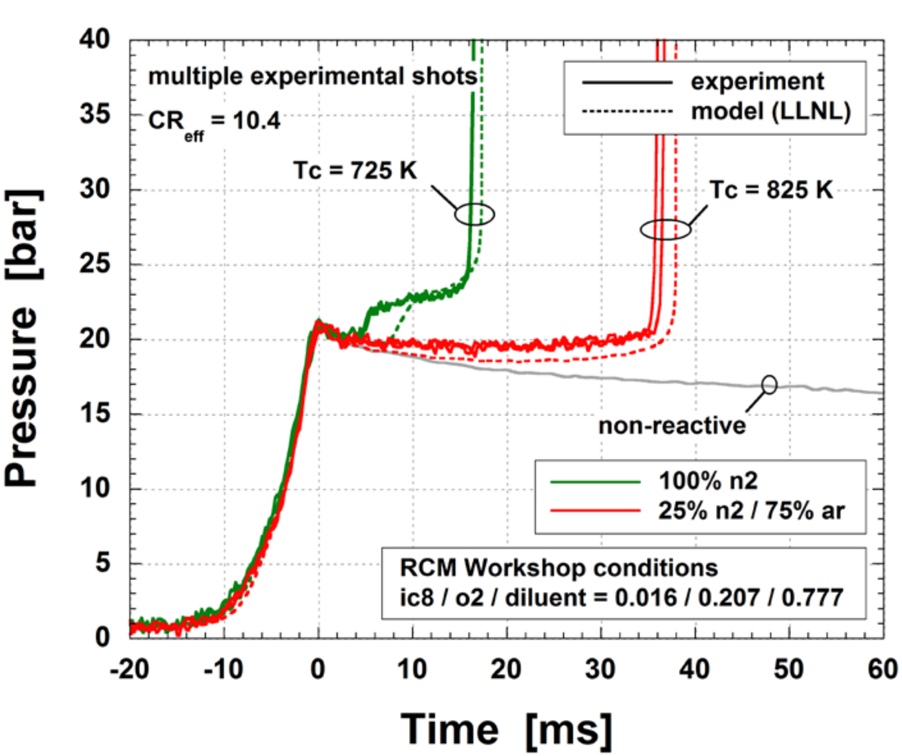
- Redesign of reaction chamber / pistons
  - Improving thermal homogeneity via creviced pistons and capability for higher fidelity heating system
  - Reducing dead volume, leakage to improve boundary conditions

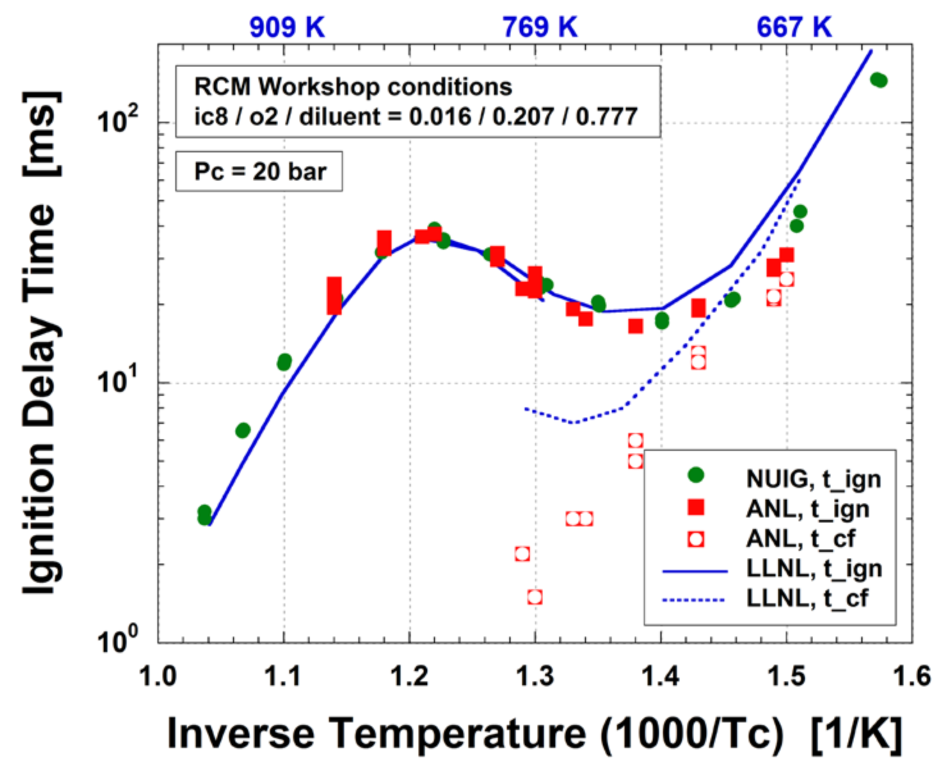


Technical Accomplishments

System Modifications

- Representative tests at **RCM Workshop** conditions
  - Excellent repeatability, comparability with existing datasets
  - Good agreement with validated chemical kinetic model (LLNL)



