Lawrence Livermore National Laboratory

Developing Kinetic Mechanisms for New Fuels and Biofuels, including CFD modeling

William J. Pitz (PI)

Russell Whitesides, Matt McNenly, Marco Mehl, Nick Killingsworth

Lawrence Livermore National Laboratory

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Project ID # FT026

DOE National Laboratory Advanced Combustion Engine R&D Merit Review and Peer Evaluation

Washington, DC

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LLNL-PRES-669706

Overview

Timeline

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

Budget

Project funded by DOE/VT:

- FY14: 500K (funding start June)
- FY15: 397K

Barriers

- Inadequate predictive tools for fuel-property effects on combustion and engine-efficiency optimization
  - Existing models for fuel-enabled engine designs are inadequate

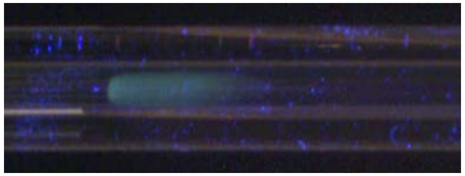
Partners

- Project Lead: LLNL – W. J. Pitz (PI)
- Part of Advanced Engine Combustion (AEC) working group:
- – 15 Industrial partners: auto, engine & energy
- – 5 National Labs & 10 Universities
- LSU: Prof. Schoegl on MicroFit experiments
- Sandia: Provides experimental data for validation of engine simulations
- FACE Working group of the Coordinating Research Council (CRC)

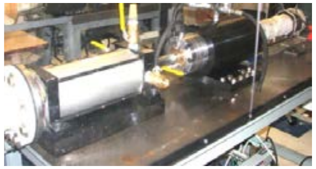
Objectives and relevance to DOE objectives

- Objectives:
  - Develop predictive chemical kinetic models for surrogate components and mixtures to represent advanced fuels. Use these models in CFD simulations to optimize fuel formulations for advanced engine combustion for maximum engine efficiency and very low pollutant emissions, thereby allowing the utmost petroleum displacement

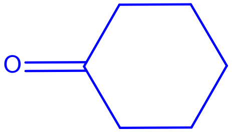
- FY15 Objectives:
  - Design and build a prototype micro-liter fuel tester, and perform initial modeling effort (LSU and LLNL)
  - Develop an accelerated, rapid compression machine (RCM) model
  - Use detailed chemical kinetic modeling to interpret DISI experiments on intermediate blends of gasoline-ethanol
  - Develop reduced mechanisms for biodiesel and long-chain alcohols for use in CFD engine simulations
  - Develop mechanism for biofuel cyclopentanone



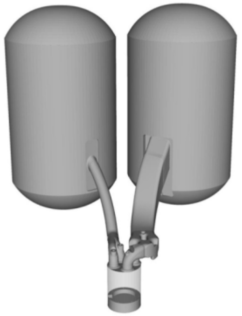
microFIT



RCM

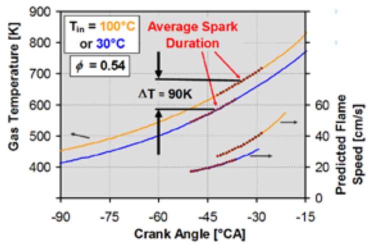


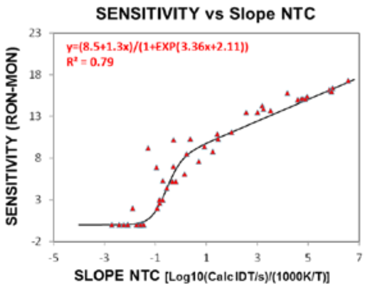
FY2014 milestones: (Funding started mid-June, 2014)



- ✓ Develop multi-dimensional model of Direct Injection Engine Experiments

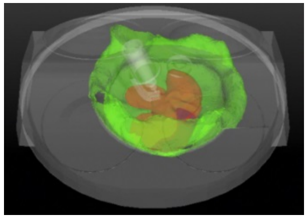
- ✓ Perform ethanol-gasoline kinetics model calculations to guide DISI operating conditions



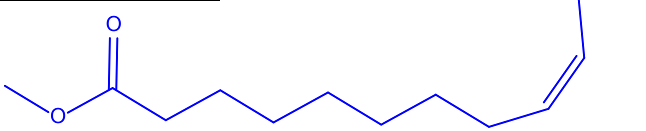


- ✓ Develop an ethanol/gasoline surrogate mixture correlation for higher levels of ethanol

- ✓ Perform multi-dimensional simulations of ethanol-gasoline DISI engine operation to inform experiments

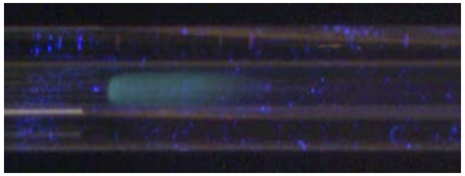


5. Improve and validate chemical kinetic models for saturated and unsaturated large methyl esters (To be completed Sept. 2015 due to late start)

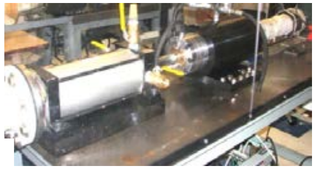


FY2015 milestones: on-schedule

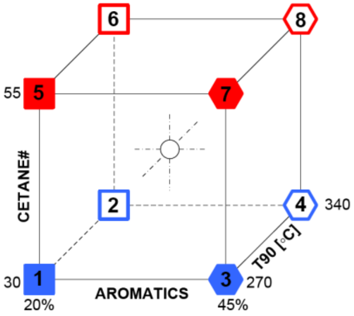
1. Initial model of micro-liter fuel tester developed (June, 2015)
2. Accelerated, Rapid Compression Machine model developed (June, 2015)
3. Perform CFD simulations of FACE Diesel engine experiments (June, 2015)
4. Development of reduced mechanisms for an improved biodiesel surrogate and a long-chain alcohol for CFD applications (Sept, 2015)
5. Cyclopentanone mechanism developed (Sept, 2015)



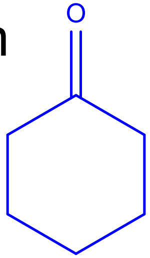
microFIT

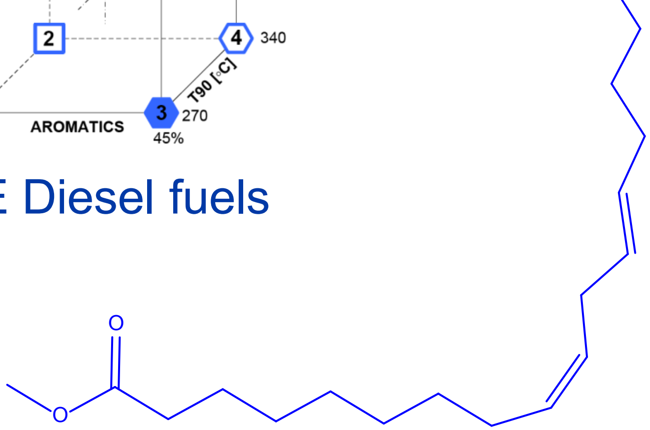


RCM



FACE Diesel fuels





Approach

- Develop surrogate fuel models for gasoline, diesel, and next-generation fuels to enable the prediction of the effect of fuel properties on advanced engine combustion. Use these mechanisms in CFD simulations of engines to gain insight into engine experiments.

