Collaborative Combustion Research with BES

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Project ID # ACE054
DOE Manager: Gurpreet Singh

Overview

Timeline

- Started Jan 2010

Barriers

- Lack of ***fundamental*** knowledge of advanced engine combustion regimes
- Lack of modeling capability for combustion and emission control

Budget

- Total project funding
  - DOE share 100%
  - Contractor share 0%
- Funding received in
  - FY11 $400K
  - FY12 $315k

Partners

- Argonne is project lead
- Partners are
  - University of Akron
  - Marquette University
  - Argonne-CSE
  - LLNL
  - UW-Madison

Objectives (Relevance)

- To support DOE-EERE's efforts to develop chemical mechanisms of various IC engine fuels so as to gain a predictive capability of in-cylinder combustion and emissions formation
  - Special emphasis has been placed on understanding LTC regimes, necessitating a better understanding of Negative Temperature Coefficient (NTC) region chemistry
- To provide complementary experimental data to enhance DOE-BES's efforts to develop improved chemical kinetic mechanisms of transportation fuels
  - Improve kinetics model quality across a wide range of conditions
  - Develop experimental capabilities to study high boiling point fuels
- To replicate high-pressure and low-temperature conditions that are typical of IC engines by using Argonne's Rapid Compression Machine (RCM)
- To develop control oriented models for use in ignition prediction and data analysis

Milestones

Month/Year	Milestone
November-11 (Complete)	• Complete installation of pre-heating and pre-mixing system • Enable transportation liquid fuel tests
February-12 (Complete)	• Installation and use of Rapid Sampling Valve and Sample Dump Tank • Facilitate chemical speciation

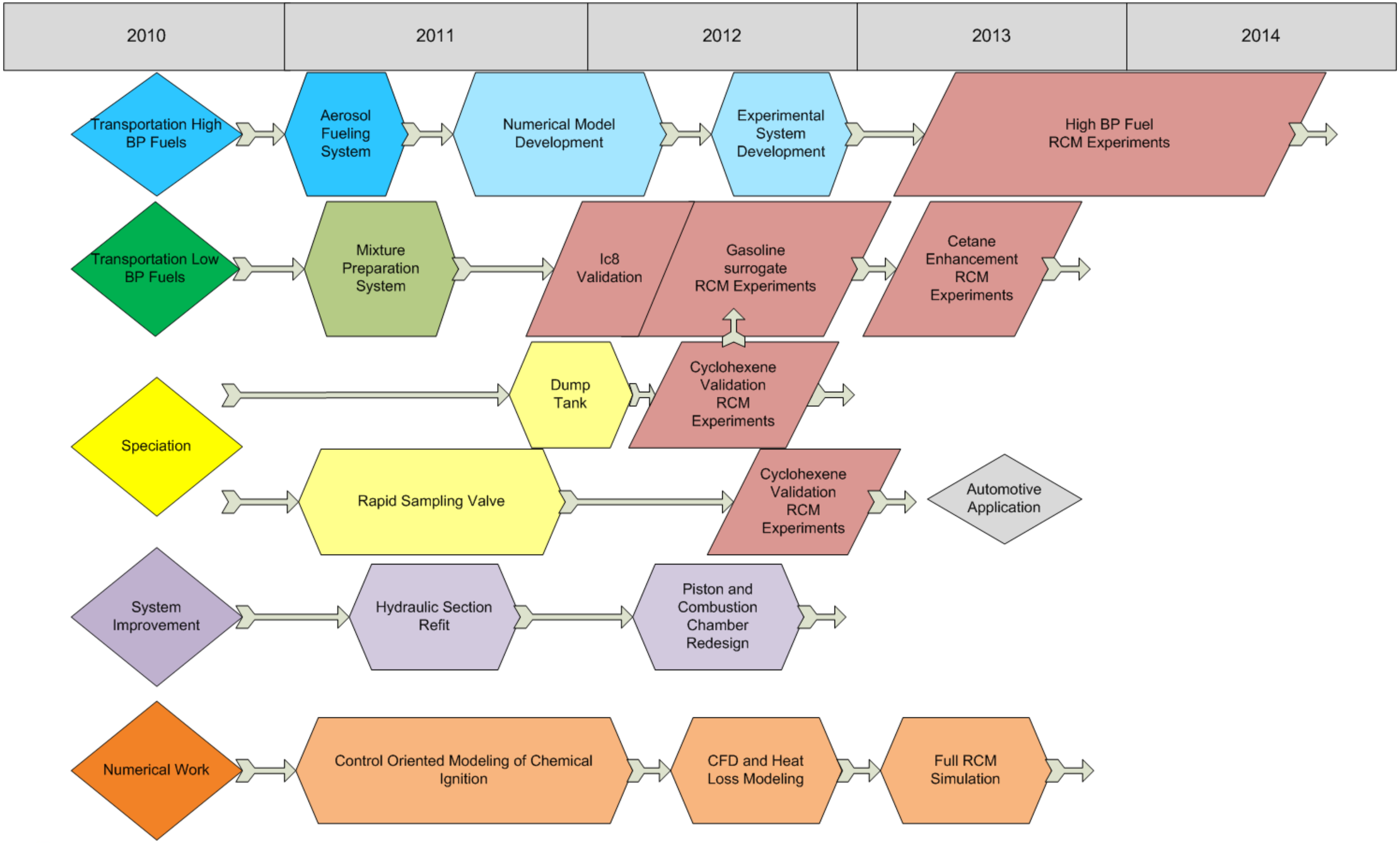
March-12 (Complete)	• Conduct tests on low boiling point fuels
	  • iso-Octane – method validation
	  • 4-component gasoline surrogate (LLNL)
	• Speciation Method Validation
	  • Cyclohexene
	• Develop 0-D heat loss model for RCM
	  • Improve data analysis

August-12 (Ongoing)	• Conduct tests on low boiling point fuels
	  • 4-component gasoline surrogate (LLNL)
	  • Real fuel – gasoline
	•Speciation Studies

FY13 (Ongoing)	•Aerosol Fueling Development
	  • Add capability for high boiling point fuel studies, such as diesel and biodiesel
	  • Modeling and Experimental development
	•Ignition Correlation Evaluations and Development