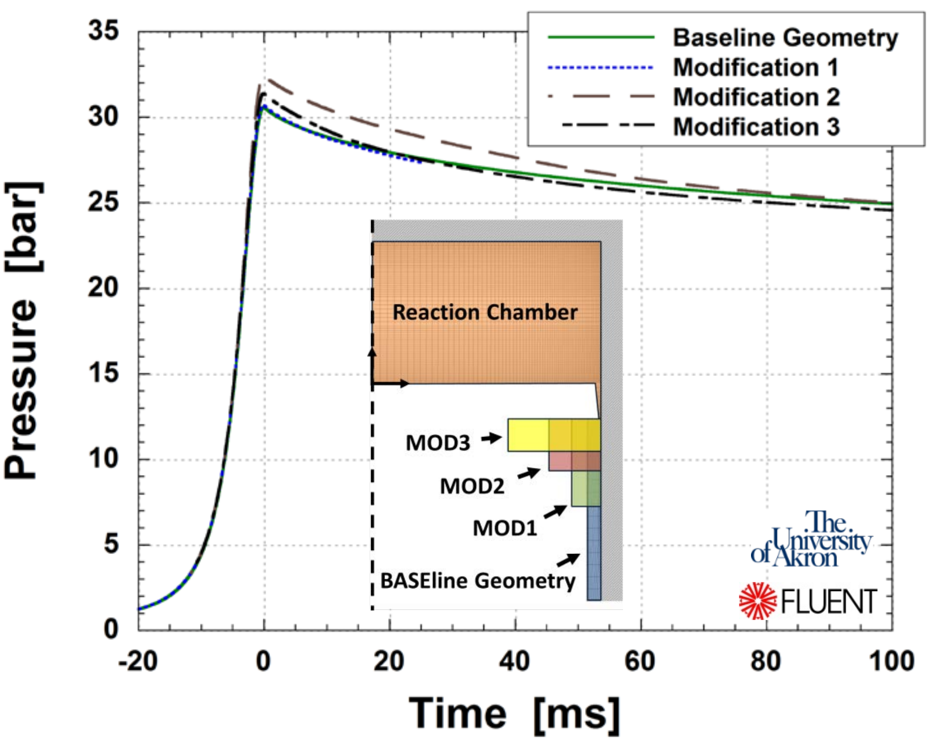


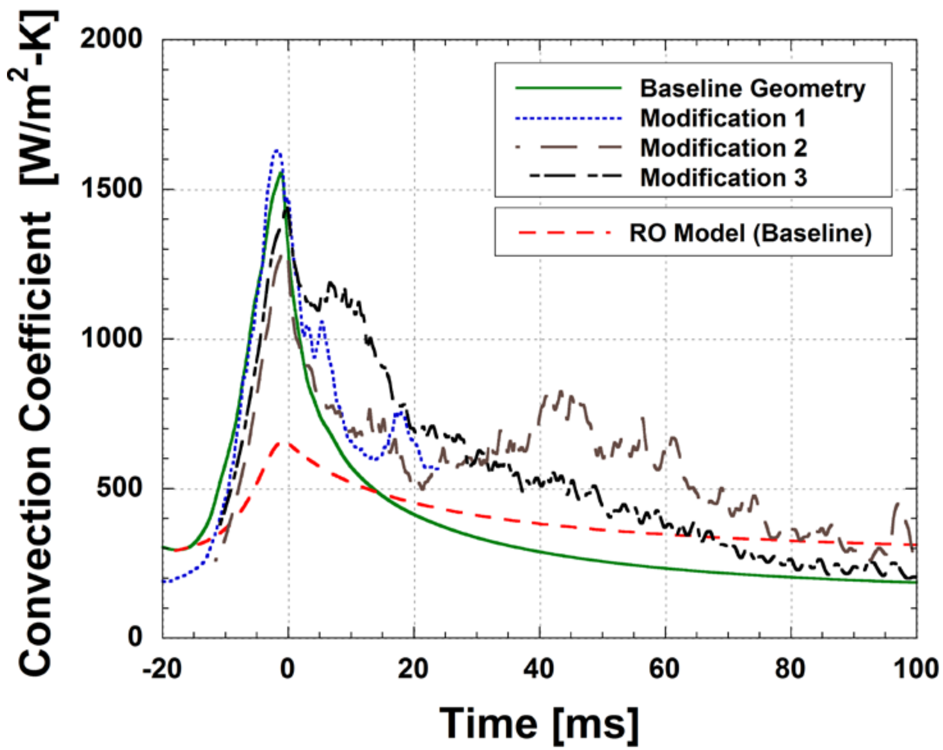
Some differences in cool flame / preliminary heat release

Technical Accomplishments

RCM SYSTEM MODEL

- **Refining sub-models for gap and crevice for various piston geometries used within different machines**
  - **Are some configurations better than others?**



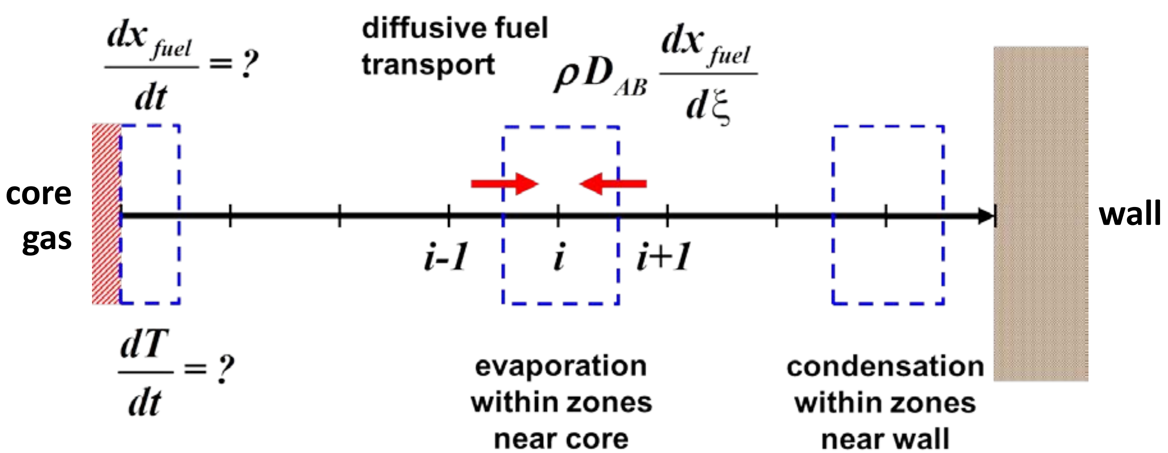


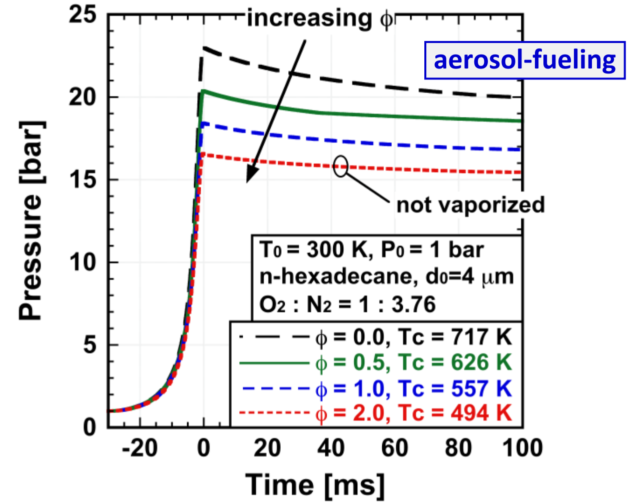
Gas motion in crevice drives heat loss, RC pressure / temperature history

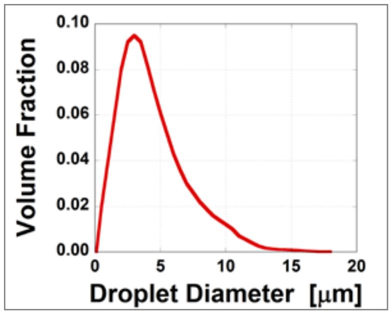
Technical Accomplishments

RCM System Model

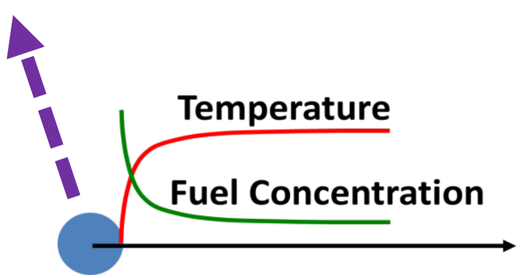
- **Incorporating sub-models for phase change that can occur in experiments using high boiling point fuel blends**



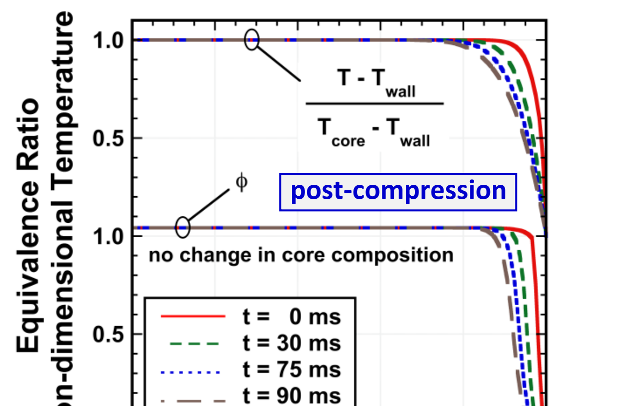




Many droplets



Single droplet evaporation

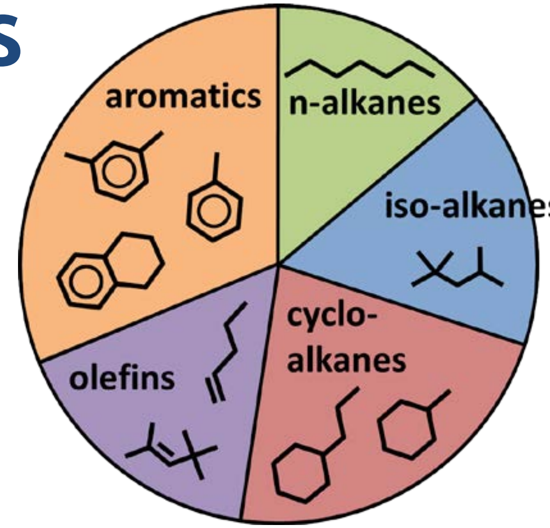


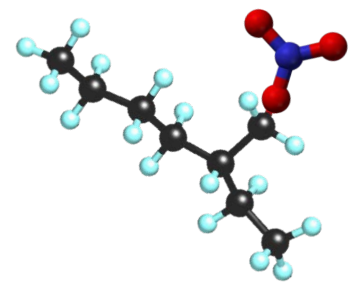
Preliminary simulations indicate core gas not affected by near-wall condensation