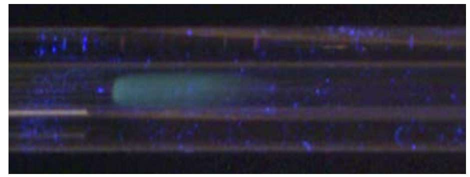
- Develop chemical kinetic reaction models for each individual fuel component of importance for fuel surrogates for gasoline, diesel, and next generation fuels
- Combine mechanisms for representative fuel components to provide surrogate models for practical fuels
  - diesel fuel
  - gasoline (HCCI and/or SI engines)
  - addition of ethanol and other biofuels
- Reduce mechanisms for use in CFD and multizone engine simulations to improve the capability to simulate in-cylinder combustion and emission formation/destruction processes in engines
- Use the resulting models to perform CFD simulations of diesel, spark-ignition and advanced-engine combustion to access fuel property effects
- Iteratively improve kinetic models as needed
- Make kinetic models available to industry

- Addresses barriers to inadequate predictive tools for fuel property effects on combustion and engine-efficiency optimization

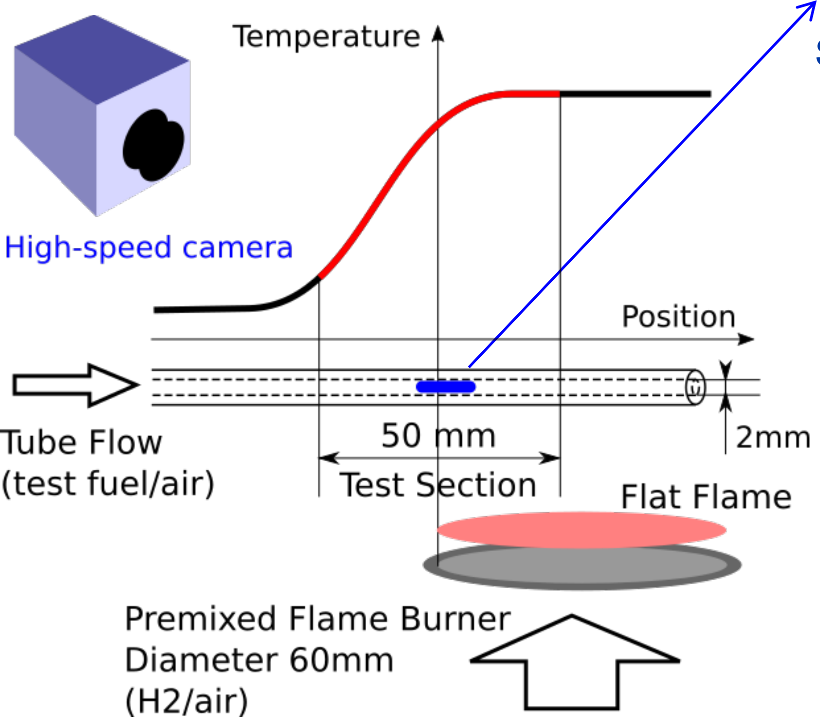
Technical Accomplishments: Micro-FIT: Goal: combustion-fuel properties with only microliters of fuel

- **Tests of fuel properties (e.g. ignition/extinction behavior)**
- **Fuel consumption of 5-20 µg/s**

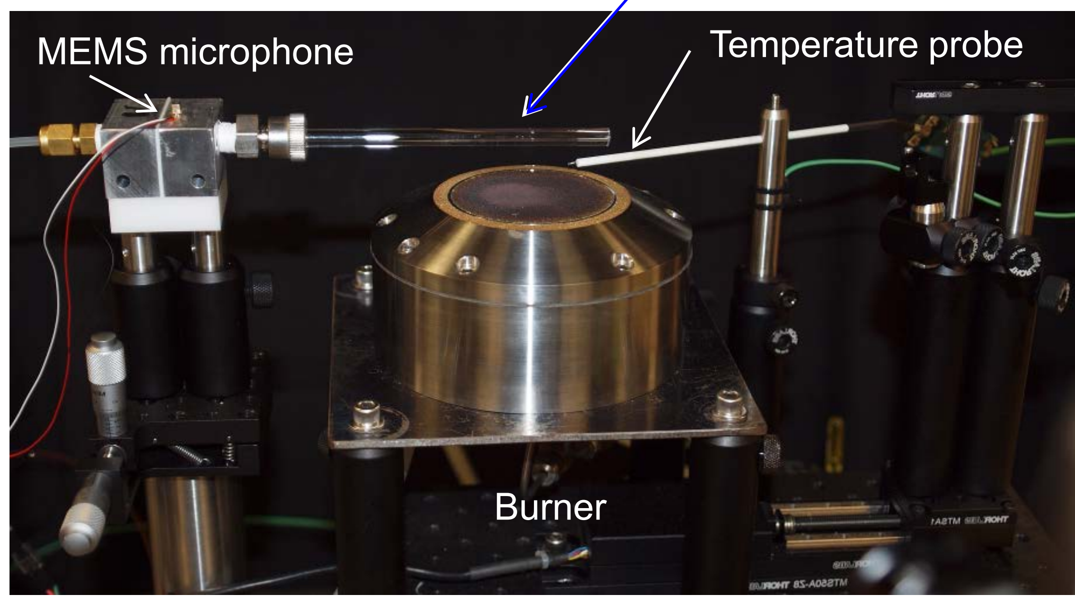
Experiments: LSU, Prof. Ingmar Schoegl,



Still image of flame (long exposure)

