DOE Bioenergy Technologies Office (BETO) 2019 Project Peer Review

MISR: Miniature Ignition Screening Rapid Compression Machine for Kinetic Measurements of Novel Fuels

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Co-Optimization of Fuels and Engines Area Review

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Goal Statement

- *The goal of this project is to develop a low-volume high-throughput approach for ignition screening of fuels/blends with co-optima relevance.*
- *When successful, the project will result in a miniature ignition screening rapid compression machine suitable for high-throughput small quantity testing, the testing and Livengood-Wu based analysis method, a survey of characteristics of co-optima relevant fuels and blends, and improved fuel ignition criteria more suitable for boosted SI and ACI engines.*
- *Current methods for testing the ignition performance of new fuels and blends are slow, costly, and require large quantities of fuel. These considerations make the current methods unsuitable for searching for new co-optimized fuel blends. Furthermore, the existing performance methods are most suitable in the conditions they are applied (for instance CI engines, or SI engines) and less suitable for the conditions of ACI engines. A new method is needed.*

Quad Chart Overview

Timeline
- Project start date: 01/15/2017 (work began: 06/25/2018)
- Project End: 05/14/2020
- Percent complete ~20%

	FY 18 Costs	Total Planned Funding (FY 19-Project End Date)
DOE Funded	$107,104	$459,359
Project Cost Share*	$47,740 UIC and Oakland	$53,387

•Partners:

•UIC, Oakland University (38% Subcontract)

•National Lab Liaison: S. Goldsborough, ANL

Barriers addressed
ADO-E: Co-Development of Fuels and Engines

Objective
Build a Miniature Ignition Screening Rapid Compression Machine. Use it to measure fuel ignition properties.

End of Project Goal
The goal of this project is to design, develop, and produce a high throughput ignition screening device capable of quickly assessing the properties of small quantities of fuels and blends relevant to co-optima.

End of project technical targets: MISR complete, assessment of commercial viability, provision of data to support merit function development, measurement of Co-Optima relevant fuels and blends.

1 - Project Overview

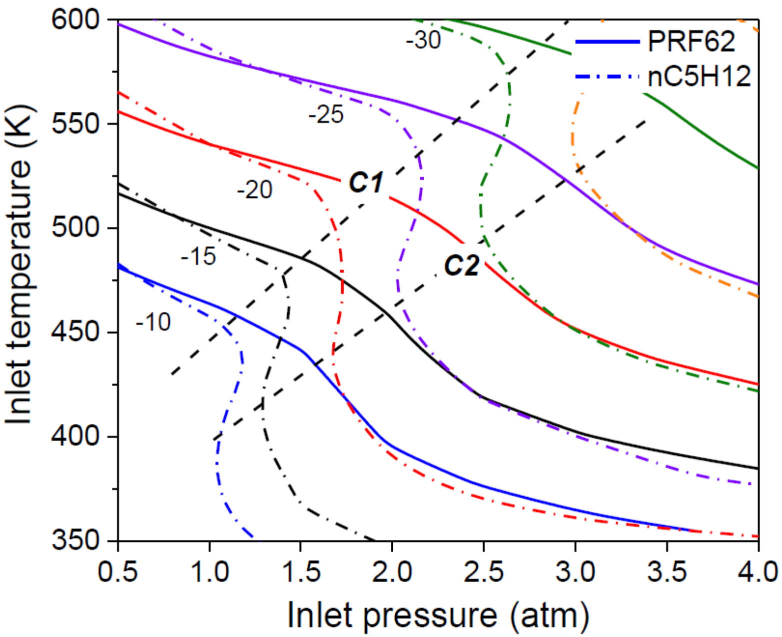
- *Current methods for testing the ignition performance of fuel blends are slow, costly, and require large quantities of fuel.*
  - *For SI: CFR engine (RON + MON)*
  - *For CI: cetane tester, IQT, etc. (CN, DCN)*