Technical Accomplishments

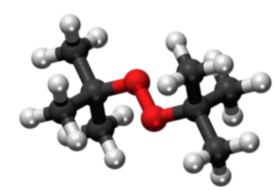
Reactivity Modifiers

- **Additives used to dynamically control combustion in advanced regimes (e.g., LTC, RCCI), multi-mode switching**
  - **Investigating fuel / additive sensitization using gasoline surrogates and FACE gasoline**
  - **Developing / validating chemical kinetic models for blends to understand kinetic and exothermic influences**
  - **Is there an optimal additive for ACE's?**

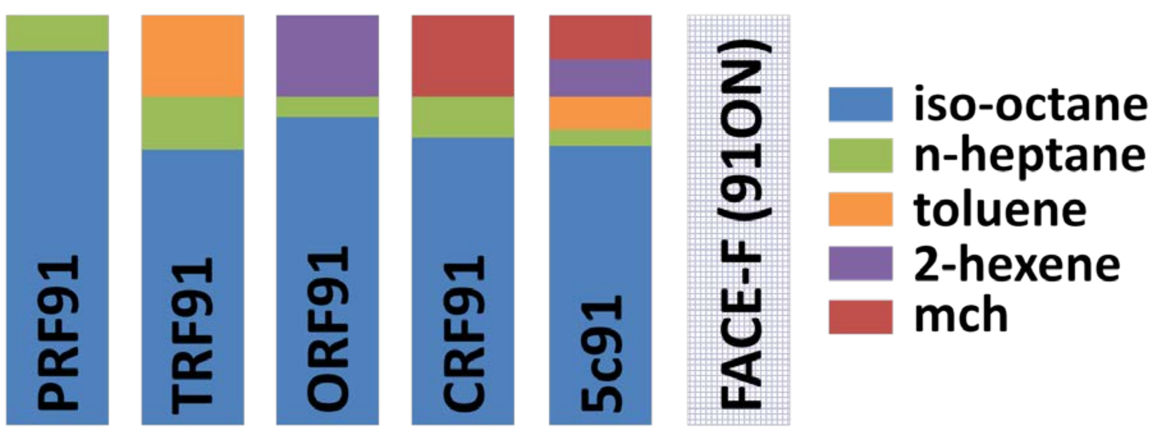




EHN



DTBP

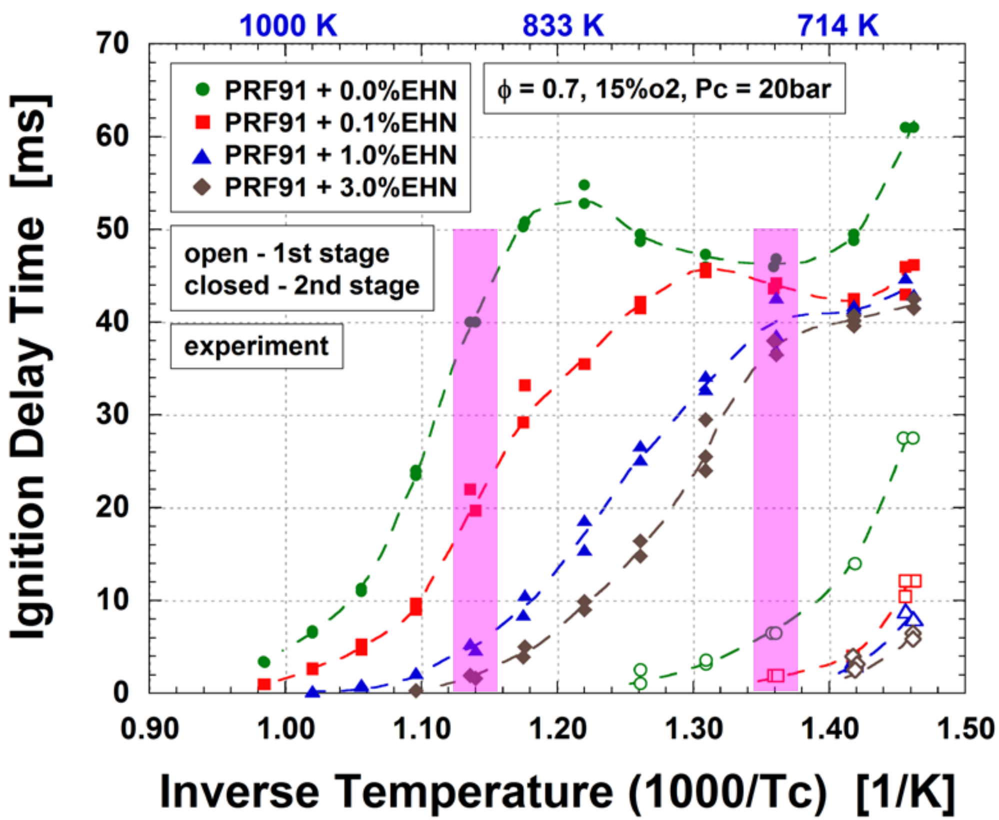


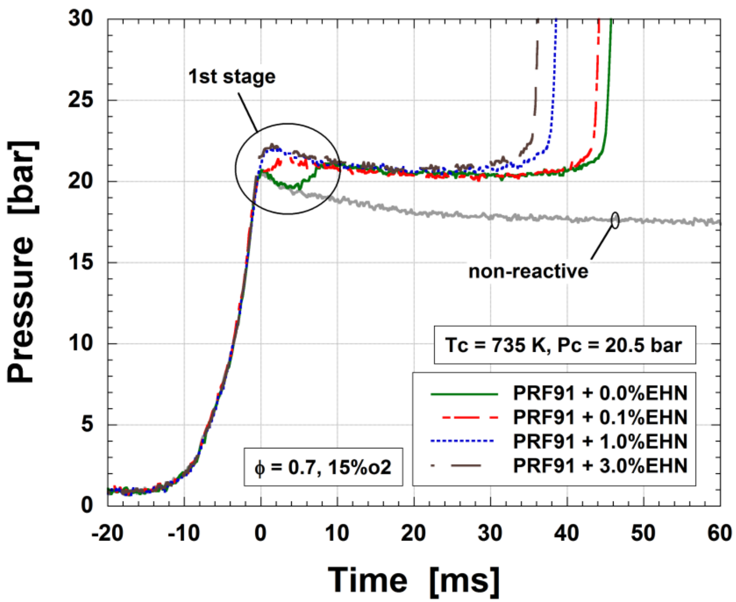
Others??