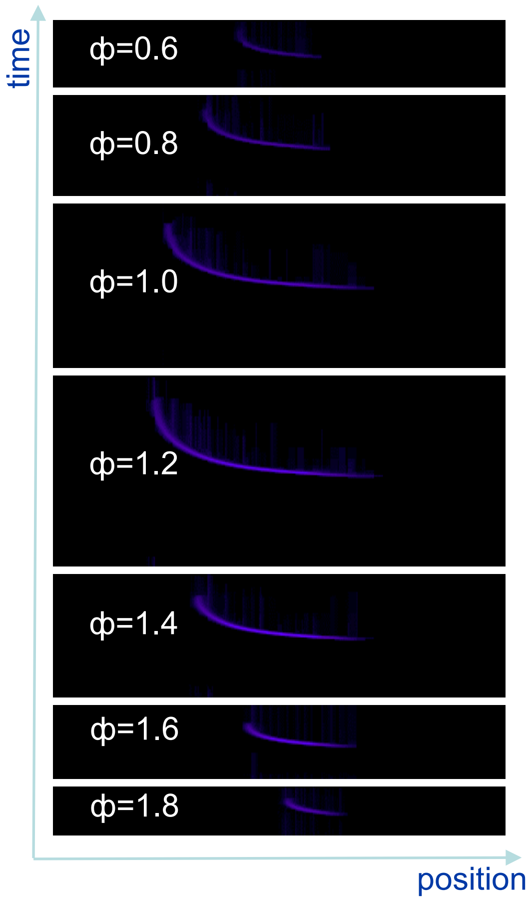


Flow tube

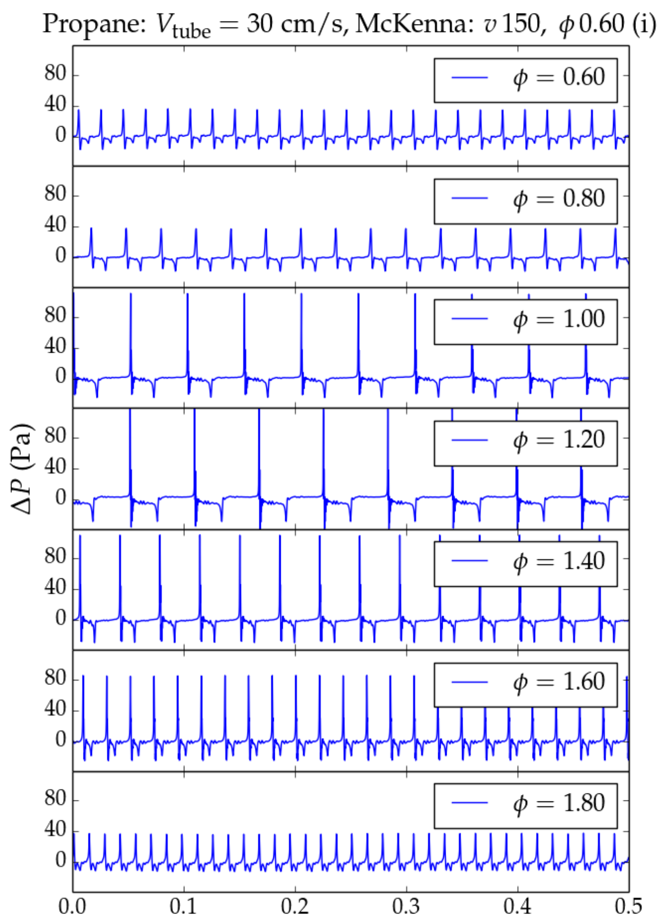


Examining wealth of data to identify fuel property fingerprints

Flame front traces

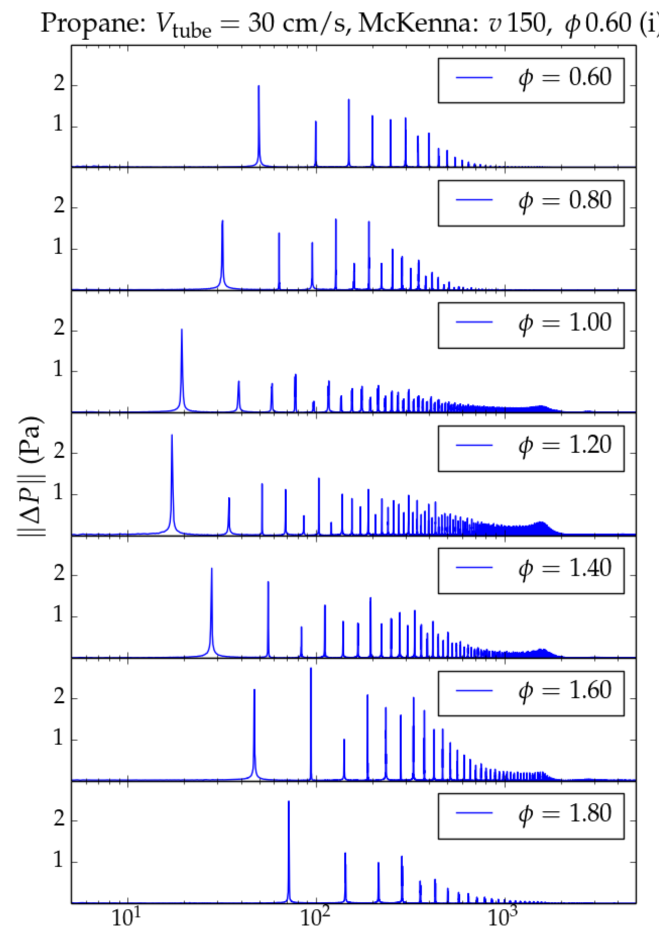


Pressure histories



Time (s)

Pressure frequency modes

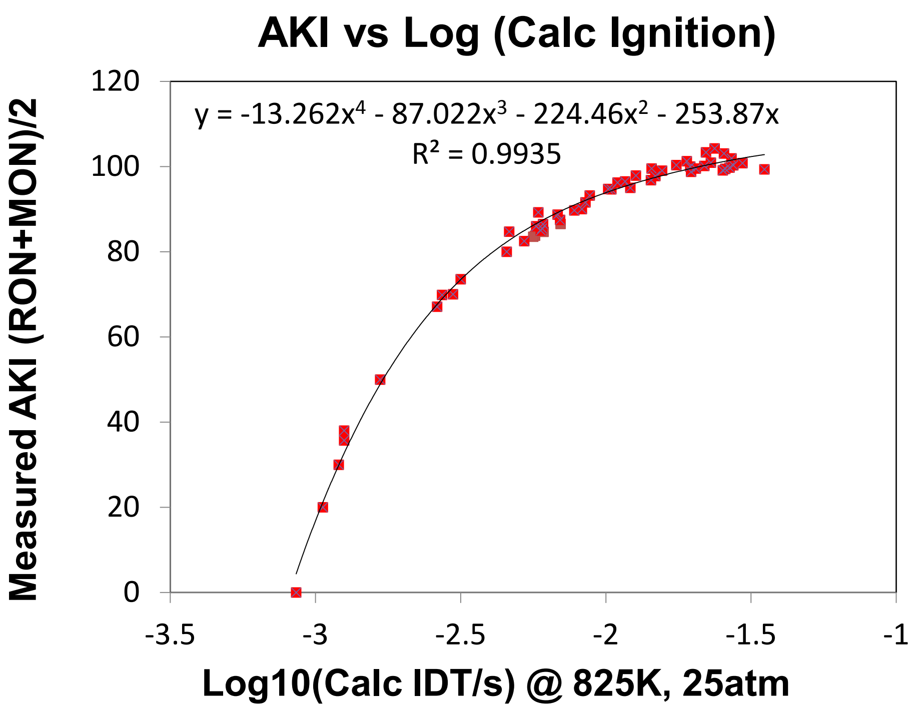


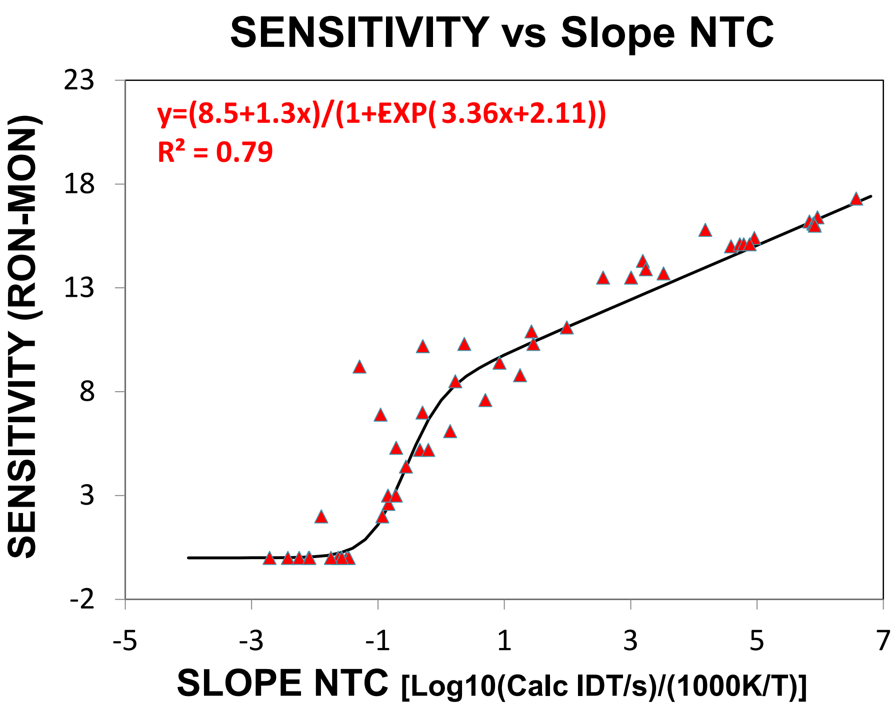
Frequency (Hz)

Validated surrogate model used to obtain Octane Number correlations for gasoline surrogate fuels, including ethanol