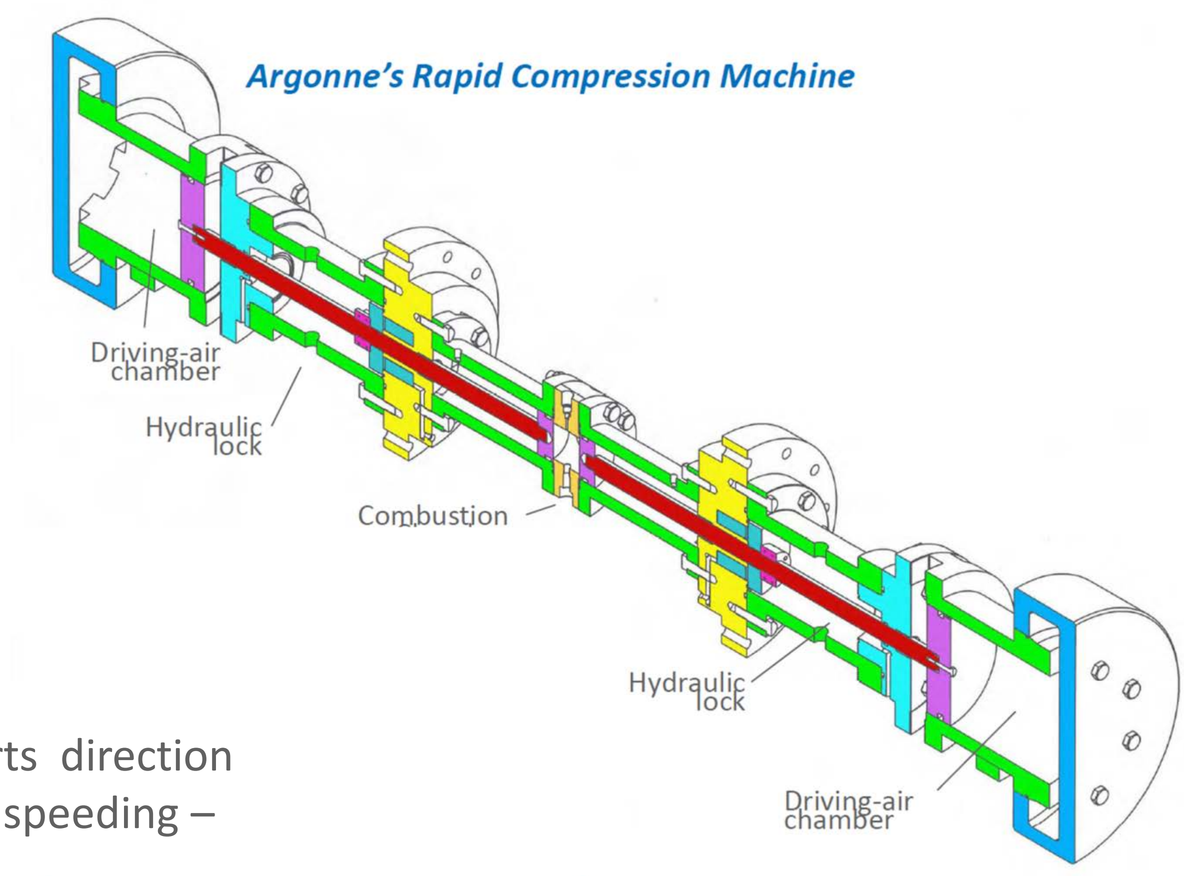
Approach

- Use Argonne's Rapid Compression Machine (RCM) to generate chemical kinetic data of transportation relevant fuels



RCM Specifications

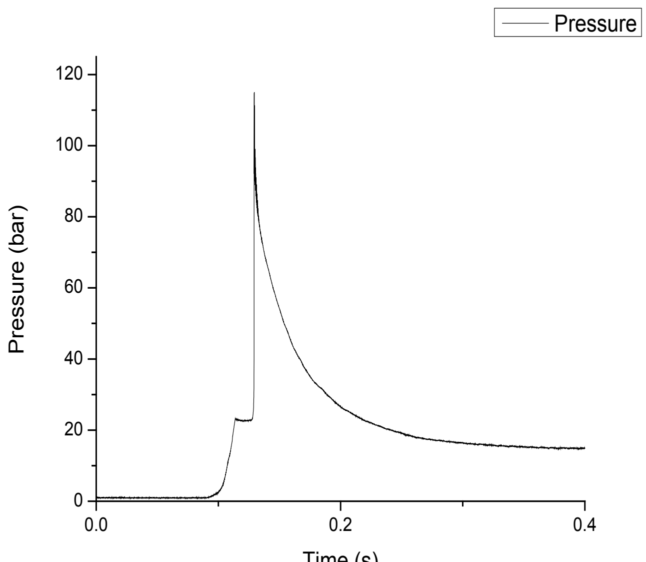
Based on MIT design	
Bore	2.5”
Stroke	6.25”
Compression Ratio	~9.5:1
Compression Time	<17 ms
Peak Pressure	362 bar



High pressure capability supports direction in engine downsizing and downspeeding – higher torque engines.