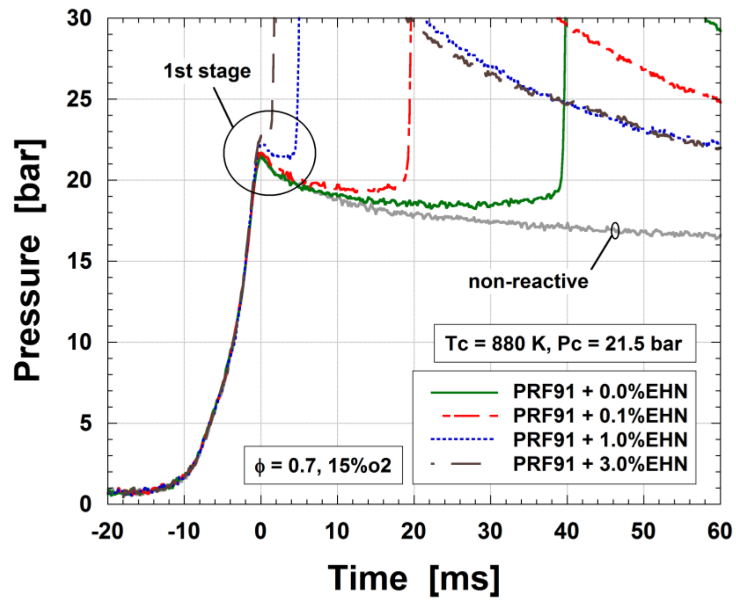
Technical Accomplishments

Reactivity Modifiers

- PRF91 + EHN, experiments
  - Early heat release with most additive concentrations





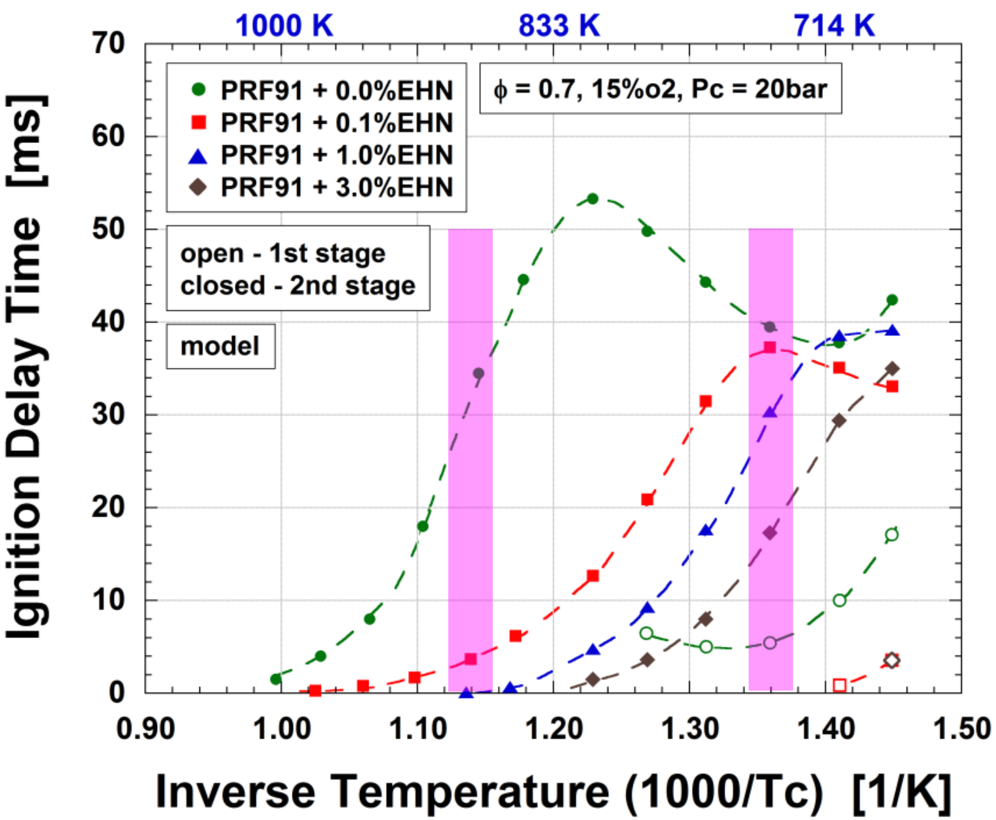


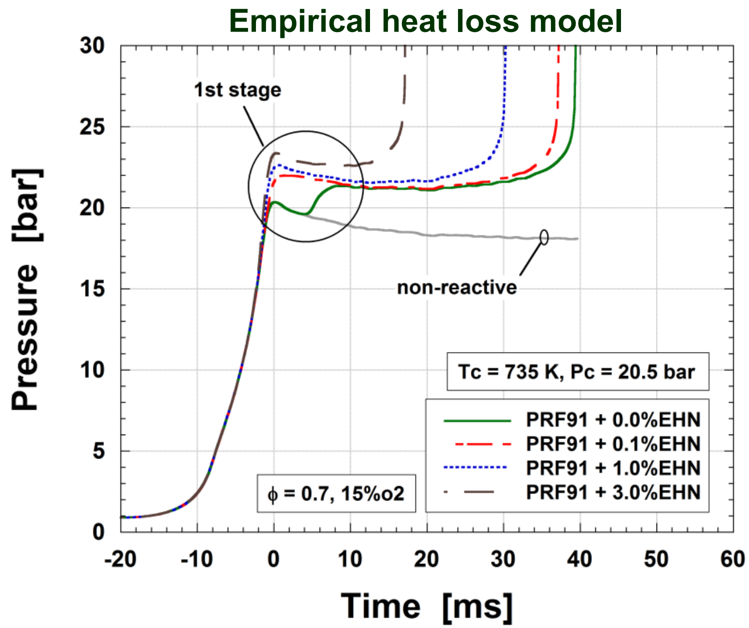
EHN influential throughout NTC regime

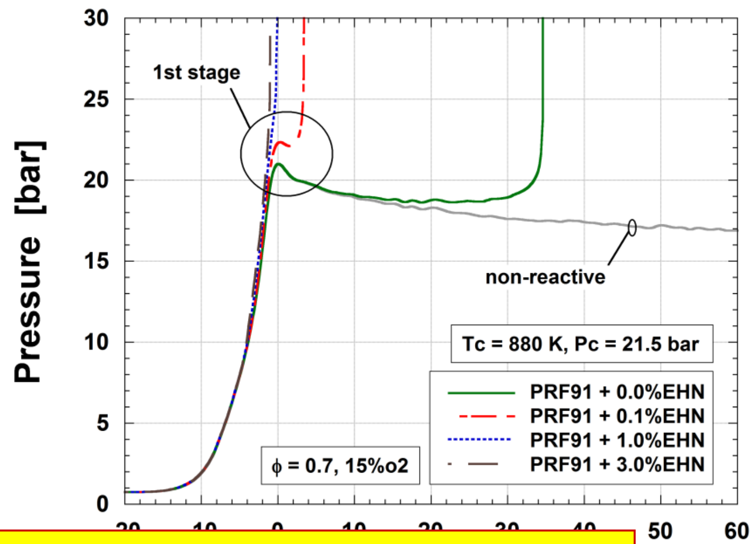
Technical Accomplishments

Reactivity Modifiers

- PRF91 + EHN, simulations
  - Over-predicting additive effects; excessive LTHR, esp. at higher T