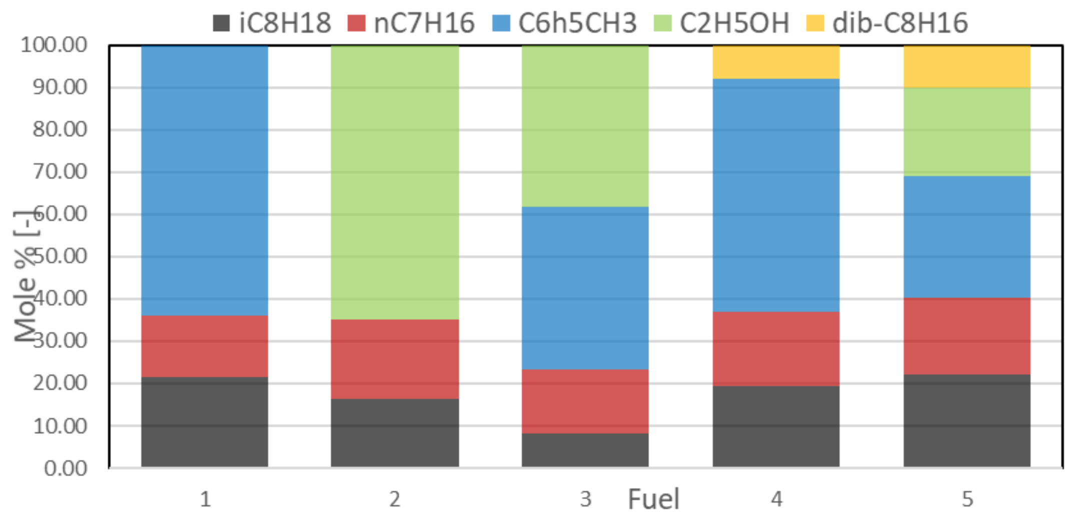
  ~liters of fuel

  - *Can be prohibitive for new biofuels + blends before scaled production, μl to ml*

At the same time they are not always suitable for boosted SI and ACI conditions

	RON	MON	OS
n-pentane	62	62	0
PRF 62	62	62	0

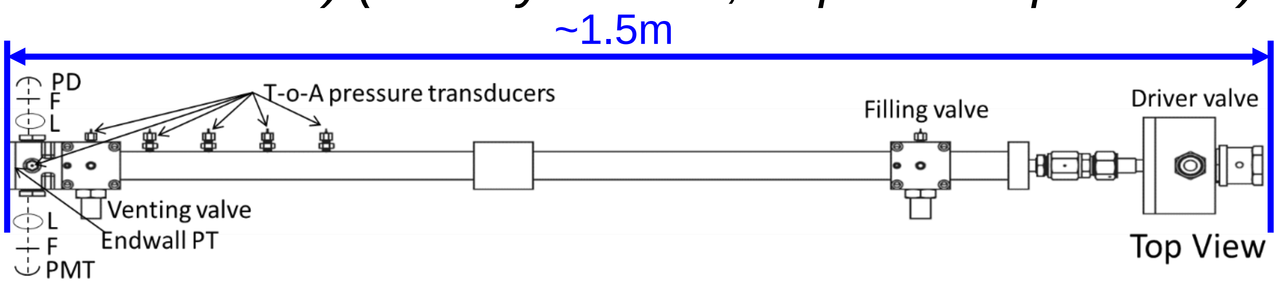


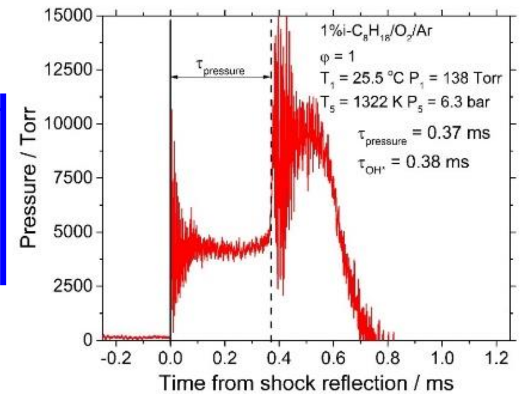


- The significance of traditional fuel metrics varies with operating conditions.
- Fuel composition does matter for combustion phasing under ACI conditions. **Better approaches to screen fuels and blends and tools to evaluate performance are needed…**

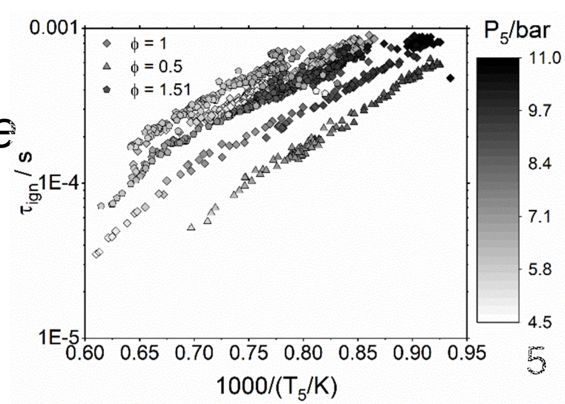
1 - Project Overview (cont.)

- ***Ignition delay based** analyses are experimentally reliable, but generally have low throughput, and not always low fuel quantity.*
  - *Also need approach for analyzing fuel characteristics in engines from those in ideal chemical reactors. Different thermodynamic conditions.*
- *We have <u>expertise in using miniature high-throughput reactors for kinetic studies: including ignition delay</u> (HRRST: high repetition rate shock tube) (~1 s cycle time, ~1µl fuel/experiment)*





- *Conditions for ACI engines are lower temperature and longer induction time than suitably measured in the HRRST, but the miniature high repetition rate reactor approach can be applied to other reactors.*