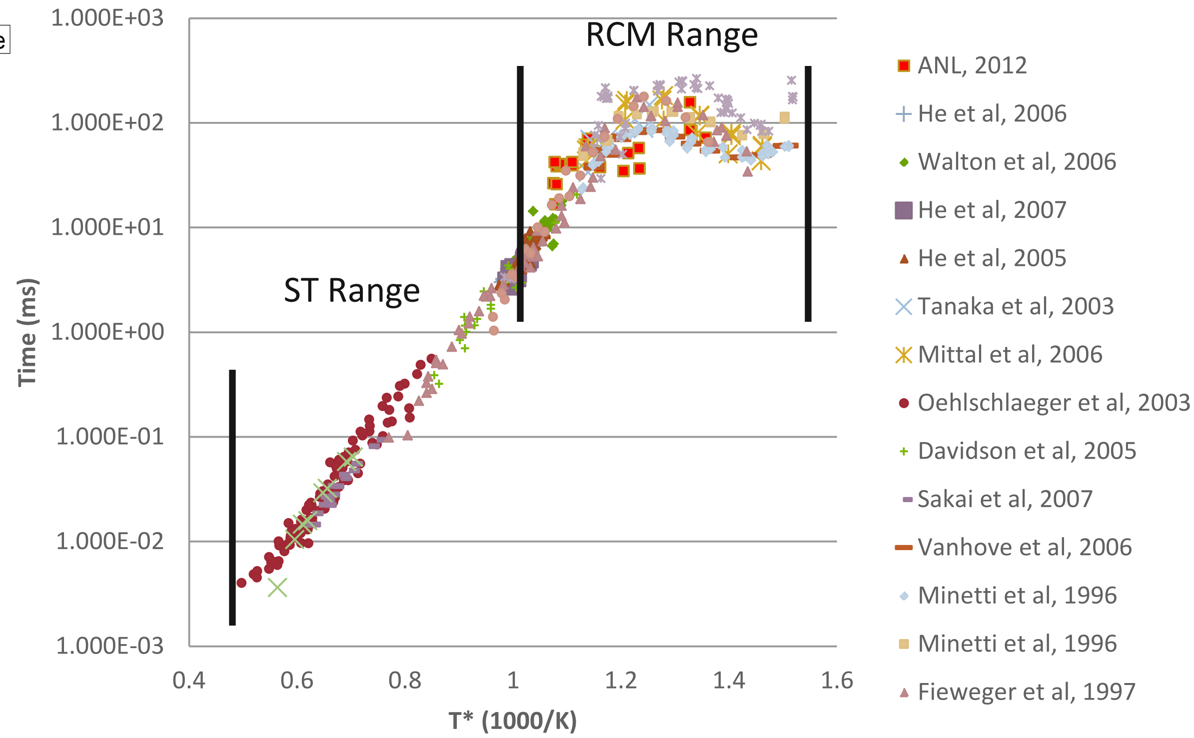
Technical Accomplishments

- *iso*-Octane tests
  - Well characterized fuel used to validate experimental technique
    - Raw data shown normalized with corrected data from a wide range of experiments
  - Diluent gases varied to enable access to wider experimental range
  - Development improvements to reduce data scatter



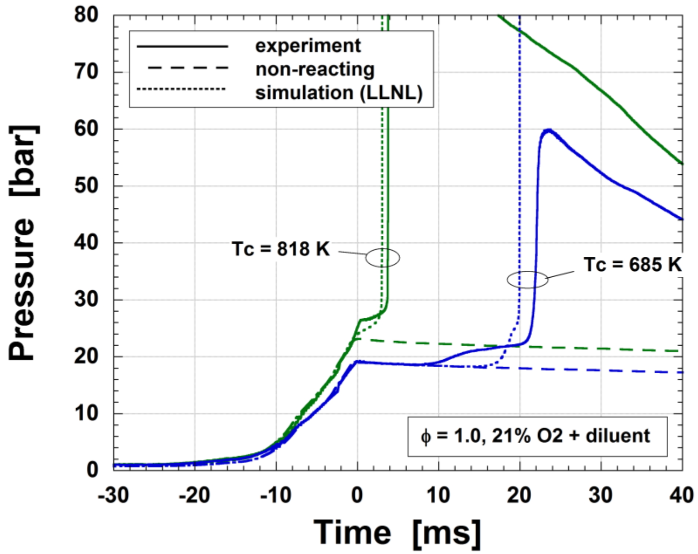
79% Ar, 21% O2, Phi =1.0
T = 919K, P = 23.23 bar

Normalized *iso*-Octane Ignition Delays

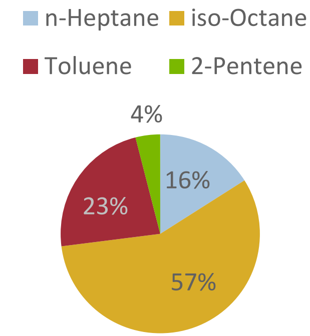


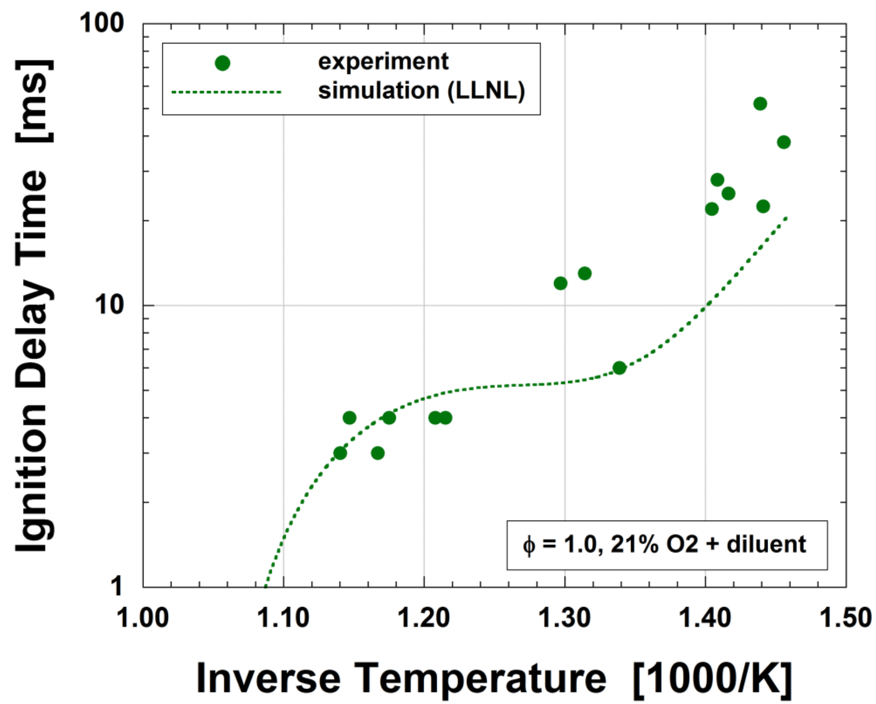
Technical Accomplishments

4 Component Gasoline Surrogate

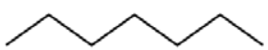


- 4 component surrogate – LLNL

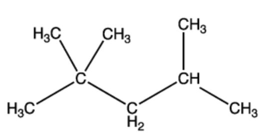




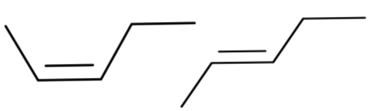
n-Heptane



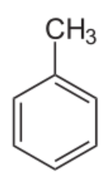
iso-Octane



2-Pentene (2 isomers)