FY14 Milestone

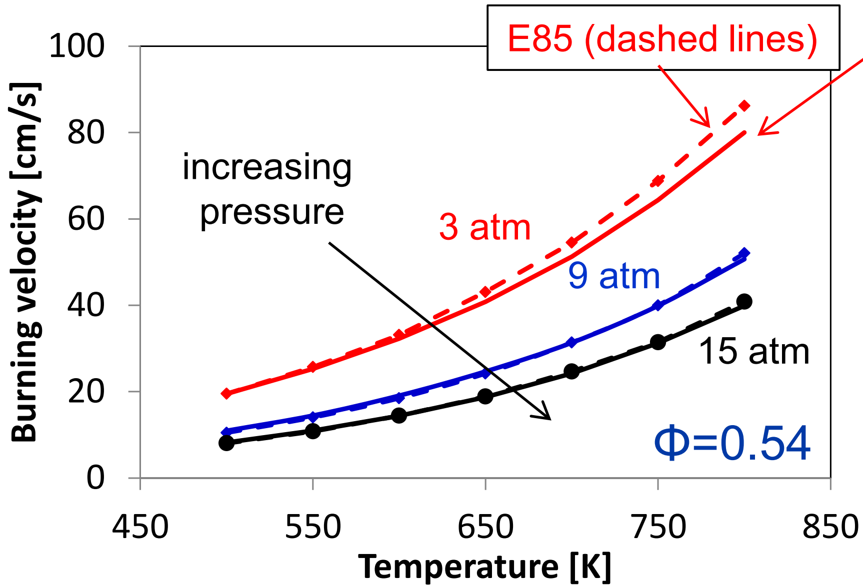
Mixtures including ethanol have been included in the pool and a new sample of 60 surrogates was selected considering only the mixtures having realistic compositions (aromatic fraction below 50%).





The burning velocity of gasoline and E85 have been evaluated at the conditions corresponding to the spark timing in DISI engine

Burning velocities at temperatures and pressures relevant to DISI:



Burning velocities:

- increase with temperature
- decrease with pressure

Burning velocity correlations are needed to evaluate flame speeds at engine conditions:

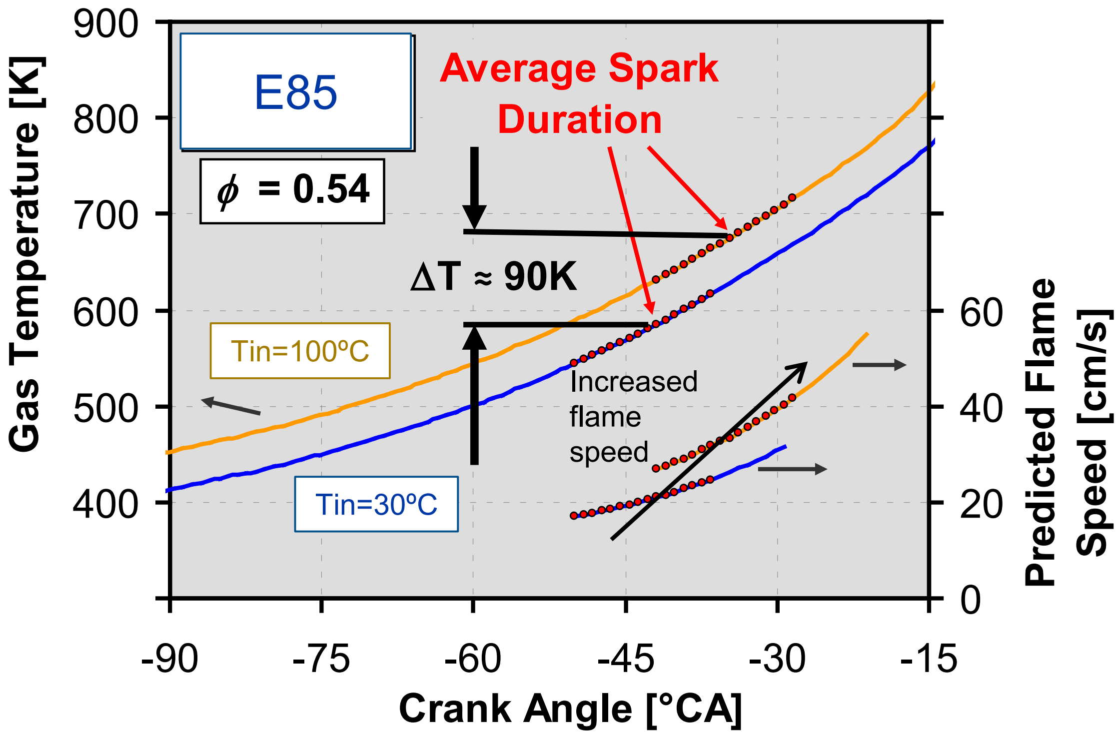
$$\mathbf{E85}: \ Burning\ velocity(T,P) = 2.49P^{-0.515}e^{(0.00522\,T)}$$

$$\mathbf{Gasoline\ (RD387)}: \ Burning\ velocity(T,P) = 2.63P^{-0.479}e^{(0.00501\,T)}$$

(Calculated with gasoline surrogate mechanism)

Flame speed calculations show why higher intake temperatures (T_{in}) improve combustion stability and efficiency for lean operation for DISI

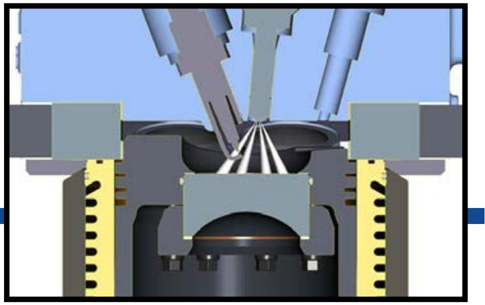
Collaboration with Sjöberg and Zeng at Sandia



From Sjöberg and Zeng, SAE 2014-01-2615

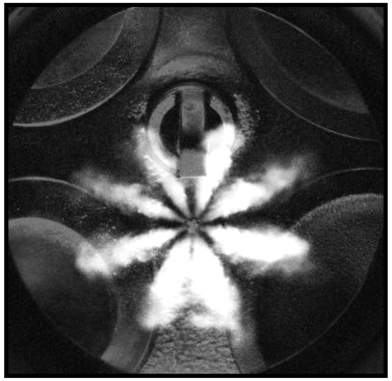
- **The calculations showed that the flame speed during the ignition event is ~ 35% higher when the intake temperature is raised by 100˚C**
- **Increased flame speed allows a delayed spark timing, with its accompanying higher charge temperature**
- **The result is increased combustion stability and efficiency**

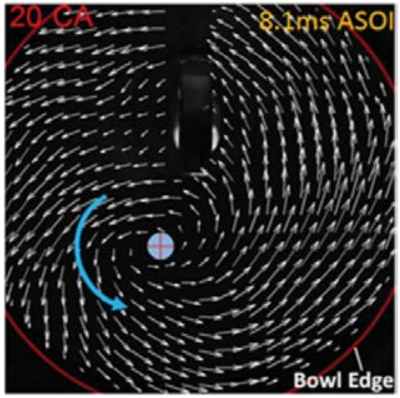
Multidimensional CFD simulations needed to understand fuel effects on Lean/Dilute DISI engine experiments at Sandia



Partial Fuel Stratification (PFS) enables good combustion efficiency with lean/dilute conditions