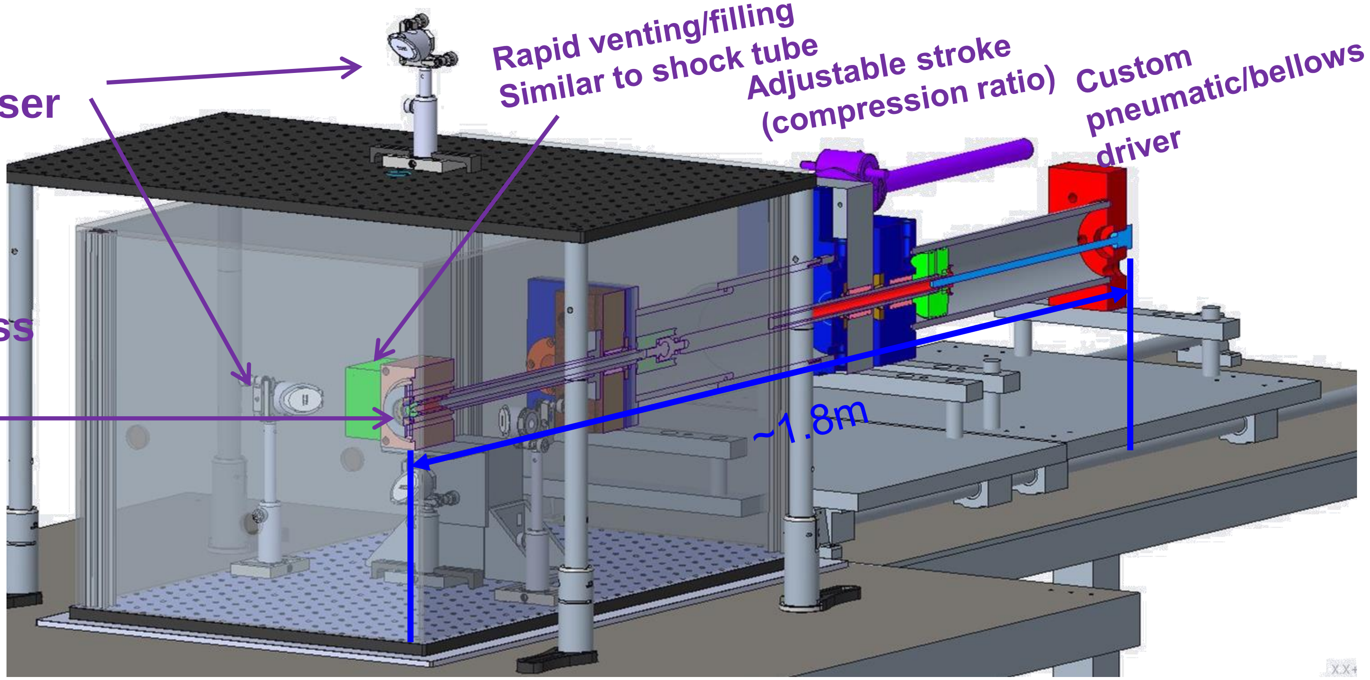


2 – Approach (Technical)

- *Develop, build, and use a* ***miniature rapid compression machine*** *based on extant rapid compression machines combined with the miniaturization + automation techniques from the HRRST.*
- *Generate Livengood-Wu based ignition kernel (ignition delay map) of Co-Optima Relevant Fuels/Blends*
  - *Does not rely on detailed chemical kinetic mechanism*
  - *Ancillary benefits: Data-set for kinetic modelers*
- *Apply this kernel to boosted SI and ACI engine thermodynamic trajectories*
  - *Ancillary benefits: Cross-correlation with different devices*
  - *Ancillary benefits: Ability to optimize with new non-standard thermodynamic trajectories (i.e. ACI engines), to predict ignition performance using staged L-W type of method.*
- *Provide data improvements to support merit function development based on this approach.*
- *Top technical challenges:*
  - *Miniaturization of RCM reactor (e.g. chamber homogeneity from thermal BL and vortices, absorption based temperature measurement at short path length higher pressure, tradeoff of size/forces/closure time). Construction/testing time. Data validation and interpretation.*
- *Go/No-Go (December 2019) Measurement of the ignition delay in miniature RCM, actually developing apparatus which can be improved and refined as needed.*

2 – Approach (Technical cont.)

MISR: Miniature Ignition Screening Rapid Compression Machine

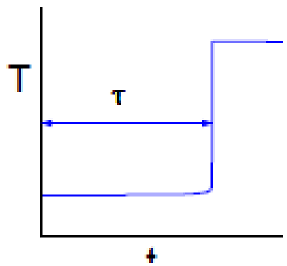


Design criteria:

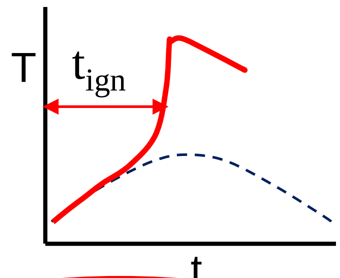
- CR 10-20
- Reactor Temperatures: 400 – 1400 K.
- Reactor Pressures: approximately 1- 100 bar
- Test gas composition < 5% total of fuel + oxidizer in an adjustable inert gas.
- **Fuel composition ~ 1µl/experiment**
- Reaction test time ~100 ms.
- **~1 Hz repetition rates**
- Modular experiments:
  - Ignition delay, tunable diode laser absorption spectroscopy