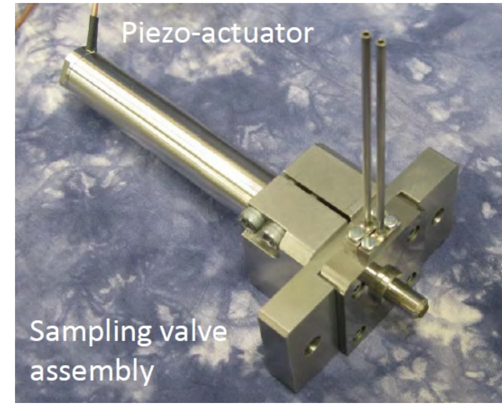


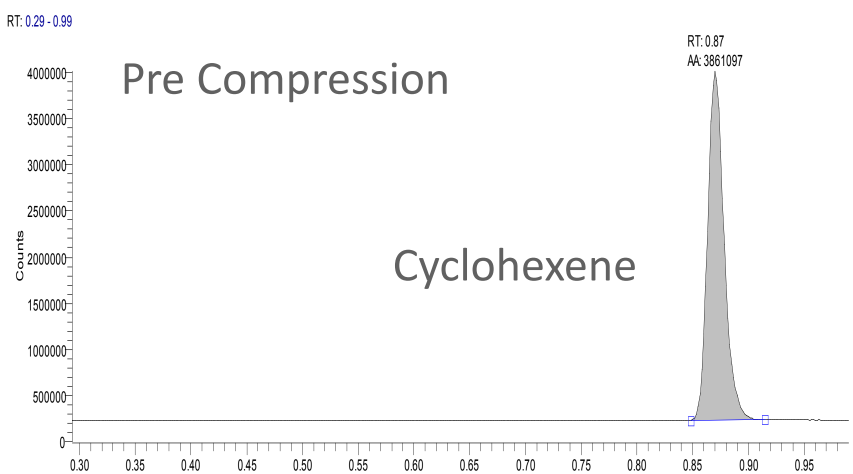
Toluene

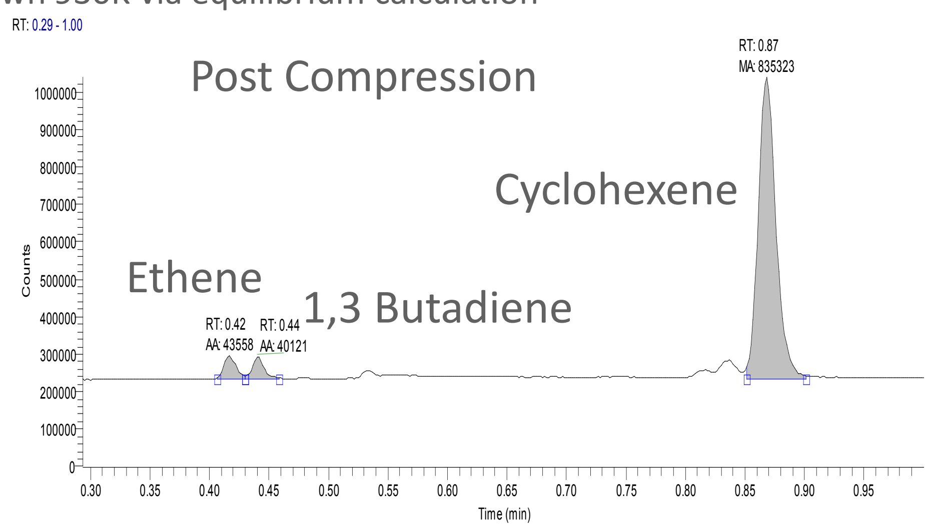


Technical Accomplishments

- Intermediate and post-combustion speciation important to support mechanism development
- Chemical Speciation using GC with Argonne-CSE
  - Rapid Sampling Valve
    - Fast acting piezo-actuated valve
      - Capable of sampling as fast as 55 μs
      - Sample volume too small for RCM work
    - Develop control strategy for engine application
- Sample Dump Tank
    - Expand reaction chamber contents to vessel, freezing chemistry
- Validated using chemical thermometer – cyclohexene
    - Estimated Temp for Experiment shown 930K via equilibrium calculation





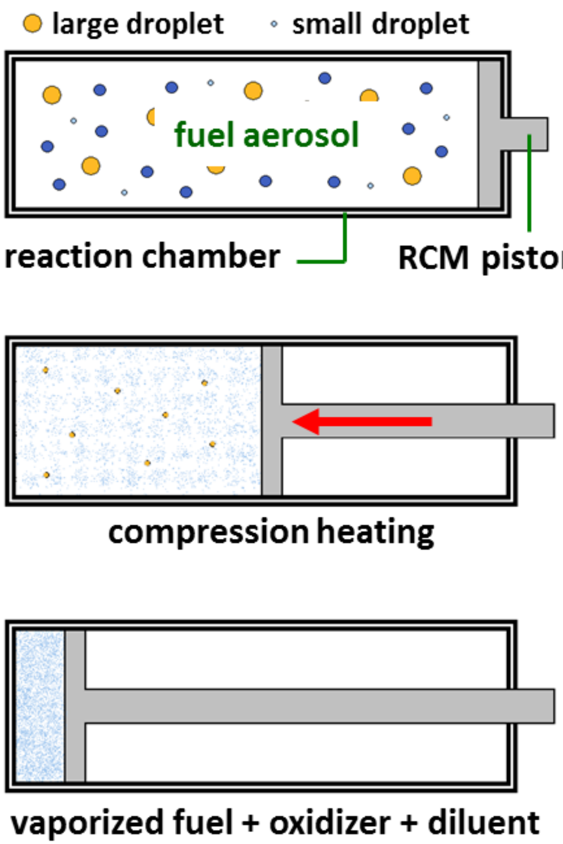


Technical Accomplishments

Aerosol Fueling for RCMs

With Marquette University

- Develop method to introduce fuel loading of high boiling point fuel in small enough droplets to facilitate vaporization through compressive heating during the compression stroke, ensuring gas phase kinetics only at TDC
- Facilitate study of diesel, biodiesel, higher hydrocarbons, FAMEs, etc.