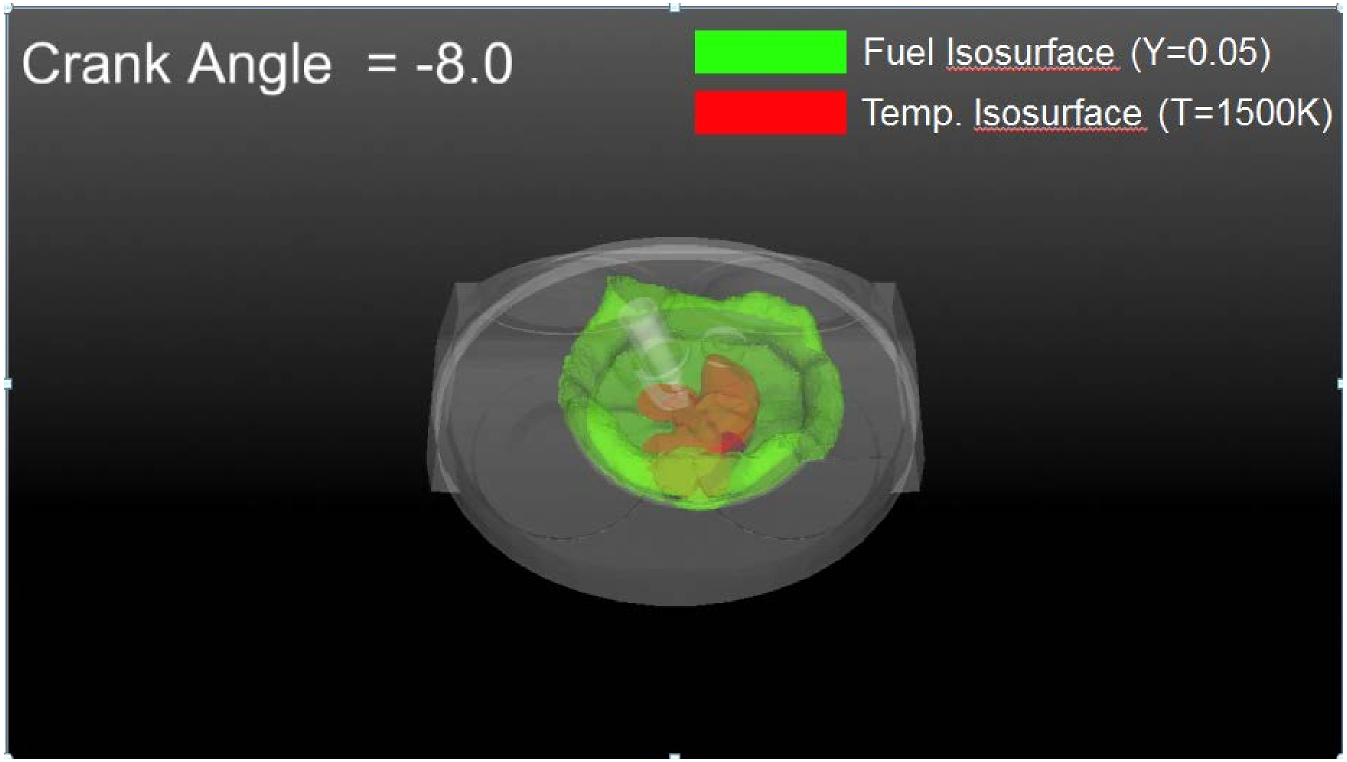
- Measured flow fields allow accurate initialization of velocities and turbulence quantities.





Images courtesy of M. Sjöberg (SNL)

Preliminary fired results: Fully-stratified combustion of E85

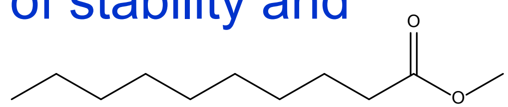


- 4mm base resolution with adaptive mesh resolution (100k-500k cells)
- 312 species Gasoline surrogate mechanism reduced from LLNL detailed mechanism
- Fine resolution MZ (ΔT = 2 K; $\Delta\phi$ = 0.02)
- LLNL Fast Chem: 11 days; Converge Std. Chem: 18 days

Modeling of experiments conducted in the Sandia in the CI Fuel Effects Optical Engine Laboratory

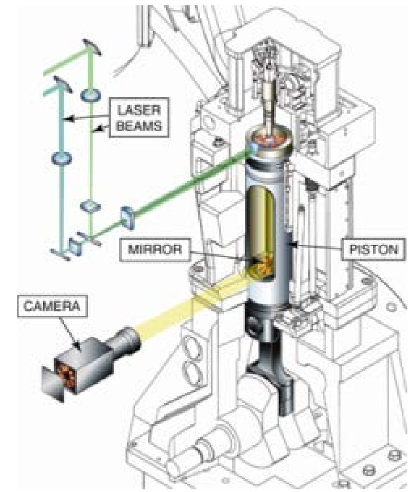
Engine fueled with methyl decanoate for soot-free, leaner lifted-flame combustion (LLFC)

- LLFC is a mixing controlled combustion strategy (ϕ<2) that does not produce soot
- Methyl decanoate is an "optimal" biodiesel methyl ester (in terms of stability and volatility)

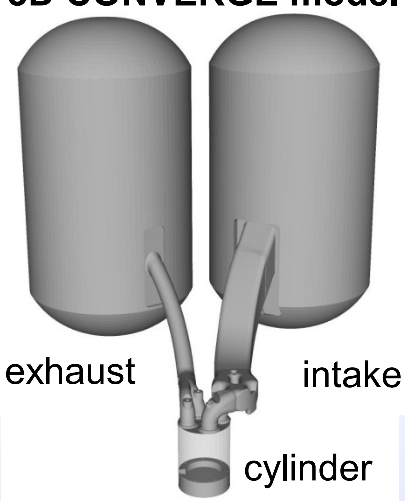


- Oxygenated fuel facilitates achievement of LLFC by providing oxygen in fuel-rich zones
- Full engine geometry modeled including intake and exhaust plenums
  - Gives accurate initial conditions at intake valve close

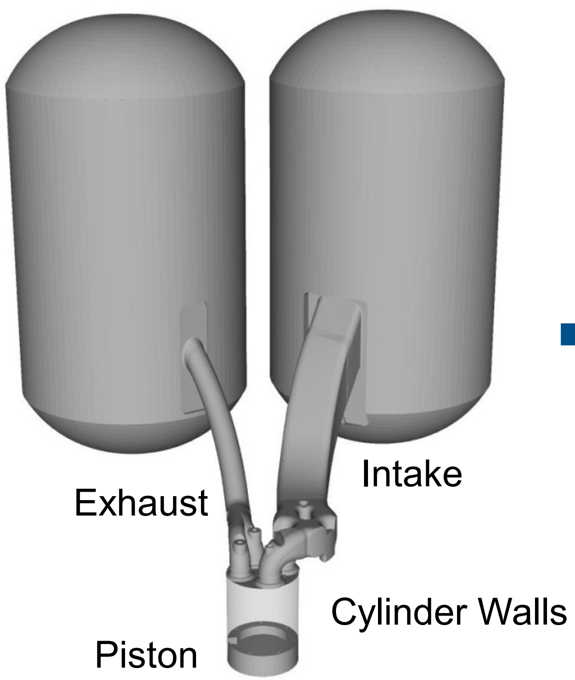
C. Mueller & co-workers heavy duty diesel engine @ SNL