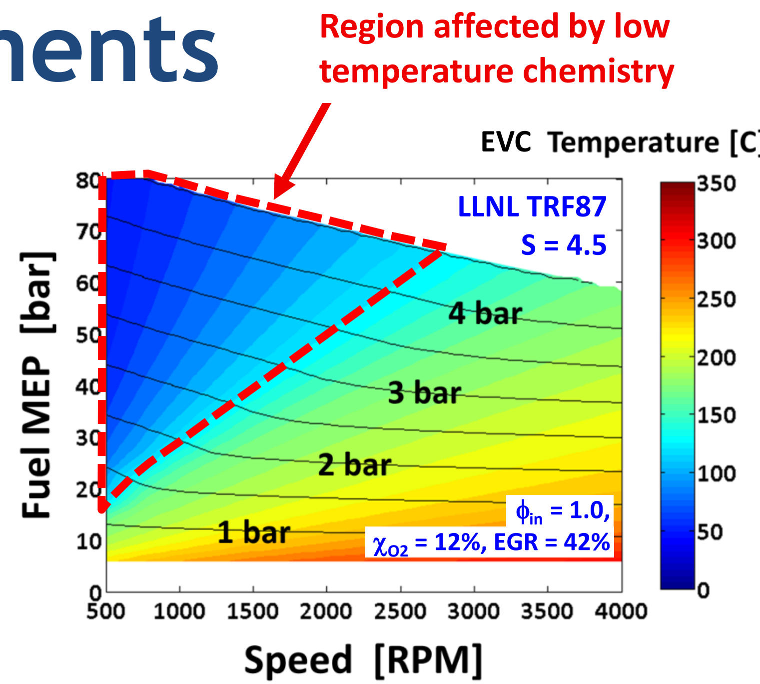




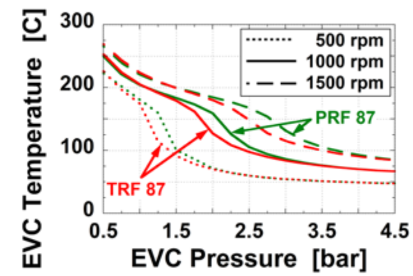
Sensitization with low temperature fuel chemistry needs better understanding

Technical Accomplishments

Reduced-order Ignition Model



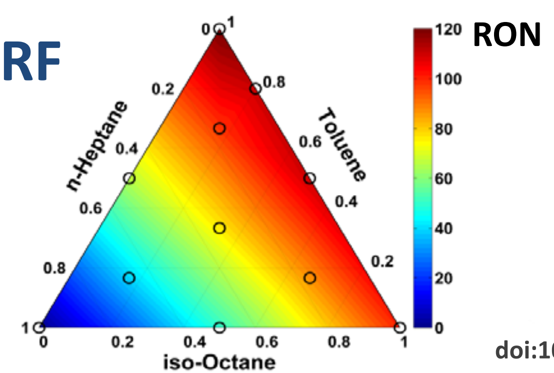
- Advanced, model-based engine control needs fast prediction of knock / autoignition
  - Lean / dilute, boosted operation affected by low temperature chemistry, esp. at lower speeds
  - Autoignition correlation covering NTC region, with range of fuel reactivity, ON sensitivity



$$\int_0^t \frac{1}{\tau(T,p,\phi,\chi_{O2})}\,dt = 1.0$$

  - Based on simulations with LLNL TRF gasoline surrogate model

T	p	ϕ	EGR
500-2000 K	10-50 bar	0.2-2.0	0-50%

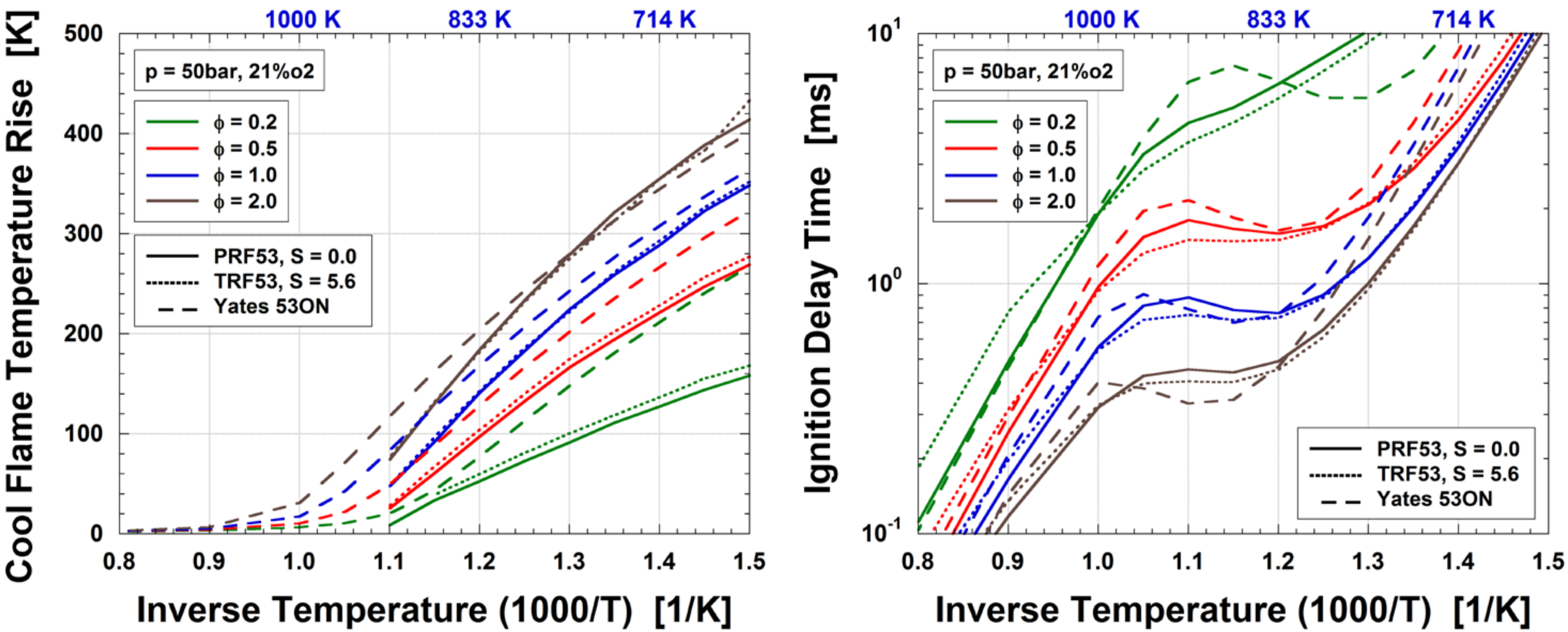


doi:10.4271/2012-01-1136

Technical Accomplishments

Reduced-order Ignition Model

- Parametric simulations provide insight for functional form of correlation and influence of ON sensitivities
  - At engine-relevant conditions ON sensitivity mainly affects NTC



Available models capture some trends; do not exhibit ON sensitivity

Collaborations

ONGOING INTERACTIONS

- **ANL:** mechanism development / refinement, global sensitivity analysis, gasoline LTC – reactivity modifiers
- **LLNL:** mechanism development / validation, FACE gasolines, surrogates and additives
- **NUI Galway:** mechanism development / validation, RCM data / model sharing
- **U. Akron:** reduced order model development / validation
- **Marquette U.:** aerosol fueling system for high boiling point fuel components / data analysis software
- **U. Lille:** RCM data and model exchange, visiting faculty appointment (summer 2013)
- **U. Leeds:** RCM data sharing