Funding for Marquette University also provided by
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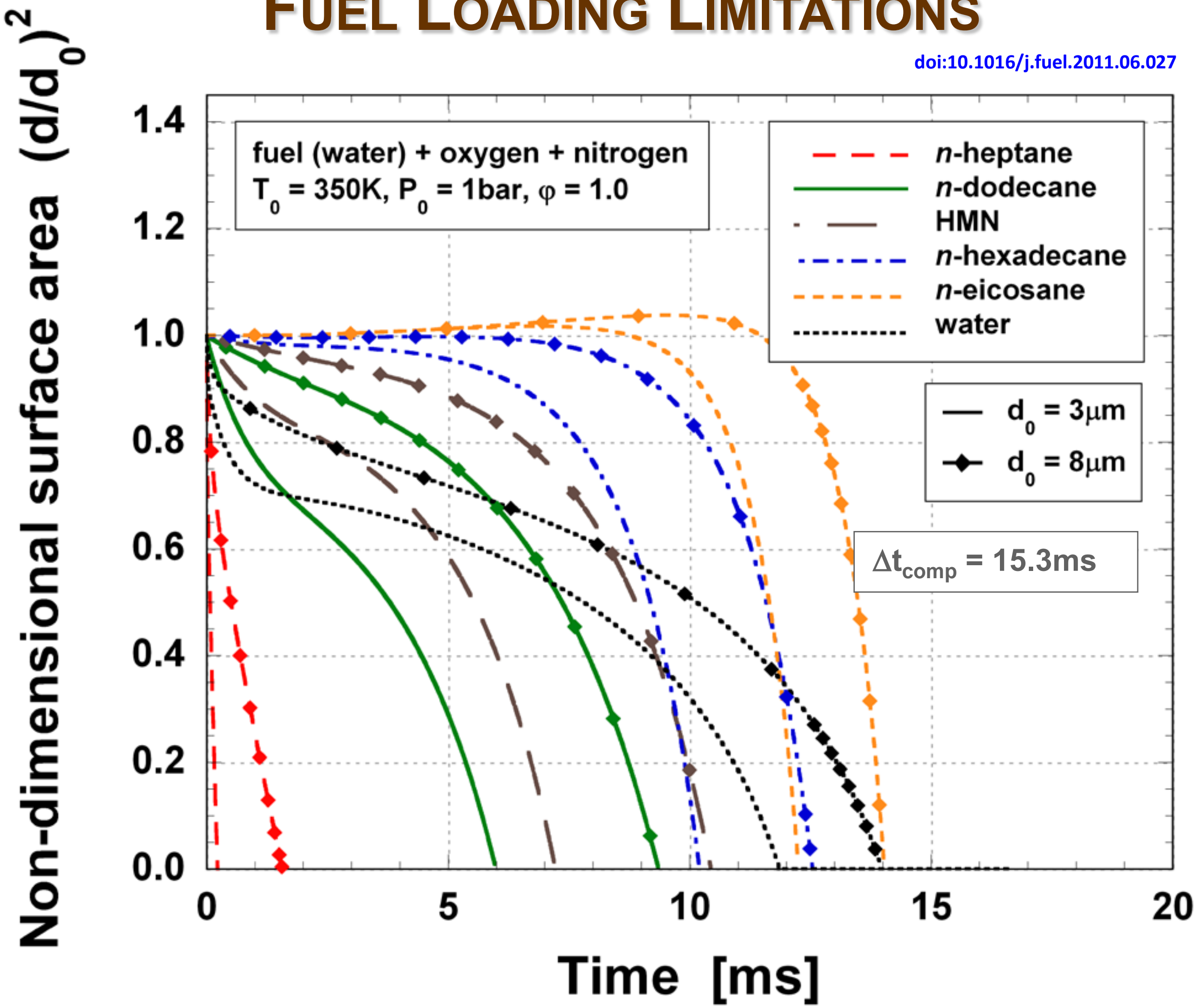
Technical Accomplishments
Aerosol Fueling for RCMs