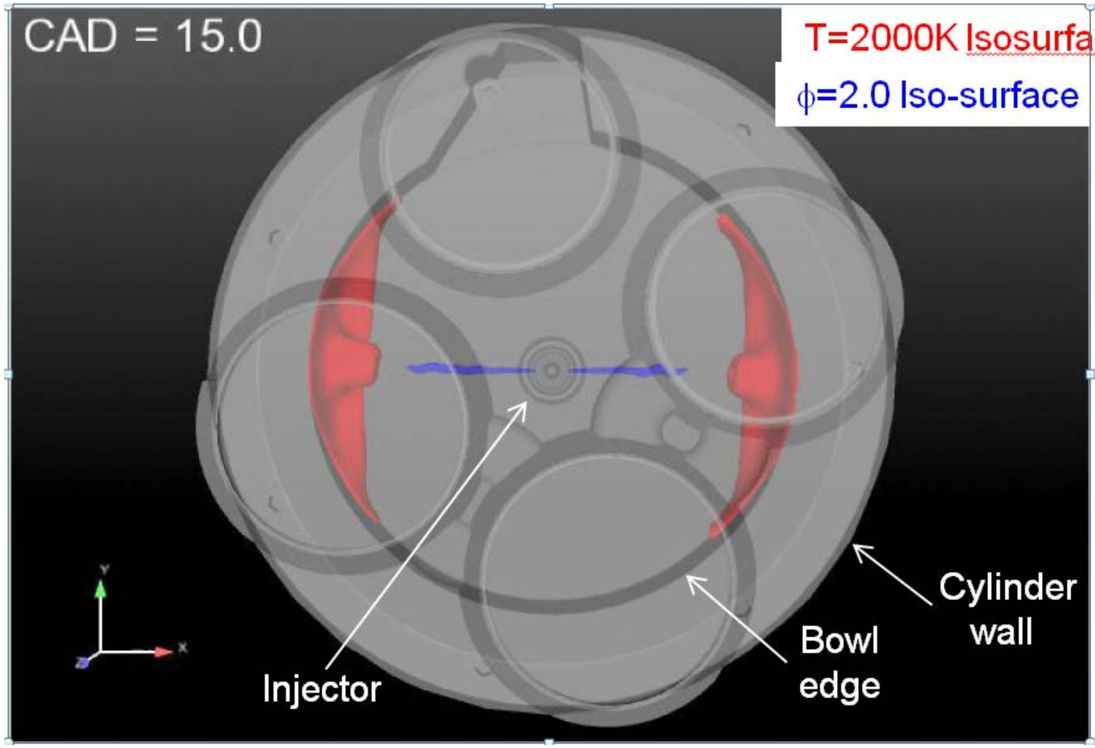


3D CONVERGE model



Preliminary results for leaner lifted-flame combustion of methyl decanoate





Full geometry simulated for 2 1/2 cycles, then mapped to cylinder-only geometry for spray combustion portion of simulation

Adaptive mesh resolution (700k-2M cells)

115 species biodiesel surrogate reduced from LLNL's methyl-decanoate + methyl-9-decenoate mechanism by UConn, ANL, and LLNL

Mechanisms are available on LLNL website and by email

https://combustion.llnl.gov

Mechanisms

Alcohols

Ethanol
Butanol Isomers
Iso-pentanol

Alkanes

2-Methyl and n-Alkanes
Heptane, Detailed Mechanism, Version 3.1
iso-Octane, Version 3
2,2,4,4,6,8,8-Heptamethylnonane

Alkenes

C5 alkene

Surrogates

Biodiesel Surrogates

Real Biodiesel
C10 methyl ester surrogates for biodiesel

Gasoline Surrogate
Diesel PRF
Diesel surrogate, detailed and reduced

Alkyl-Carbonates

Dimethyl Carbonate
Diethyl Carbonate
Cyclopentane

Gasoline Surrogate

Reviewer's comments and our response

- Project not reviewed last year (re-started in June, 2014)

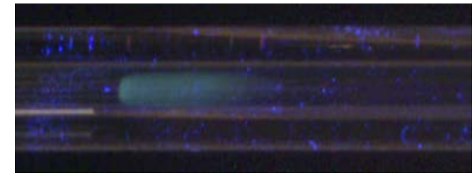
Collaborations

- Our major current industry collaboration is via the DOE working group on Advanced Engine Combustion
  - All results presented at Advanced Engine Combustion Working group meetings (Industry, National labs, Universities)
  - Multiple exchanges of chemical kinetic models with industry
  - Collaboration on gasoline/gasoline-ethanol engine experiments with Sandia:
    - John Dec on CI and Magnus Sjöberg on DISI
  - Collaboration with Sibendu Som at Argonne on diesel reacting sprays
  - Collaboration with Brad Zigler at NREL on IQT experimental validations
- Second interaction is collaboration with many universities
  - Prof. Ingmar Schoegl at LSU on Microfit combustion
  - Prof. Sung's group, U of Conn., Dr. Sarathy, KAUST, and Prof. Dibble, UC Berkeley and Prof. Oehlschlaeger, RPI on gasoline surrogates
  - Dr. Curran at Nat'l Univ. of Ireland on gasoline and diesel fuel components in RCM and shock tube
  - Prof. Reitz, Univ. of Wisc., on development of reduced chemical kinetic models for diesel surrogate components
  - Prof. Lu, U. of Conn. on mechanism reduction
  - Prof. Pfefferle, Yale, on soot chemistry
- Participation in other working groups with industrial representation
  - CRC Fuels for Advanced Combustion Engines (FACE) Working group and CRC AVFL-18a (Surrogate fuels for kinetic modeling)
- Ford: Kinetic modeling support for leaner lifted-flame combustion (LLFC)

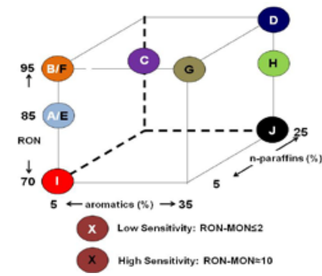
Remaining Challenges and Barriers

- Improve accuracy of CFD simulations with fuel chemistry so that desired predictability needed by engine designers can be achieved
- More accurately simulate the fuel effects with changing pressure, temperature, EGR, equivalence ratio and fuel composition
- Verify accuracy of fuel-surrogate models at high-compression ratio, boosted conditions
- Improve predictability of spray modeling

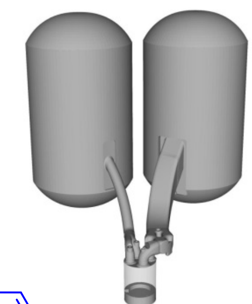
Future plans for next year:



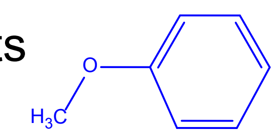
- Extend micro-FIT operation to 30 bar and enable measurement of intermediate-temperature heat-release and pressure sensitivity
- Develop gasoline surrogate mixture model for E10 gasoline RD587 to be used to simulate partially-stratified CI engine experiments at Sandia, in collaboration with RCM experiments at ANL
- Develop validated and improved gasoline surrogate mechanism for FACE fuel F with ethanol up to 30%, using RCM experiments from ANL



- CFD simulations of Chuck Mueller's diesel engine at Sandia



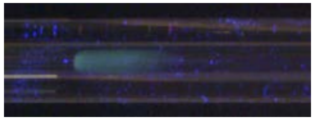
- Develop an chemical kinetic model for anisole, a model component to represent drop-in fuel components derived from upgraded, biomass pyrolysis oil



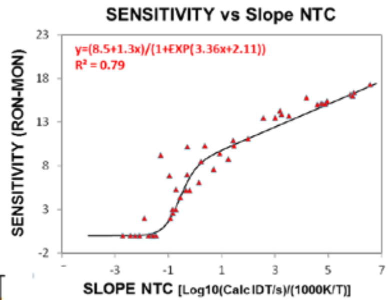
- Model end-gas autoignition as seen in DISI engine experiments at Sandia by Sjöberg et al.