Collaborations

New Developments

- **International RCM Workshop:** patterned after ECN to better understand LTC phenomena using RCMs, esp. auto-ignition chemistry, turbulence-chemistry interactions, etc.; theorists, experimentalists, modelers participating; 14 RCM laboratories contributing to first standardized tests using iso-octane, with bi-component and other blends to follow; 1st meeting held at ANL, August 2012.

http://www.transportation.anl.gov/rcmworkshop/

Collaborations

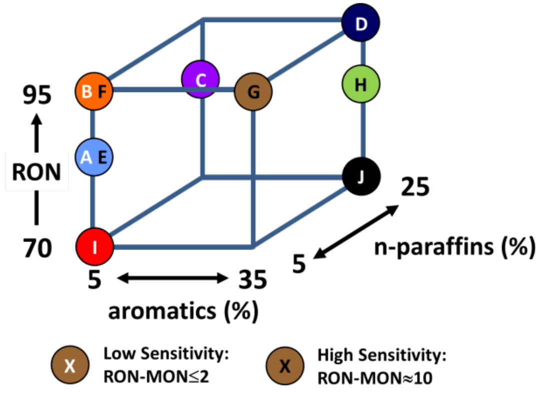
New Developments

- **KAUST:** experiments / modeling with FACE gasolines
- **U. Wisconsin ERC:** data / models using reactivity modifiers
- **U. Illinois Chicago:** biodiesel surrogates data / models
- **U. Michigan:** RCM Workshop, LTC / RCM review paper
- **Convergent Science, Sasol LTD:** sponsorship of RCM Workshop

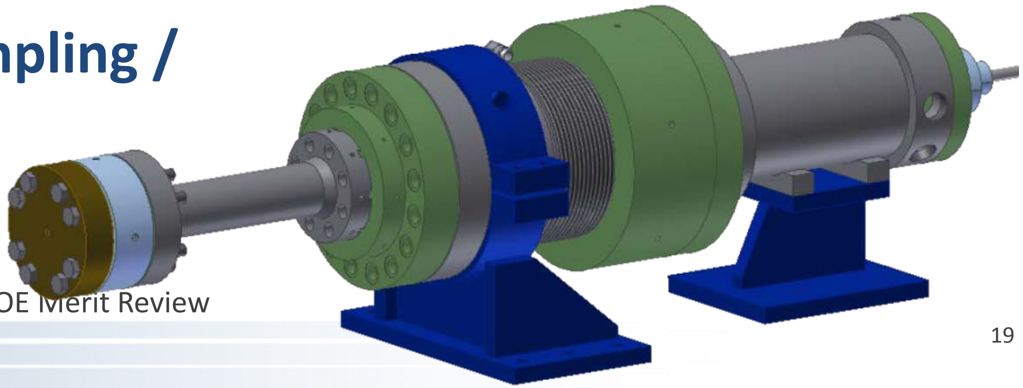
Future Work

FY2013 / FY2014

- Experiments and modeling with surrogates and additives
- Experiments using FACE gasolines
- Incorporate stratified reactor model into RCM system model
- Integrate model probing tools (GSA) with RCM system model to improve chemical kinetic models



- Fabricate new single-piston RCM via ANL LDRD
  - Aerosol-fueling capable for high boiling point fuels
  - Integrated with gas sampling / analytical unit



Summary

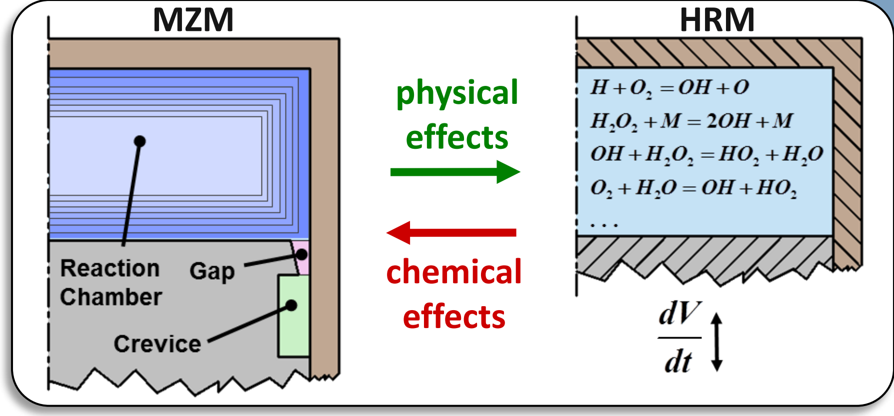
- **Objective**
  - Acquire data / develop models for transportation-relevant fuels at advanced engine conditions
- **Approach**
  - Utilize ANL's RCM and novel data analysis tools, leverage expertise of BES-funded researchers to synergistically develop predictive models
- **Technical Accomplishments**
  - Improved existing facilities, and physics-based, RCM system models
  - Acquired data and developed kinetic model for reactivity modifiers
  - Developing control-oriented, reduced-order ignition model
- **Collaborations**
  - National labs, universities and industry; International RCM Workshop
- **Future Work**
  - Reactivity modifiers, FACE gasolines, model improvement tools, and fabrication of new experimental apparatus

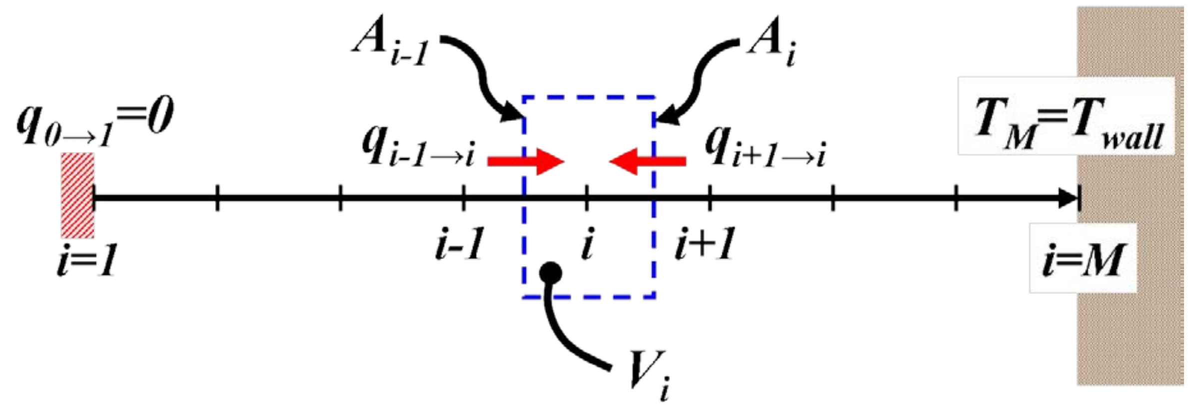
Technical Back-Up Slides

(Note: please include this "separator" slide if you are including back-up technical slides (maximum of five). These back-up technical slides will be available for your presentation and will be included in the DVD and Web PDF files released to the public.)