2 – Approach (Technical cont.)
Livengood-Wu Based Integration

- Widely used for correlating ignition delay times in IC engines
- Assumes ignition is based on the accumulation of critical chain carriers.
- The rate of accumulation can be estimated as $1/\tau$



$$\int_0^{t_{ign}} \frac{dt}{\tau(P,T)} = 1$$

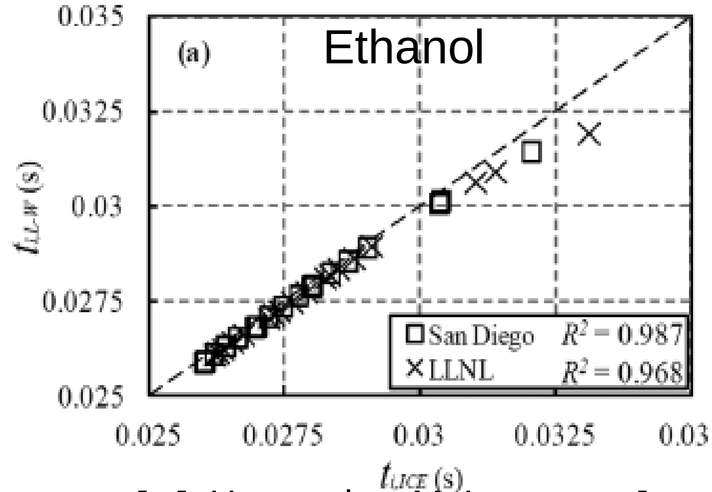


(P, T) trajectory

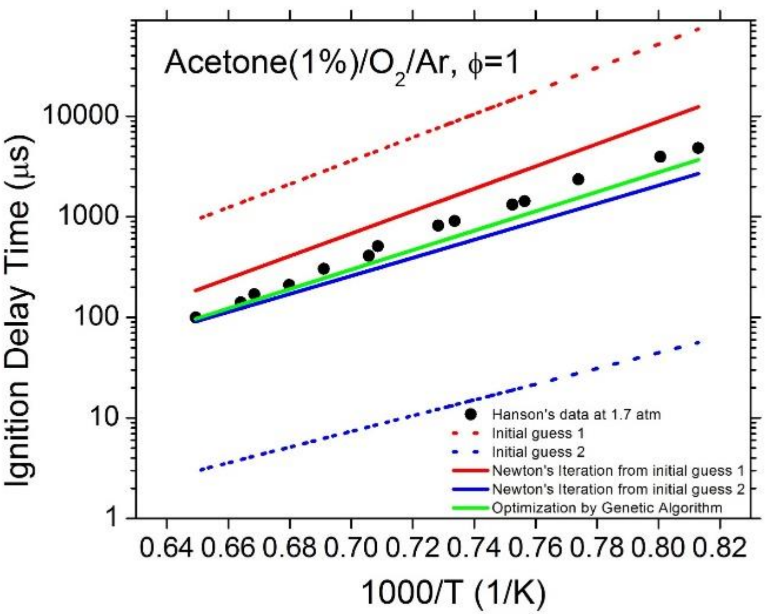
Ignition delay under varying conditions $t_{ign}(P(t),T(t))$

?

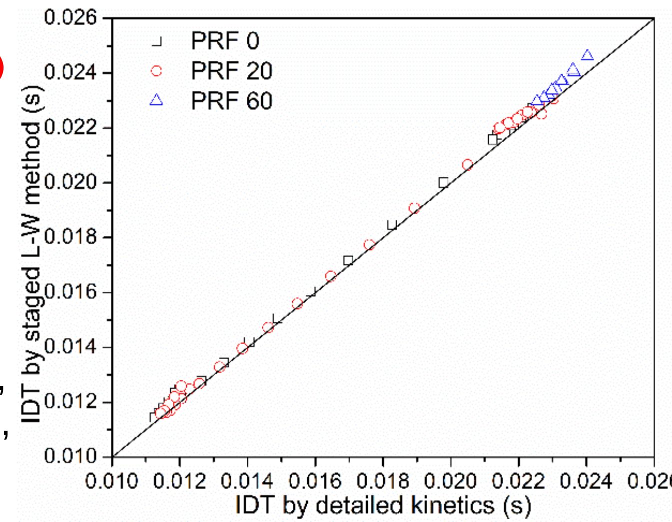
T trace



J. J. Hernandez, M. Lapuerta, J. Sanz-Argent *IJER* **2014** I-13



M. Tao, A. Laich, P. Lynch, P. Zhao, *IJCK*, 50(6) **2018**, 410-424

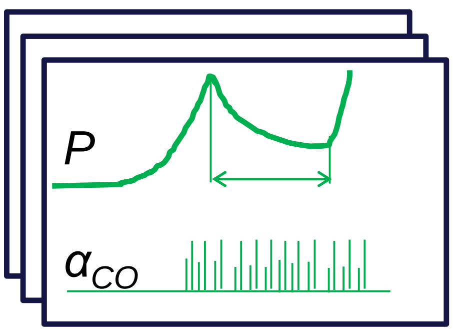


M. Tao, P. Zhao, D. DelVescovo, H. Ge *Combust. Flame* 176 **2017** 400-408

2 – Approach (Technical cont.)
Analysis and modeling technique

$$\tau_1 = AT^{\alpha}P^{\beta}\exp(T_a/T)$$
$$\Delta T = AP^{\beta}\varphi^{\gamma}(T_{ceil} - T)$$
$$\tau_2 = A(P+\Delta P)^{\beta}\varphi^{\gamma}\exp(T_a/(T+\Delta T))$$