Summary: Developing surrogate fuel models for gasoline and diesel fuels with biofuels to enable accurate advanced-engine combustion simulations to understand fuel effects

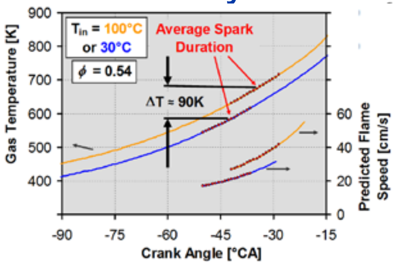
1. Designed and built prototype of micro-liter fuel-property tester



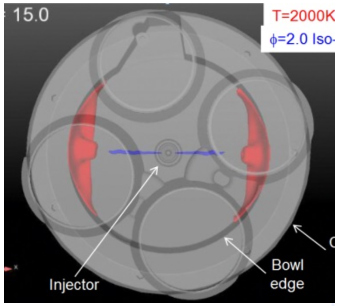
2. Developed of Octane-Number correlation with ethanol using our gasoline-surrogate mechanism with ethanol

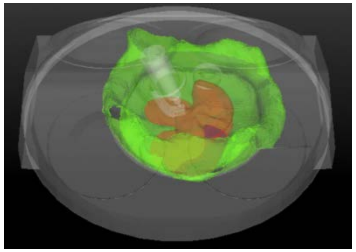


3. Flame speed calculations show why higher intake temperatures (Tin) improve combustion stability and efficiency for lean DISI operation



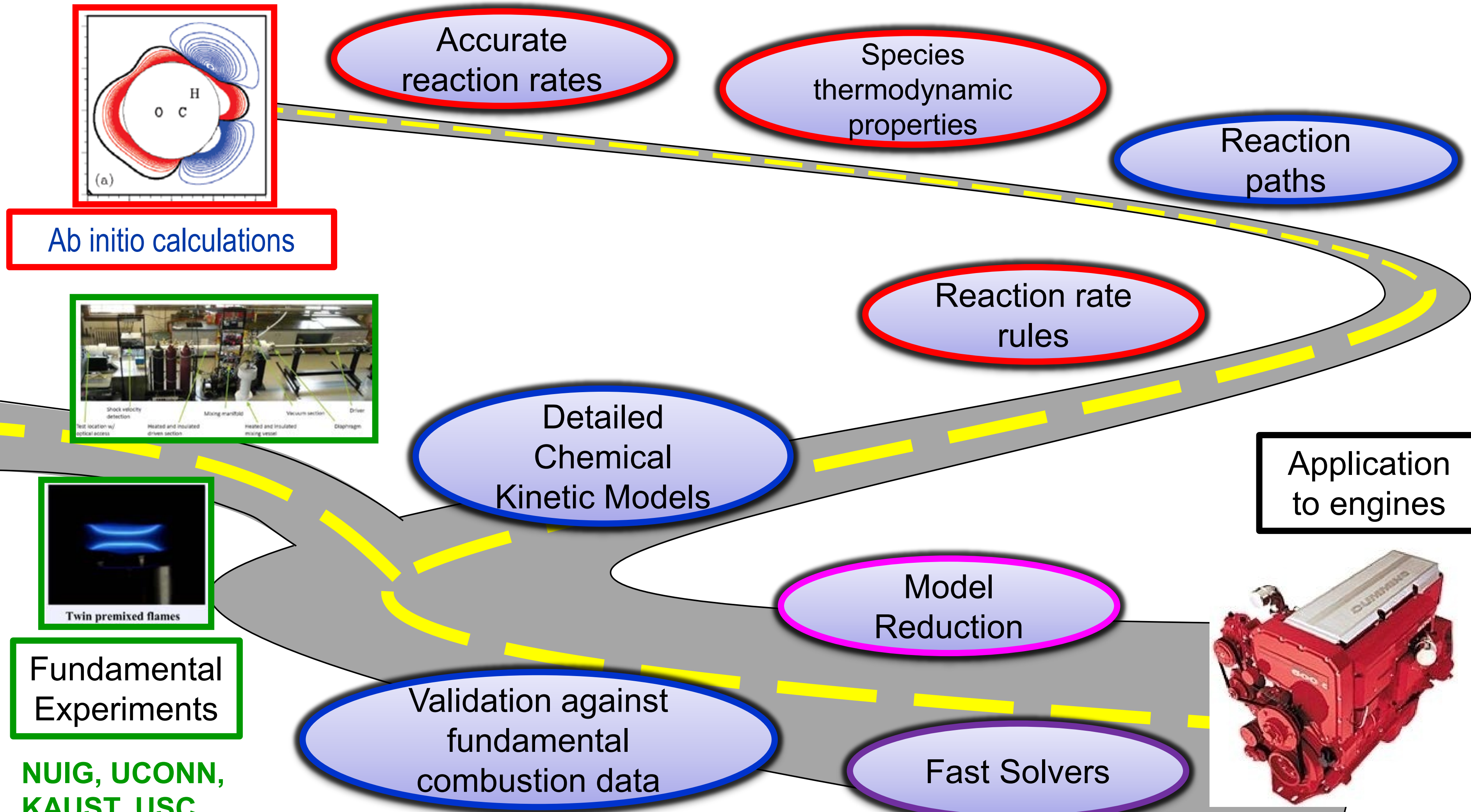
4. Preliminary multidimensional CFD simulations:
   1. To understand fuel effects on Lean/Dilute DISI engine experiments at Sandia with E85
   2. For leaner lifted-flame combustion of methyl decanoate in optical diesel engine at Sandia

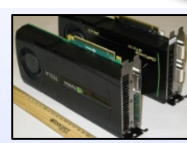




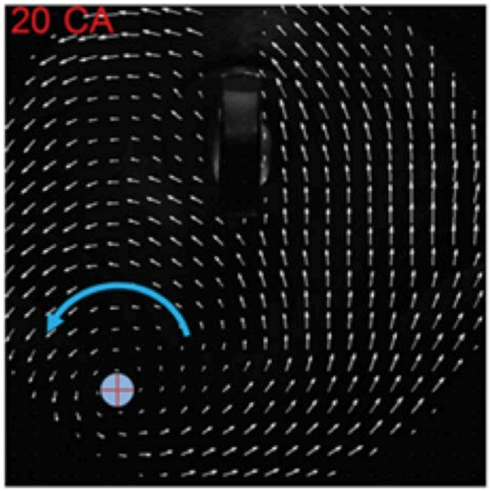
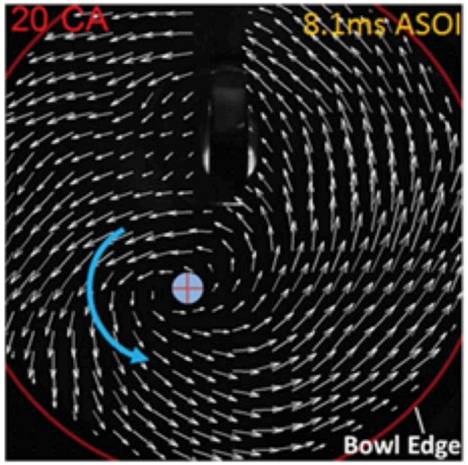
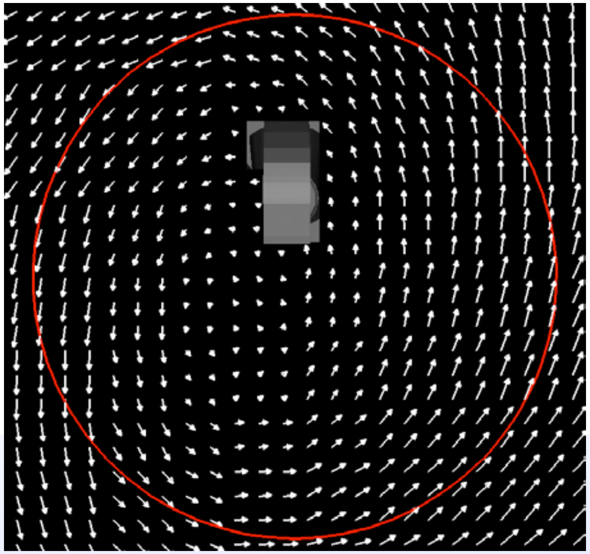
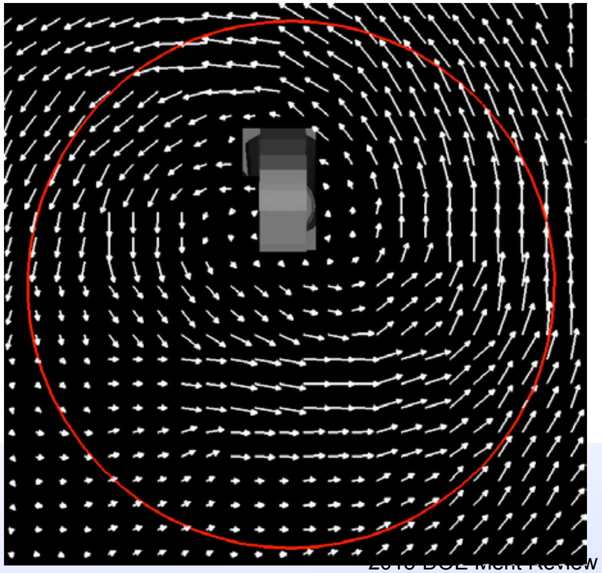
Technical Back-Up Slides