FUEL LOADING LIMITATIONS

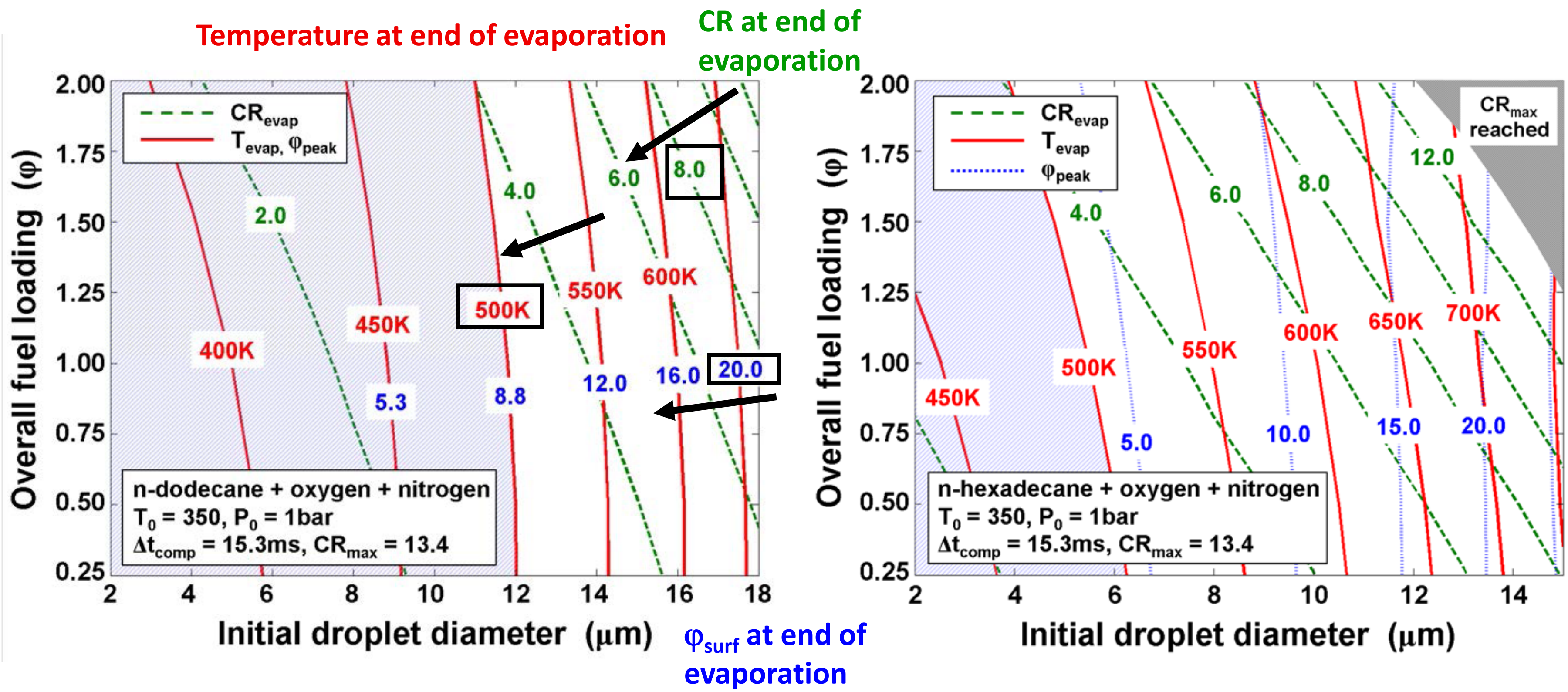
doi:10.1016/j.fuel.2011.06.027



Technical Accomplishments

Aerosol Fueling for RCMs

Fuel Loading Limitations



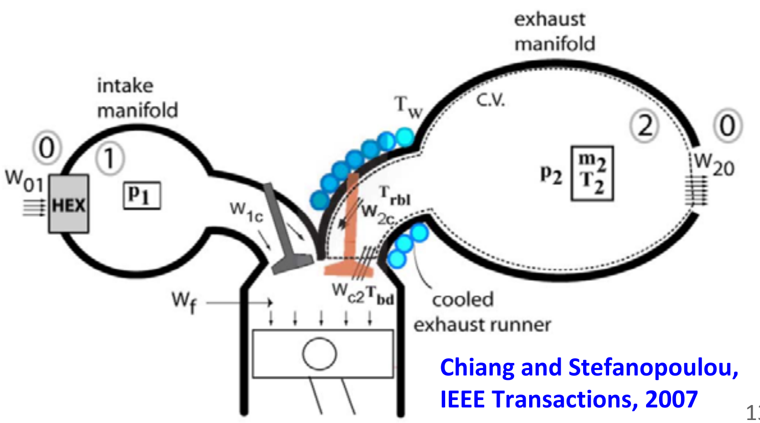
Technical Accomplishments
Control-oriented models for chemical ignition prediction

- **Motivation:** Control of advanced engine cycles, including LTC and HCCI, requires fast (e.g., algebraic) means to predict chemical ignition over range of conditions. Advanced SI engines need fast methods to accurately predict knock.

- **Objective:** Formulate ignition delay correlation applicable to wide range of conditions, including fuel reactivity (e.g., ON).

- **Approach:** Evaluate existing correlations to determine best functional form. Utilize simulation results with LLNL TRF mechanism to fit new correlation; modify functions appropriately.

$$\int_{t_{IVC}}^{t_{SOC}} \frac{1}{\tau(T,\phi,p,\chi_{O2},EGR)}\,dt = 1.0$$



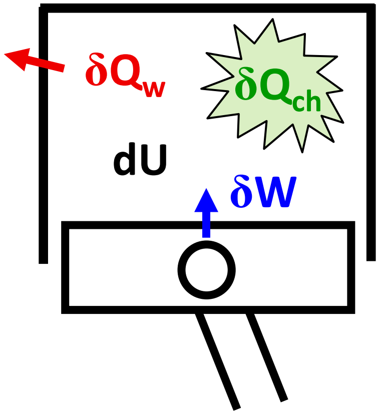
Chiang and Stefanopoulou, IEEE Transactions, 2007

Technical Accomplishments

Control-oriented models for chemical ignition prediction

EVALUATE EXISTING IGNITION DELAY CORRELATIONS

- Compare ignition timings at engine-relevant conditions, with single-zone engine simulator (like HCCI model-based control algorithm).



  - Knock-integral for ignition timing.
  - Wiebe function for ROHR.
  - Slider-crank trajectory.
  - Modified-Woschni heat loss.
  - Operating-condition dependent wall temperature.
  - Specify IVC p, ϕ, EGR, engine speed.
  - Iterate IVC temperature to achieve CA50 at +8 ATDC.

$$\int_{t_{IVC}}^{t_{SOC}} \frac{1}{\tau(T,\phi,p,\chi_{O2},EGR)}\,dt = 1.0$$

$$x_b = 1-\exp\{-a[(\theta-\theta_{SOC})/\Delta\theta]^{w+1}\}$$

	Case 1	Case 2	Case 3
ϕ_{in}	0.42	1.00	1.00
χ_{O2} (%)	19	8	12
EGR (%)	9	62	42
ϕ_{eff}	0.38	0.38	0.58
P_{IVC}	0.5 – 4.5 bar		
Speed	500 – 4000 rpm		

Displaced volume	549.5 cm^3
Stroke	94.6 mm
Bore	86.0 mm
Compression ratio	11.75:1
Exhaust Valve Open	70° bBDC
Exhaust Valve Close	5° aTDC
Inlet Valve Open	5° bTDC
Inlet Valve Close	30° aBDC
Fuel Heating Value	~44 MJ/kg

Technical Accomplishments

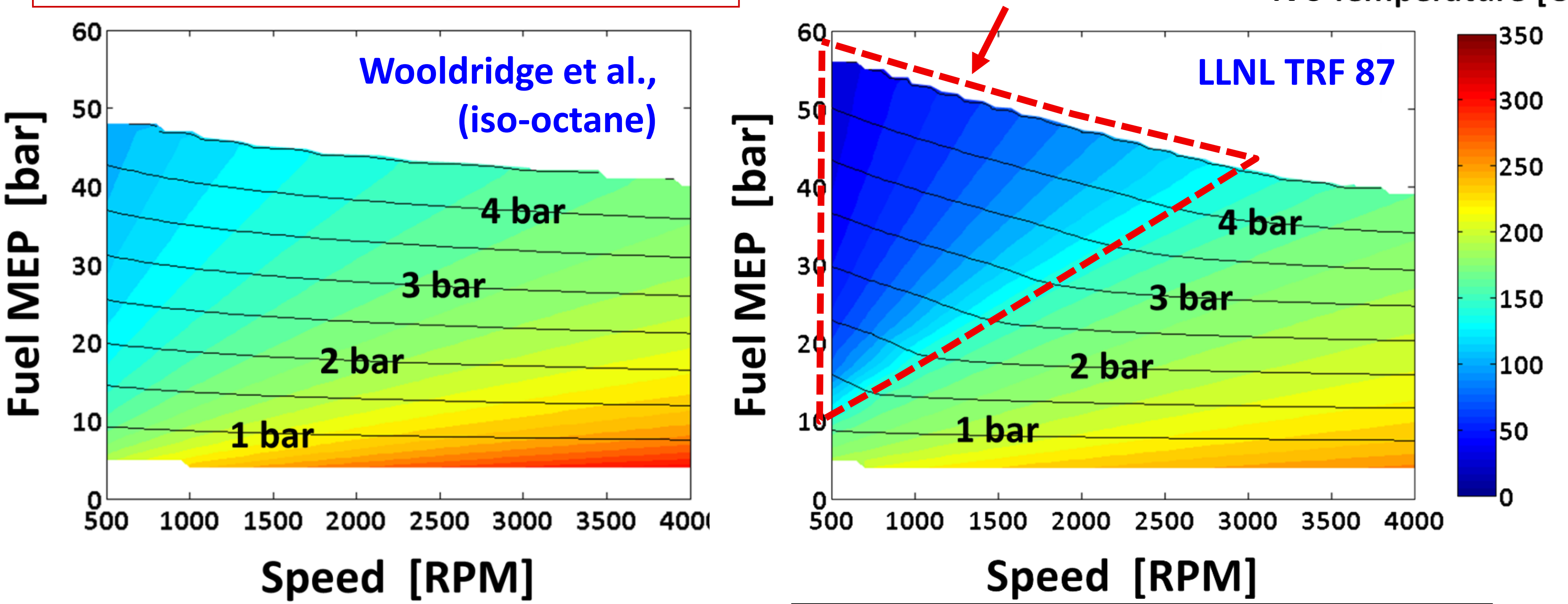
Control-oriented models for chemical ignition prediction

EVALUATE EXISTING IGNITION DELAY CORRELATIONS

- Compare ignition timings at engine-relevant conditions, with single-zone engine simulator (like HCCI model-based control algorithm).