MISR Experiments
- High throughput
- Low fuel volume
- Selectable conditions



***Deconvolve* ignition behavior from many experiments**
Each accessing different T+P conditions

Inverse 'Staged' *L-W*
- High T-LTC region
- Chemistry based

$T(t), P(t), \tau_v, \varphi$ → ***Ignition delay kernel (map)*** $\tau(T,P,\varphi)$

Optimization Schemes
- ***Relaxed Newton-iteration (fast but local minima)***
- ***Genetic Algorithm (slow but global)***

Forward 'Staged' L-W

$T(t), P(t), \varphi$ → τ

Ignition estimation
- Statistical variability
- Assessing performance

Thermodynamic Trajectories
Boosted SI or ACI Conditions, Cross Validation Exps., etc.

2 – Approach (Management)

- *Management approach: University directed research project which interfaces with Co-Optima Fuel Properties Group + Kinetics "Small Group".*
  - *To date: Receiving and testing kinetic models (e.g. w. Pitz LLNL), collaborating and expanding upon thermodynamic trajectory based approaches (e.g. w. Szybist ORNL), and receiving input on RCM design and operation (Goldsborough, ANL)*
  - *Ongoing and Future: identification of fuel blends for testing, feedback data to kinetic modelers, improvement and generalization of thermodynamic trajectory based approaches for merit function improvement.*
- *Project Structure: UIC (PI: Lynch) is lead organization. Oakland (coPI: Zhao) is subcontract from UIC. They jointly decide scientific direction.*
  - *Lynch is responsible for the design and construction of the MISR apparatus, and oversees experiments, including ancillary experiments in shock tube.*
  - *Zhao is responsible for the development of inverse Livengood-Wu based approaches for data analysis and leads modeling efforts.*
  - *Lynch and Zhao are jointly responsible for data validation, alternative approach to evaluate ignition performance under ACI conditions, etc.*
  - *Lynch is responsible for project management, reporting, etc.*
  - *Lynch and Zhao are jointly responsible for dissemination.*

3 – Technical Accomplishments/ Progress/Results

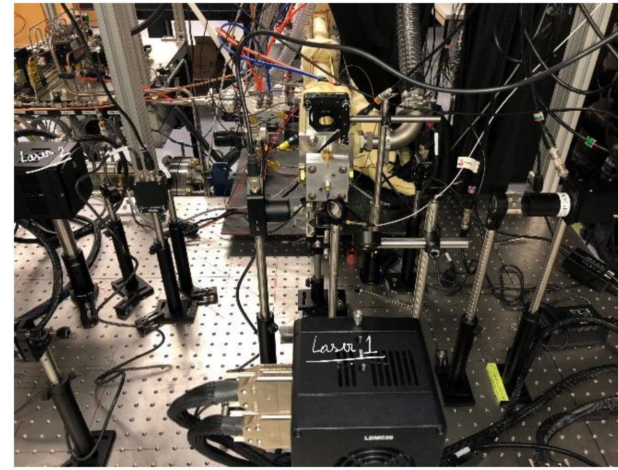
- *Project management plan:*
  - *on track after a delay in project start date. Project budget and technical progress essentially at 8 month stage, and following closely to revised PMP despite officially at 26 month.*
- *Exp. Design/measurement (Milestones to date) :*
  - *finished design of miniature RCM chamber including CFD analysis (ML1.1.2 complete 06/30/2018), procured parts. Tested mixing apparatus for involatile fuels and met repeatability target (ML 1.1.3 complete 12/30/2018) Procured analytical equipment for MISR (2 tunable diode lasers + ancillary equipment). Equipment works with miniature shock tube reactor in configuration similar to MISR (still needs improved calibration upcoming milestone ML 1.1.1 3/31/2019)*
- *Analysis and modeling side (Milestones to date) :*
  - *Inverse Livengood-Wu approach used to measure ignition delay times in high temperature conditions in miniature shock tube (ML 1.2.1 9/30/2018). Analysis strategy with approximated temperature trace and measured pressure trace works well.*
- *Ancillary accomplishments aligned with PMP / ahead of schedule:*
  - *Methodology for using miniature high repetition rate reactors (HRRST and MISR) with chemical kinetic data for mechanism comparison/validation.*
  - *Framework for alternative approach to analyzing autoignition in engines with ACI conditions by overlapping fuel-ignition delay isocontours with thermodynamic trajectory (w/ Szybist, ORNL)*
    - *Method is further generalizable, extendable with Livengood-Wu based ignition delay maps, and a framework for optimization.*