RCM System Model
SUB-MODEL DESCRIPTION

- Reaction Chamber





$$\frac{d(nu)_i}{dt} = -P_i\frac{dV_i}{dt} + \left(q_{i-1\to1} + q_{i+1\to1}\right) - h_i\frac{dn_i}{dt}$$

Compression Work
(piston motion)

Conductive Transport
(important to ensure surface area of reaction chamber equals surface area of RC mesh (i=M))

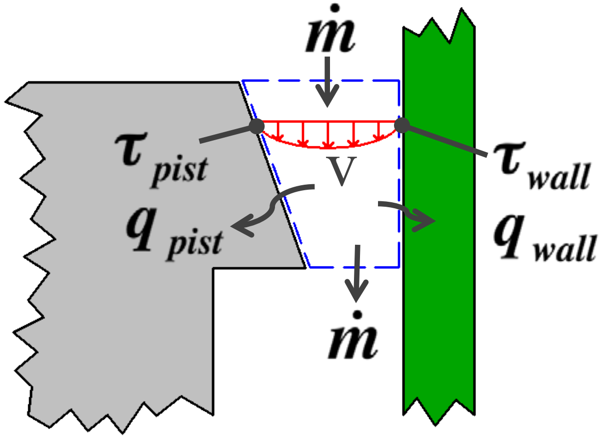
Enthalpy flow to crevice
(most cells contribute mass)

doi:10.1016/j.combustflame.2012.07.010

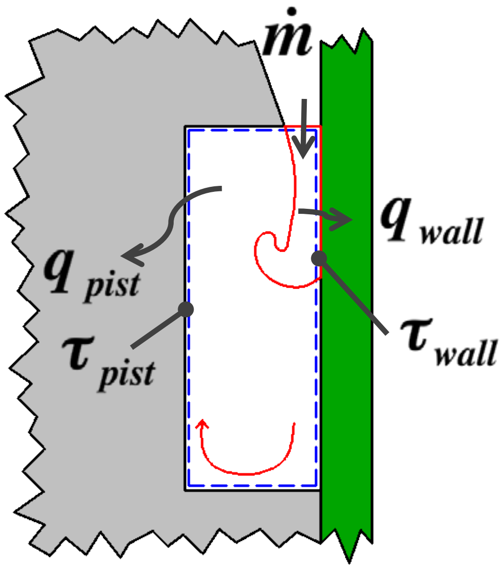
RCM System Model

Sub-model Description

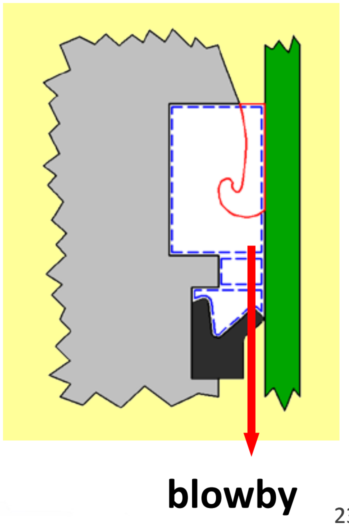
- **Tapered Gap**
  - Quasi-steady flow driven by pressure differential
  - Fluid shear on piston and wall using mean friction coefficient, $\tau_s = 0.5\, C_f \rho\, v^2$
  - Convective heat loss, using annular, developing flow correlation, $q = h_{conv} A(LMTD)$



- **Crevice Volume**
  - Fully unsteady analysis
  - Entering flow modeled using jet correlation
  - Crevice flow modeled using annular pipe correlation
  - Different crevice geometries require modifications to shear and convection correlations



- **Ringpack Volume**



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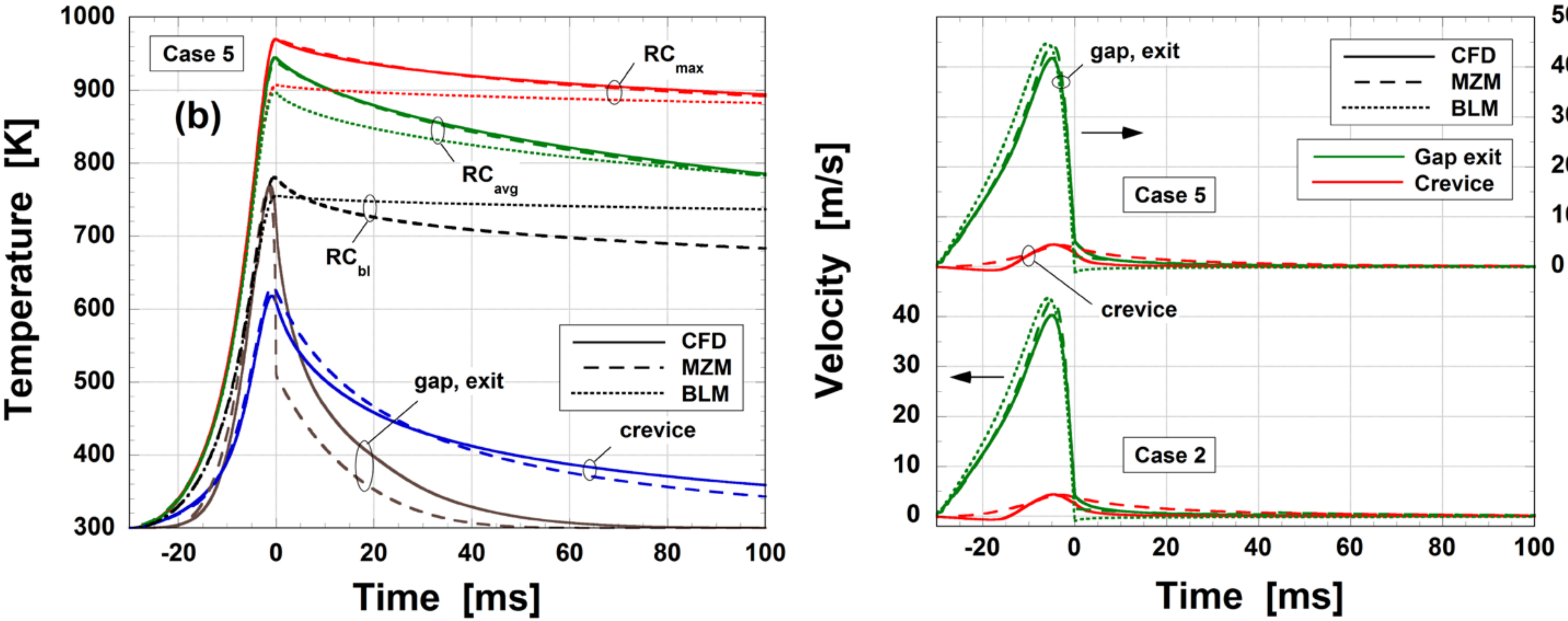
RCM System Model

VALIDATION

- Using non-reacting / reacting CFD, and experiments



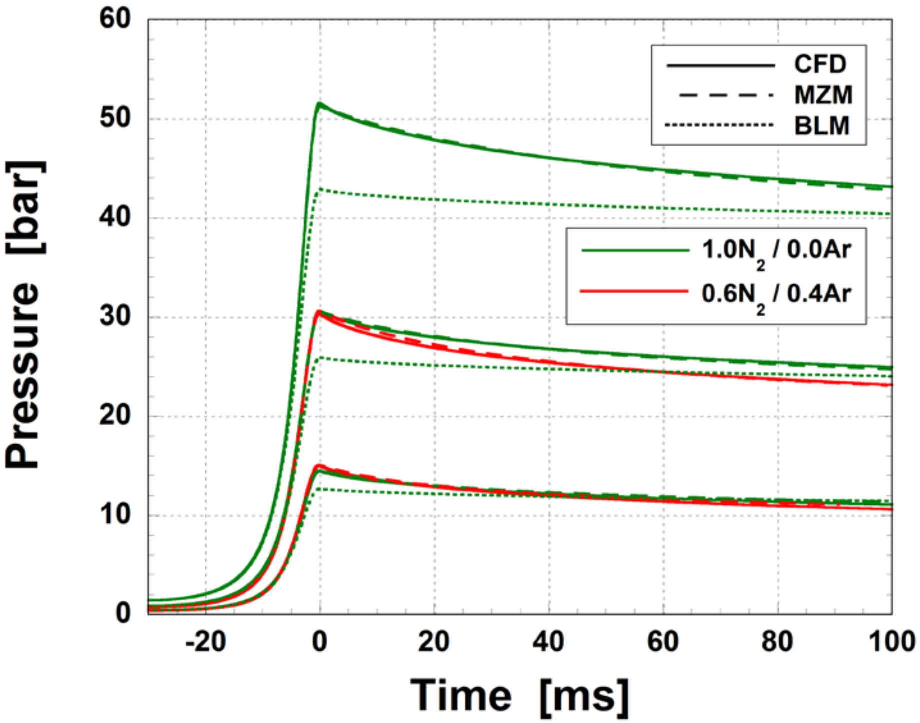
- Good agreement in trends of temperature decay within reaction chamber and in gap / crevice regions between CFD and multi-zone model (MZM).
- Gap and crevice velocities also show reasonable agreement.
- Some discrepancies seen due to sub-model approximations, e.g., quasi-steady assumption, shear and convection correlations in crevice volume.