Region affected by low temperature chemistry

$$\tau = 2.80\times10^{-3}\,\phi^{-0.79}\,p^{-1.25}\,\chi_{O2}^{-1.14}\times\exp(13{,}788/T)$$



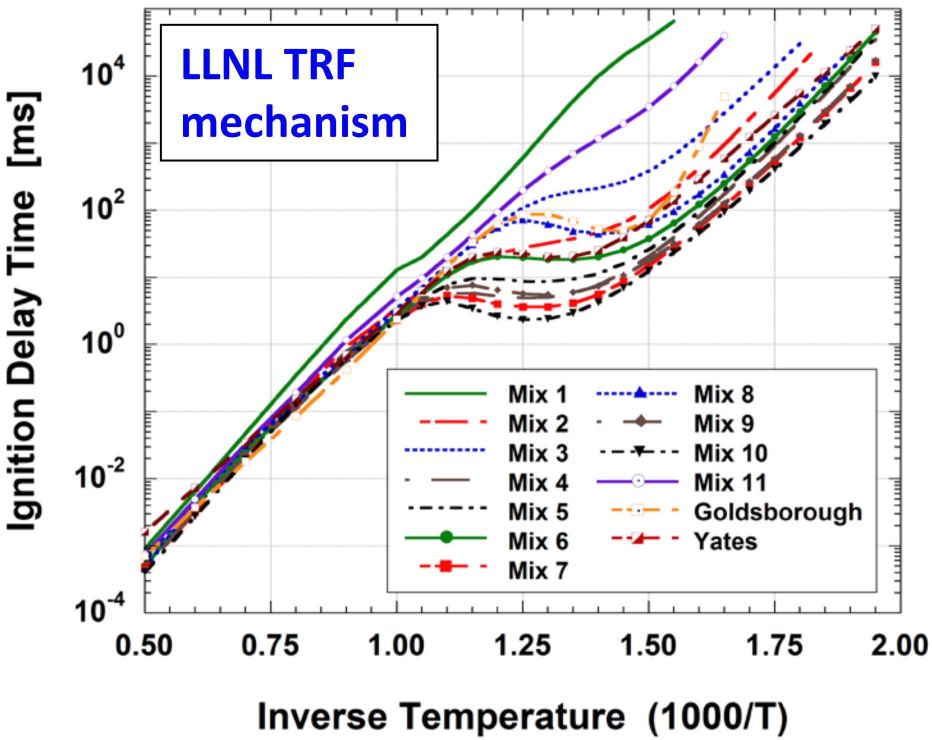
Case 1: ϕ_{in} = 0.42, χ_{O2} = 19%, EGR = 9%

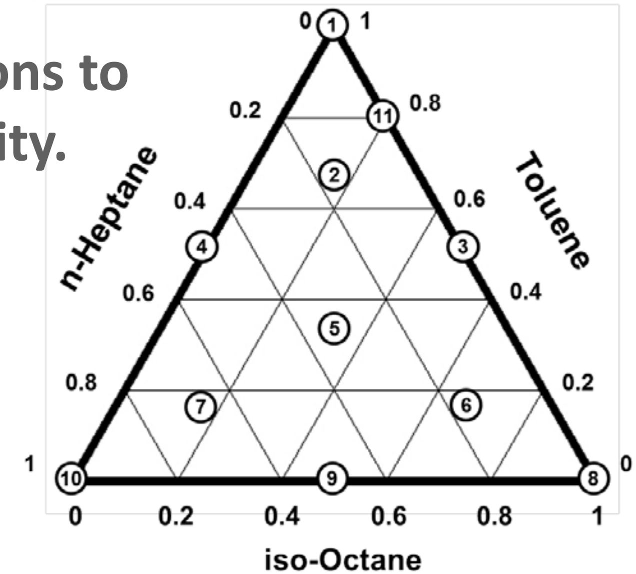
Technical Accomplishments

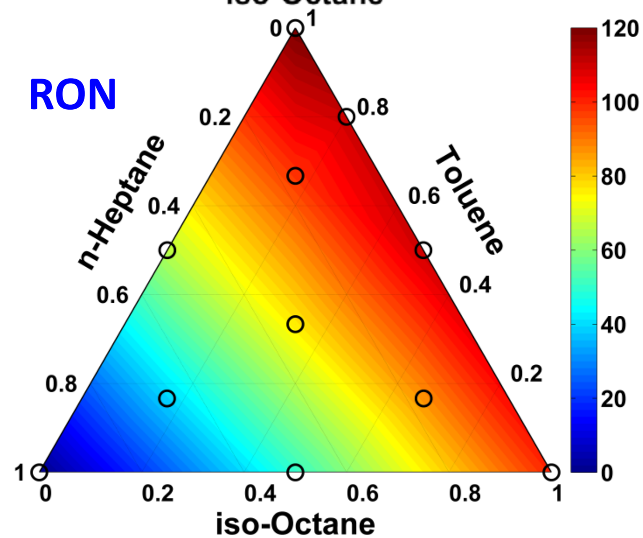
Control-oriented models for chemical ignition prediction

Correlation Development – Analysis of TRF Results

- Compare <u>simulated</u> τ at various conditions to illustrate <u>trends</u> with T, ϕ, p, and reactivity.