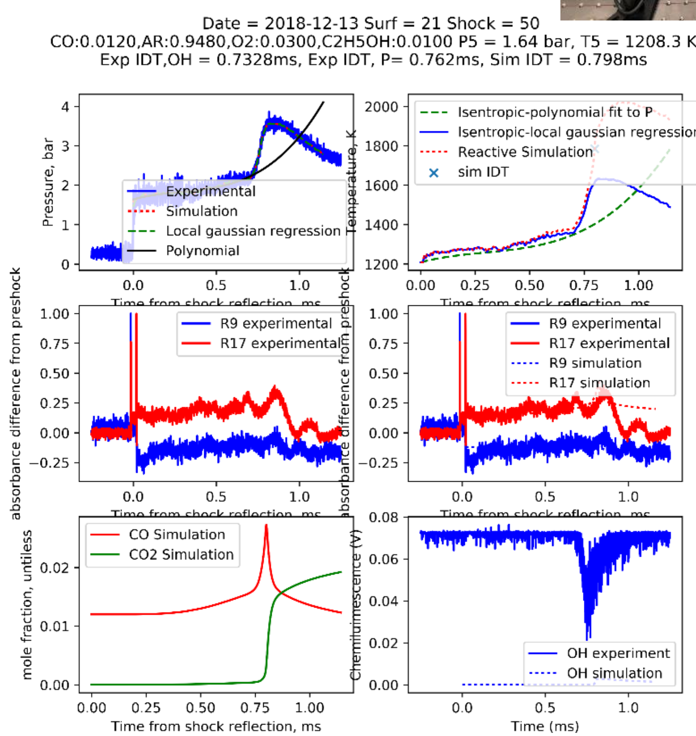
3- Recent Progress (cont.)

***ML 1.1.3* Automated gas mixing rig for high throughput ignition delay devices commissioned**

Composition repeatability <1.5% measured using GC/FID
Ongoing Refinements: Improved handling of very involatile liquid fuels, accuracy of automated set point for composition.

Measurement of two lines of CO in absorption in the miniature shock tube
Ongoing Refinements: High temperature calibration, improvement of signal level, signal averaging, extending time scales to that of the MISR.

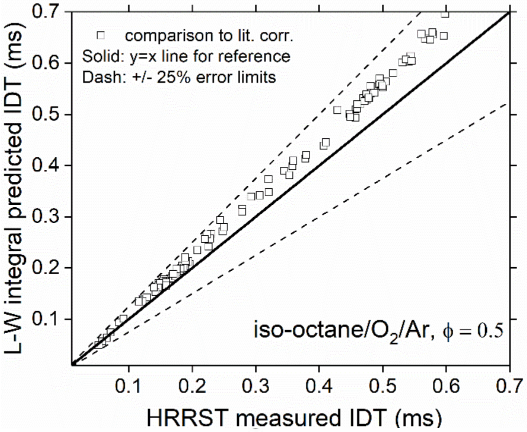




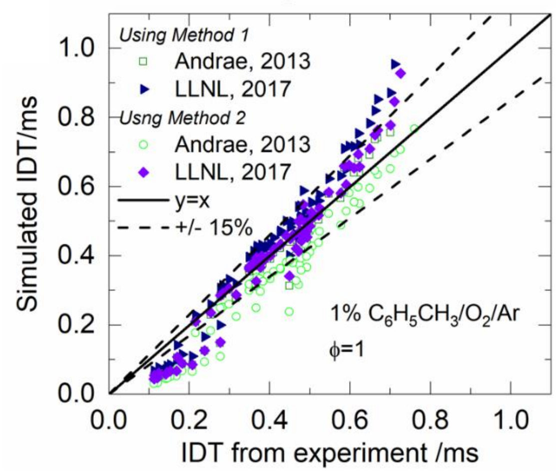
Measurement of ignition delay times in the miniature shock tube:
High T conditions
ethanol
PRFs,
PRF components,
TPRF,
toluene,
acetone

3- Recent Results (cont.)

Miniature reactors (shock tube) with *proper account of complex thermodynamic trajectory* compare well with:



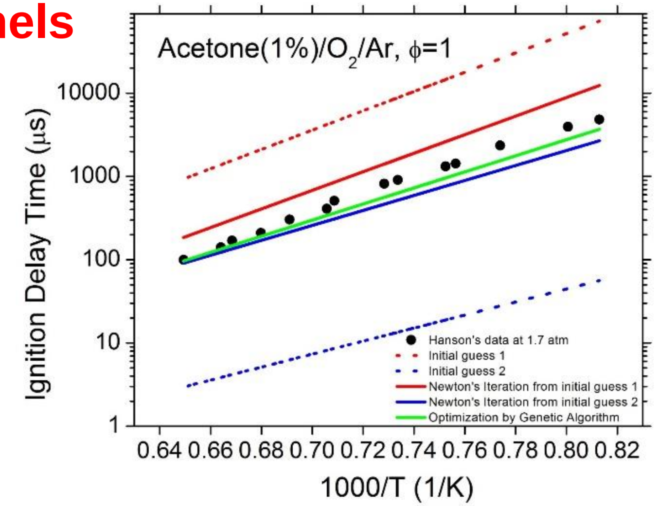
Experimental ignition delay data from conventional reactors