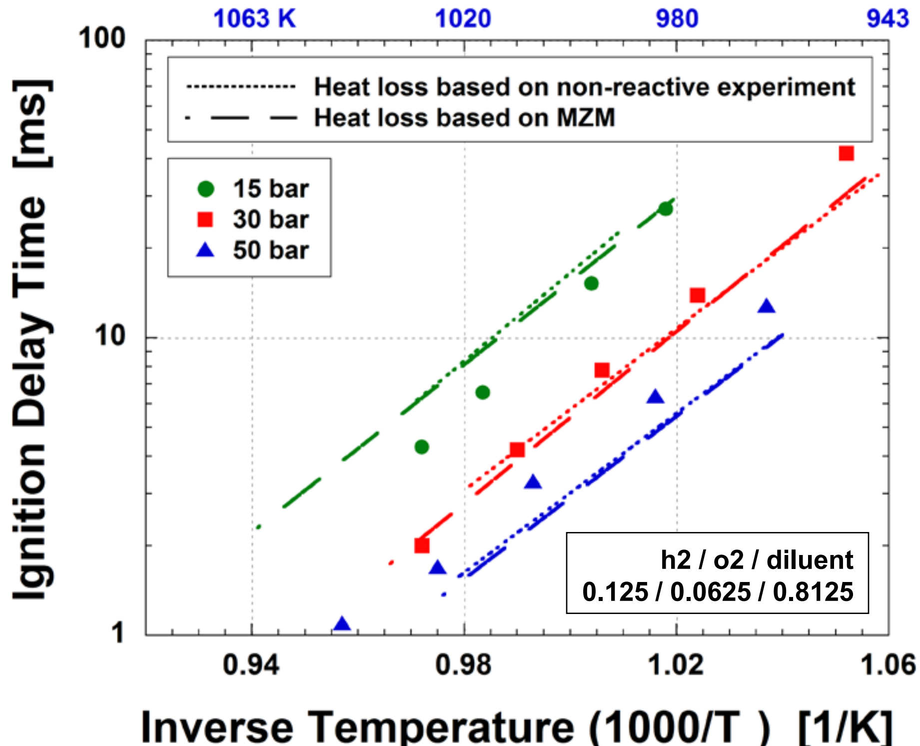
doi:10.1016/j.combustflame.2012.07.010

RCM System Model

VALIDATION

- Using non-reacting / reacting CFD, and experiments





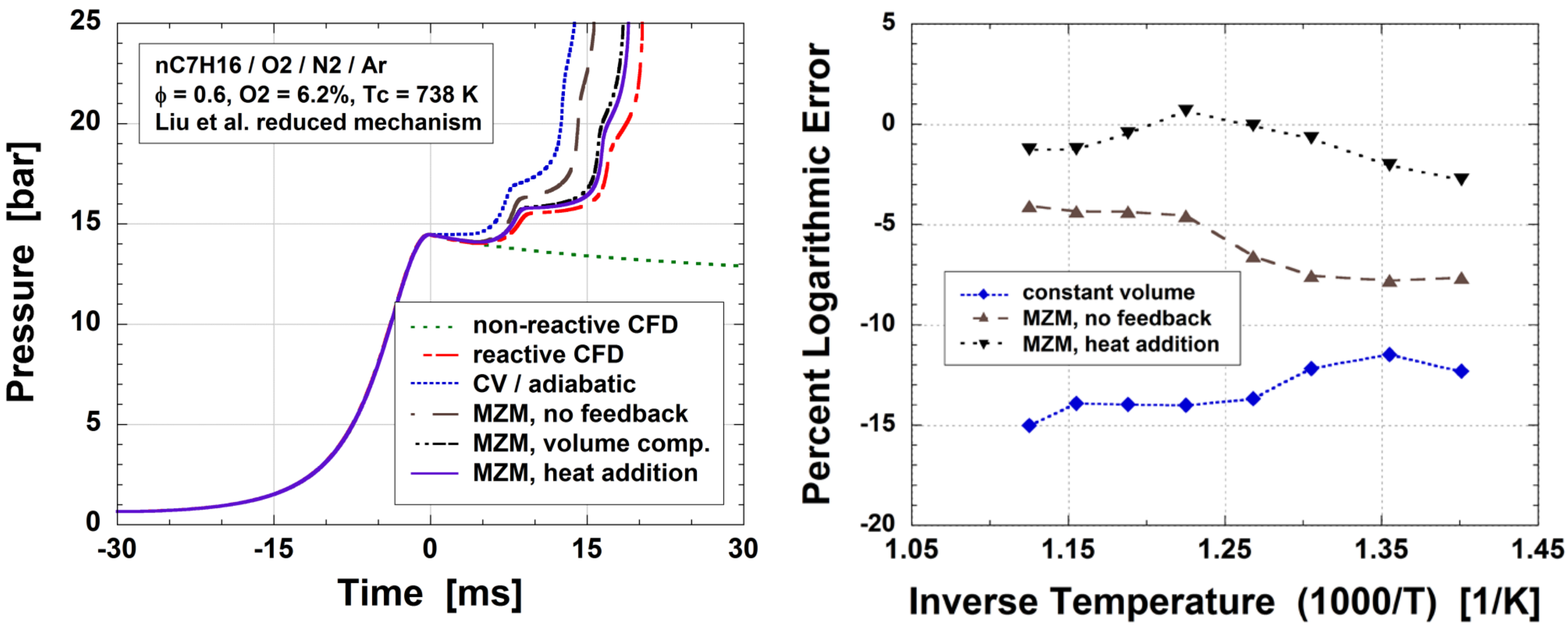
- MZM captures effects of pressure ($\alpha=k/\rho c_p$), and composition (T_{peak}, α) changes, as well as compression ratio. Effects of crevice design currently under investigation.
- Comparison with experiments indicate MZM performs just as well as conventional, empirical heat loss model for single stage fuels.

doi:10.1016/j.combustflame.2012.07.010

RCM System Model

ADVANTAGES

- **Multi-stage ignition – chemical-physical interactions**



- NTC regimes can experience substantially increased ignition delay when preliminary heat release causes flow into crevice (leading to increased heat loss).
- Analogous physics in shock tubes yield decreased ignition times.
- Coupled MZM / HRM accounts for these effects during RCM simulations.

doi:10.1016/j.proci.2012.05.094