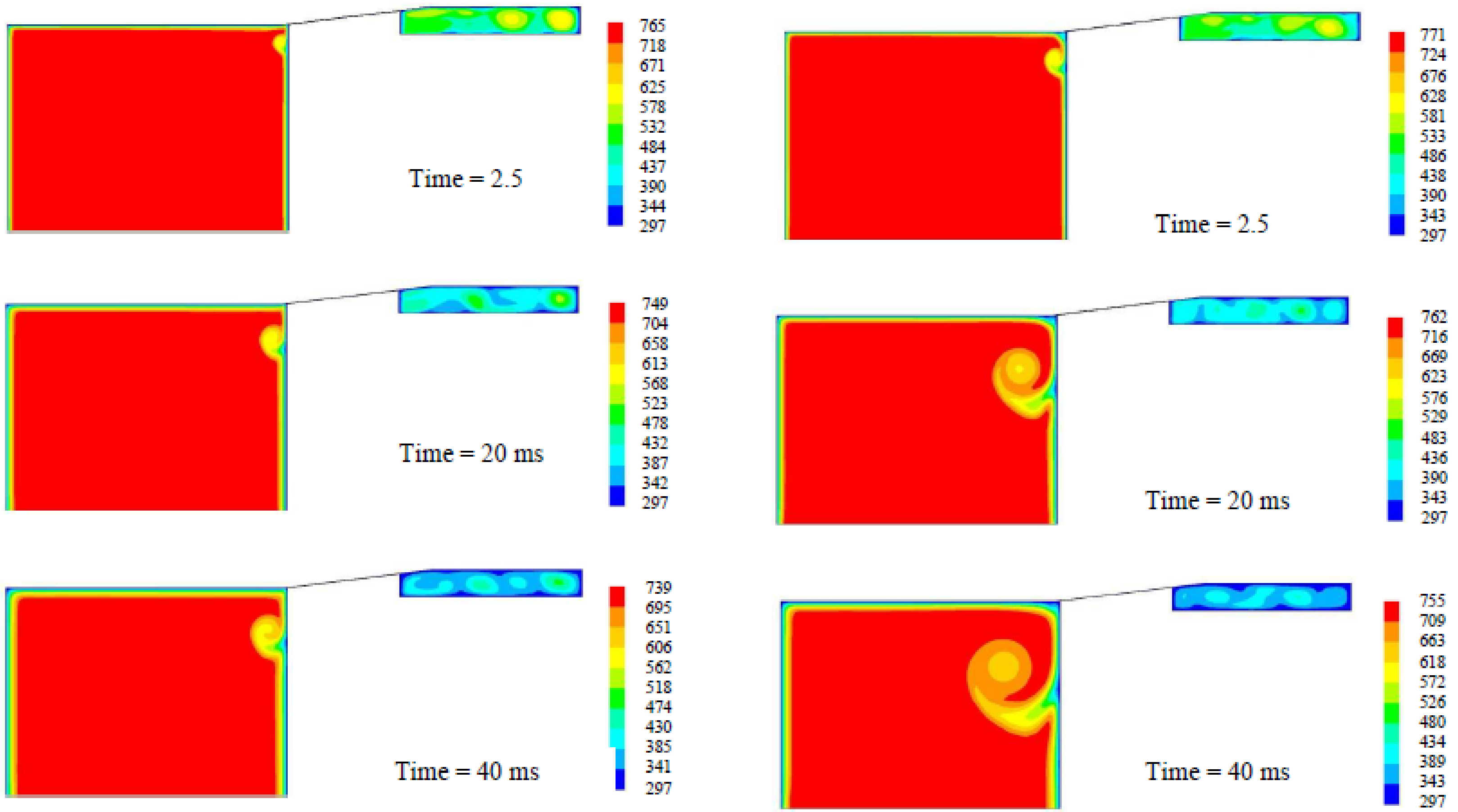




Technical Accomplishments

- RCM Improvement effort – Contained Crevice Piston
  - Piston design and CFD analysis by University of Akron

With Crevice Containment | Without Crevice Containment



Collaborations

- Partners
  - University of Akron
    - Empirical heat loss model development to improve data analysis
    - RCM design improvements to piston design with CFD analysis
  - Marquette University
    - Develop aerosol fueling approach for low vapor pressure fuels
    - Physics-based heat loss model development to improve data analysis
  - University of Wisconsin – Madison
    - Cetane enhancement of gasoline
  - Argonne-CSE
    - GC/MS Speciation
  - LLNL
    - Provided gasoline surrogate mechanism for correlation development
    - Develop capability to provide experimental data to support diesel surrogate work
      - n-Dodecane and m-Xylene

Future Work

- Continue to refine and improve RCM hardware to improve data quality
- Developing advanced RCM design to apply lessons learned and expand operating range to new combustion operation regimes
  - Internal Argonne funding
- Expand experimental matrix of fuels and conditions
  - 4 component gasoline surrogate – expanded experimental range
  - Real gasoline
  - Diesel surrogate work
    - n-dodecane, m-xylene
  - Biodiesel surrogate
    - methyl decanoate
- Simulation of RCM operation and comparison to experimental data
  - CFD, Heat Transfer and Chemical Kinetics
- Continue development of aerosol fueling to enable investigation of high boiling point fuels
- Provide speciation data to partners
  - Argonne-CSE
  - LLNL

Summary

- Relevance: Low temperature, high pressure chemical kinetic data is needed to advance transportation modeling efforts
- Approach: Rapid Compression Machine experiments using transportation fuels coupled with efforts to develop numerical models of fuel ignition
- Technical Accomplishments: ic8 data as a method validation study, 4 component gasoline surrogate, chemical thermometer speciation validation, heat loss models, ignition correlations, aerosol fuel system development
- Collaborations: Work with University of Akron and Marquette University continues to develop analytical and experimental tools, speciation work with Argonne-CSE, cetane enhancement with UW-Madison, future work guided by needs of LLNL

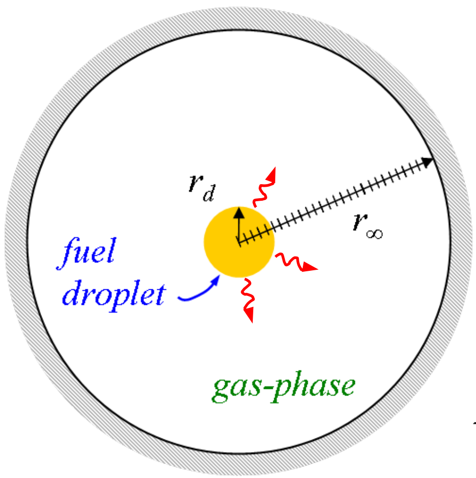
Technical Back-Up Slides

Aerosol Fueling

- Aerosol model equations

$$\phi = \frac{(m_f / m_a)}{(m_f / m_a)_{\text{stoich}}} = \frac{1}{0.067} \frac{\rho_{f,0}\, r_{d,0}^3}{\rho_{a,0}\,(r_{\infty,0}^3 - r_{d,0}^3)}$$

$$CR(t) = \frac{r_{\infty,0}^3}{r_\infty^3(t)}$$



$$u_\infty = \frac{\partial T_\infty}{\partial r} = 0$$

$$\frac{\partial \rho_{k,\infty}}{\partial r} = \frac{\partial \rho_\infty}{\partial r} = 0$$