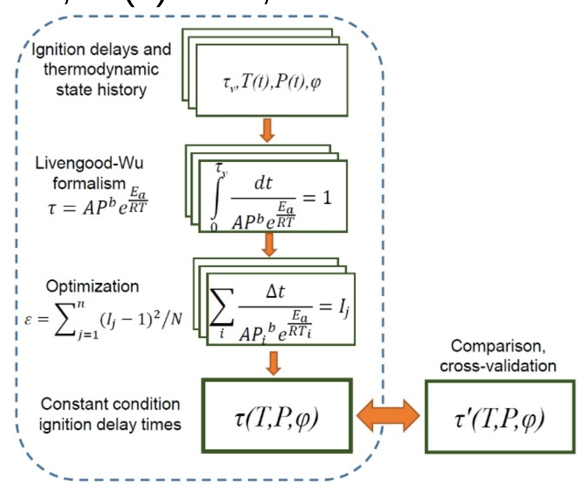
Livengood-Wu integral based modeling or direct chemical modeling

Use of miniature reactors (HRRST) for validation of chemical mechanism for ignition delay time (high temperature) M. Tao, P.T. Lynch and P. Zhao, *Proceedings of the Combustion Institute 37,* **2019** *593-601*.

ML 1.2.1 Inverse Livengood-Wu integral approach can extract ignition kernels



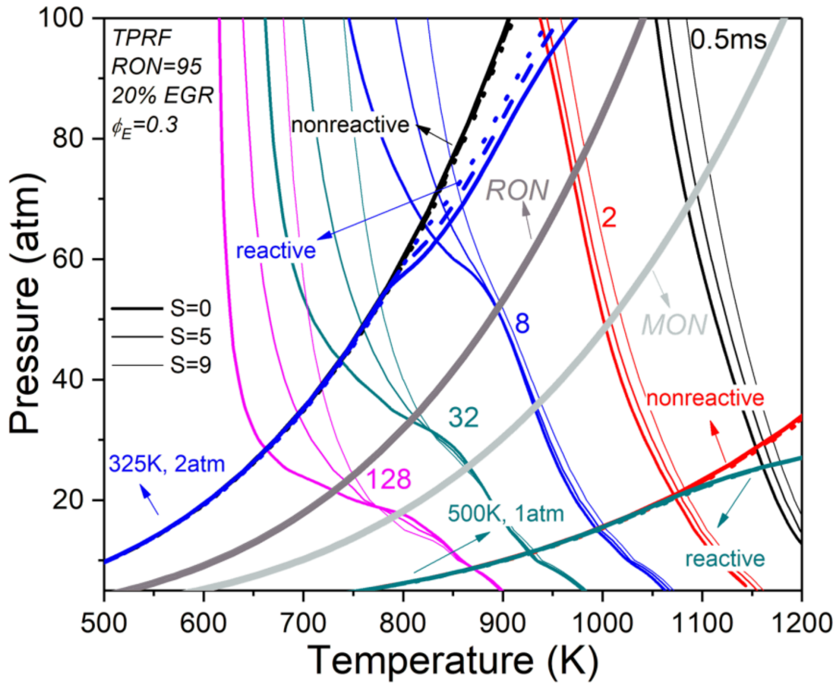
Analysis strategy developed, used, and published (M. Tao, A. Laich, P.T. Lynch, and P. Zhao, *International Journal of Chemical Kinetics*, 50(6) **2018**, 410-424.



3- Recent Accomplishments (cont.)

- We have explored the entire range of SI and ACI engine conditions by overlaying modeled engine P-T trajectories onto fuel ignition-delay contours.
- In the analysis shown, the auto-ignition impact of S was small (closely spaced ignition-delay contours) at high T and low P, but large (widely spaced ignition-delay contours) at low T and high P; to predict performance accurately, the weighting of S would need to vary according to ACI P-T regimes.
- This approach clarifies the chemistry- and condition-dependent impacts of numerous factors needed to predict fuel performance under SI and ACI conditions.
- **The insights obtained for knock under boos ted SI cannot be taken for granted under ACI conditions.**

M Tao, P Zhao, JP Szybist, P Lynch, H Ge *Combustion and Flame*, 200, **2019**, 207-218



Example pressure vs temperature plot showing auto-ignition analysis: engine thermodynamic trajectories (rising from left to right) overlaid onto ignition-delay contours for toluene primary reference fuel (TPRF) with three different S (falling from left to right, labeled with delay in milliseconds). EGR = exhaust gas recirculation, φ_E = actual fuel/air ratio divided by stoichiometric fuel/air ratio.

4 – Relevance (cont.)