Chemical kinetic model development for practical fuels:





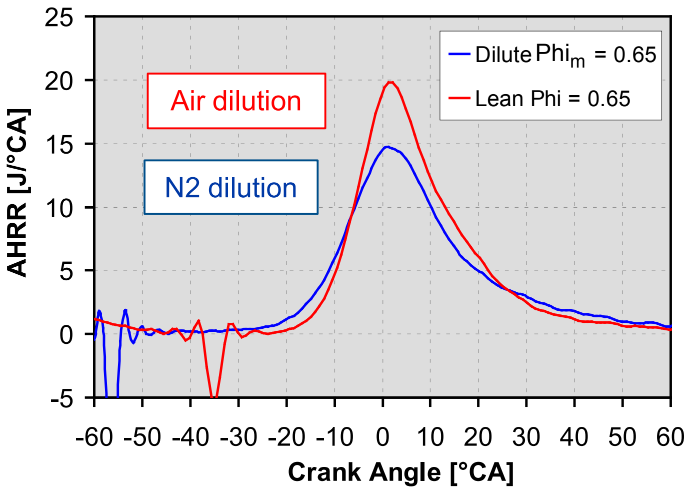
Initial results for lean/dilute DISI experiments at Sandia: Qualitative agreement for swirling flow with and without spray

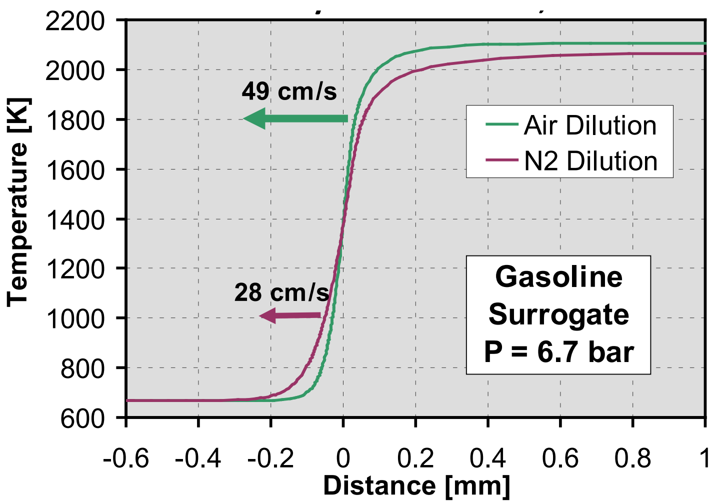
	Without Spray	With Spray
Experiment		
CFD		

Laminar flame speed calculations were used to compare fuel-lean combustion vs stoichiometric-diluted combustion in DISI engine experiments at Sandia

Experiments highlighted how dilute $\phi = 1$ operation leads to much slower spark-to-CA50 although the overall fuel/oxidizer mixture mass ratio is conserved.

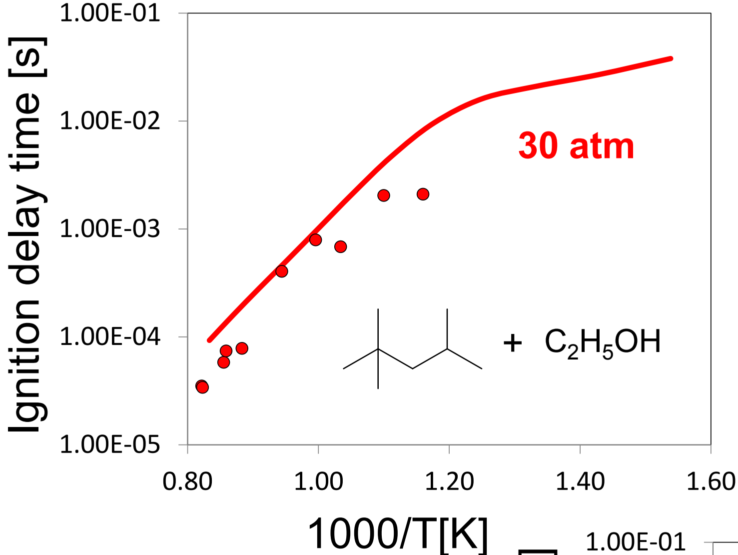
- **Courtesy of Magnus Sjoberg, SANDIA**

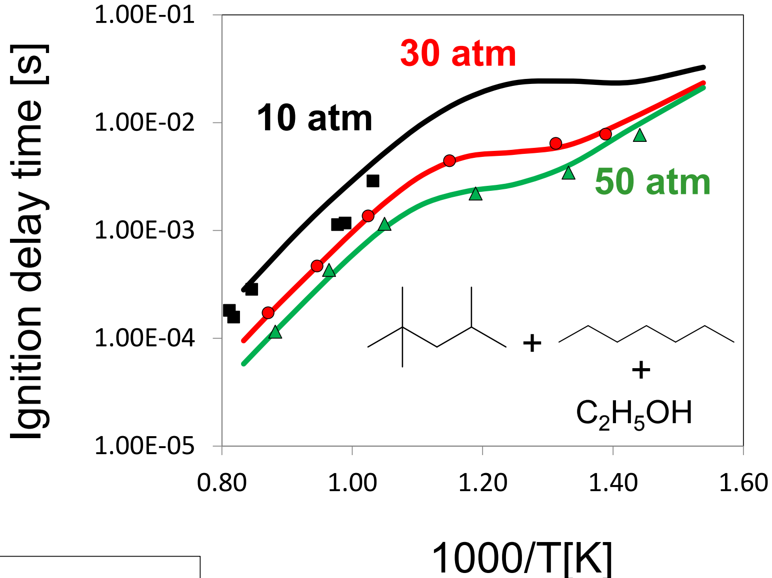




Kinetic calculations obtained using a E30 gasoline surrogate showed that in the nitrogen dilute case the combustion is 40% slower

Validated gasoline-surrogate mechanism with ethanol using shock tube ignition experiments:





Experiments:
Schulz et al., Germany

Stoichiometric mixtures