- *The goal of this project is to develop a low-volume high-throughput approach for ignition screening of fuels/blends with Co-optima relevance.*

- *Ignition performance is a key target within Co-Optima's central fuel hypothesis.*
- *Our approaches contribute to the search for a general fuel property relevant to ignition in ACI engines (kinetically controlled ignition).*
  - *Such a property is very complicated if it is to be independent of composition.*
  - *Merit function based on weights of RON/MON alone may miss valuable fuel/engine configurations.*
  - *More useful and predictive fuel properties permit engine designers to exploit* ***higher vehicle engine efficiency*** *configurations.*

4 – Relevance

- *The goal of this project is to develop a low-volume high-throughput approach for ignition screening of fuels/blends with Co-optima relevance.*

- *This project further contributes to identifying key bio-derived fuels/blends that exhibit this fuel property relevant to ignition.*
  - *This can capitalize on desirable properties available from bio-derived blend stocks.*
  - *Can provide value proposition when coupled to efficient engine configurations.*
  - *Improved understanding of the suitability of bio-derived fuels/blends from µl samples **lowers costs,** reduces development/decision time on the discovery side, and feeds back into BETO's portfolio planning role.*
  - *Ultimately can contribute to a reduction of petroleum based fuels for transportation.*
- *If reliable+ commoditizable, MISR analysis technique could furthermore be competitive or complementary with standard ignition characterization tools including CFR engines, cetane testers, ignition quality testers.*

5 – Future Work

- *Next 10 months: Building and testing MISR, perfecting inverse – Livengood Wu integral analysis scheme with independent temperature measurement from two-line measurement*
  - *Key Challenges: procurement, assembly, testing, etc., small size of reactor, signal levels, calibration, quantification and reduction of uncertainty in analysis method*
- *Following 8 months: Use of the MISR on Co-Optima relevant fuels*
  - *Key Challenges: standardizing and reducing computational complexity of analysis scheme, further reduction of uncertainty.*
- *Upcoming milestones:*
  - *Characterization of MISR: High Speed Imaging for rollup vortices and ignition homogeneity (ML 1.1.4 approx. Sept 2019)*
  - *Demonstration of 2-line measurement of temperature in HRRST first (ML 1.1.1 approx. March 2019)*
  - *Use of proper i-L-W method with independent temperature in HRRST (ML 1.2.2 approx. June 2019)*
- *Go/No-Go Decision Point (BP1 Planned Dec 2019)*
  - *Major challenge: Building and commissioning of MISR*
  - *Measurement of the ignition delay for a high octane rating fuel (100 experiments in one calendar month, IDT, two line absorption of CO, spec'd pressures, fuel consumption rate, repeatability, and agreement with conventional RCM*

Summary

1. Overview: Traditional fuel performance metrics are not always suitable/predictive for new biofuels/blends, especially in boosted SI and ACI conditions, new analysis and modeling strategy is needed.
2. Approach: Miniature Ignition Screening Rapid Compression Machine + *Livengood-Wu based analysis* technique for quickly measuring a critical fuel property under relevant conditions and assessing performance in those conditions
3. Progress: *Project on track after delay in start date*. Procurement/production of MISR on schedule. Major components of ancillary equipment procured. Measurement and analysis scheme on track with high temperature data in shock tube. Collaborating and developing methodology for modeling + thermodynamic trajectory based approach for fuel quality for merit function.
4. Relevance: Improved understanding of the suitability of bio-derived fuels/blends from μl samples **lowers costs** and reduces development/decision time on the discovery side.
5. Future work: Developing and testing MISR. Improving Livengood-Wu based analysis method and measuring Co-Optima relevant fuels + blends.

Additional Slides

Publications, Patents, Presentations, Awards, and Commercialization

Publications resulting from the work on this project.

- M. Tao, P.T. Lynch and P. Zhao, "Kinetic Modeling of Ignition in Miniature Shock Tube", *Proceedings of the Combustion Institute,* 37*,* **2019,** *593-601.* doi: 10.1016/j.proci.2018.05.048
- M. Tao, A. Laich, P.T. Lynch, and P. Zhao, "On the Interpretation and Correlation of High Temperature Ignition Delays in Reactors with Varying Thermodynamic Conditions" *International Journal of Chemical Kinetics*, 50(6), **2018**, 410-424. doi: 10.1002/kin.21170
- M. Tao, P. Zhao, D. DelVescovo, H. Ge "Manifestation of octane rating, fuel sensitivity, and composition effects for gasoline surrogates under advanced compression ignition conditions" *Combustion and Flame,* 192, **2018,** 238-249. doi: 10.1016/j.combustflame.2018.02.015
- M Tao, P Zhao, JP Szybist, P Lynch, H Ge "Insights into engine autoignition: Combining engine thermodynamic trajectory and fuel ignition delay iso-contour" *Combustion and Flame*, 200, **2019**, 207-218 doi:10.1016/j.combustflame.2018.11.025

Presentations to Government/Laboratories acknowledging Co-Optima Support:

- P. Lynch, "High Pressure Combustion Kinetic Measurements in Shock Tubes" Naval Air Weapon Center, China Lake, CA, 25 June 2018.