CFD Simulations and Experiments to Determine the Feasibility of Various Alternate Fuels for Compression Ignition Engine Applications

Sibendu Som

Douglas E. Longman, Anita I. Ramirez, Zihan Wang

Argonne National Laboratory

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Team Leader: Kevin Stork

Project ID # FT022

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Overview

Timeline

Project start: May 1st 2012

Partners

Project Lead: Sibendu Som

Argonne National Laboratory
Leadership Computing Facility

Convergent Science Inc.
Lawrence Livermore National Laboratory
Sandia National Laboratory
University of Connecticut
US Department of Agriculture (USDA)
National Renewable Energy Technology Laboratory (NREL)
Indian Institute of Technology, Kanpur (IIT-K)

Advanced Engine Combustion (AEC) Working group

Barriers

- ❑ "Inadequate understanding of stochastics of fuel injection for bio-derived fuels"
- ❑ "Improving the predictive nature of spray and combustion models for biodiesel fuel"
- ❑ "Incorporating more detailed chemical kinetics into fluid dynamics simulations for biodiesel fuels"

Budget

FY 12: 150 K
FY 13: 150 K

Objectives

- Biodiesel is a lucrative alternate for compression ignition engines. However, differences in physical & chemical properties of biodiesel and petrodiesel are significant
- The physical and chemical properties of biodiesel from different feedstocks also vary significantly. Of specific interest: (1) Soy methyl ester, (2) Tallow methyl ester, (3) Cuphea methyl ester, (4) Rape-seed methyl ester
- Obtain fuel properties such as density, viscosity, surface tension, vapor pressure, heat of combustion, heat of evaporation, distillation curve etc. for different these different “drop-in” biodiesel fuels
- Predict differences in inner-nozzle flow behavior of these fuels in terms of cavitation inception, turbulence levels, injection velocity, discharge coefficient etc.

Significant interest within industry and academia for using reliable mechanisms to predict biodiesel combustion

- Simulate biodiesel combustion using four published mechanisms
- Quantify their performances under engine conditions

Relevance

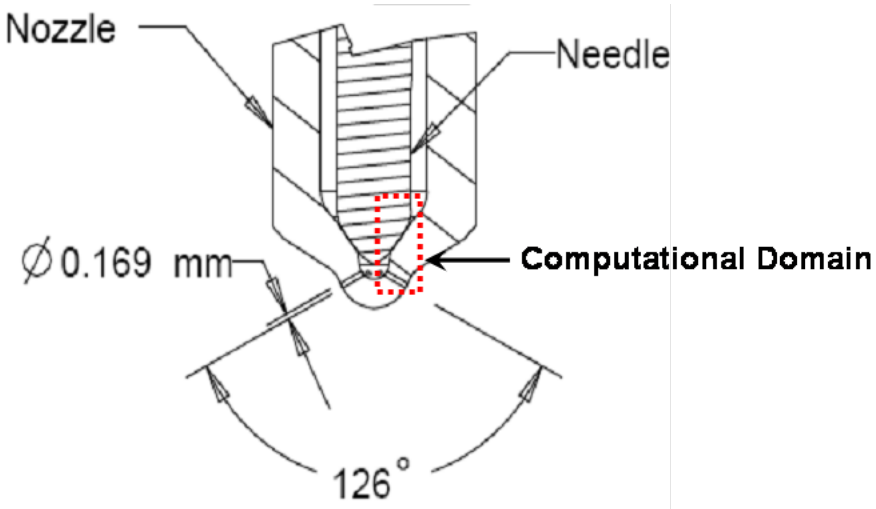
- **Nozzle flow and Spray research**
  - Fuel spray breakup in the near nozzle region plays a central role in combustion and emission processes for biodiesel fuels
  - Understanding and improving in-nozzle flow and turbulence predictions is key towards the development of predictive models for biodiesel fuels
- **Combustion modeling using detailed chemistry**
  - Accurate detailed chemical kinetics for biodiesel fuel surrogates are key towards developing predictive combustion modeling capability
  - Reduced chemical kinetic mechanisms are necessary for comprehensive CFD simulations with biodiesel fuels
  - Mixture of methyl decanoate, methyl 9-decenoate, and n-heptane is a suitable biodiesel fuel surrogate
- **Well-validated spray and combustion modeling approaches for biodiesel fuels are necessary for biodiesel fuels similar to diesel and gasoline fuels**
  - Significant differences in fuel properties between conventional compression ignition engine and biodiesel fuels

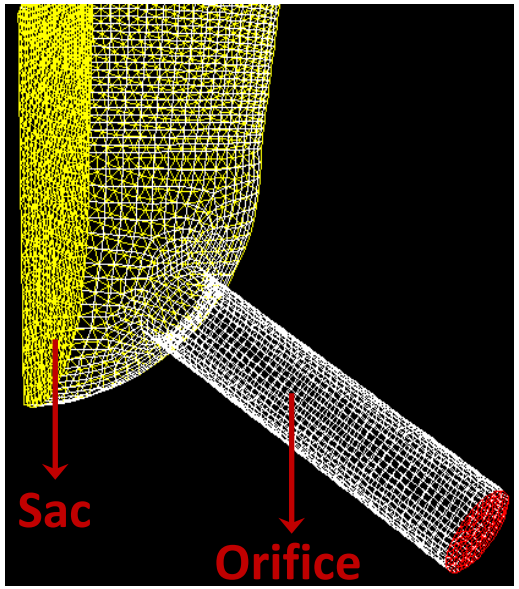
Milestones, FY 13

- In-Nozzle flow Simulations for biodiesel from different feedstocks
  - ✓ Determine temperature dependent fuel properties of these biodiesel fuels of interest and compare them against diesel fuel {Complete}
  - ✓ Compare in-nozzle flow characteristics such as cavitation and turbulence levels inside a conventional diesel injector for different biodiesel fuels of interest {Complete}
  - ✓ Comparison of flow characteristics between biodiesel from different feedstocks and diesel fuel {Complete}
- Combustion Modeling with Detailed Chemistry for soy-based biodiesel
  - ❑ Develop a reduced chemical kinetic model for the three component biodiesel surrogate for CFD simulations {Complete}
  - ❑ Comprehensive validation of the developed reduced kinetic mechanism against experimental data available from Sandia National Laboratory {Complete}
  - ❑ Compare the results of this new three component surrogate mechanism against other mechanisms available in literature {Complete}

Computational Approach and Model Set-up

- Simulations performed in FLUENT v6.3
- Mixture based cavitation model
  - No slip between liquid and vapor phases
  - Thermal equilibrium
  - Compressible flow simulations
  - Rayleigh-Plesset equation for phase change
  - Separate transport equation for vapor mass fractions
- RNG K-ε Turbulence model, non-equilibrium wall-functions
- 3D simulations
- 6 hole production nozzle, only one orifice simulated
- Total number of grid points: 150K at peak needle open position





* S. Som, PhD thesis, **2009**

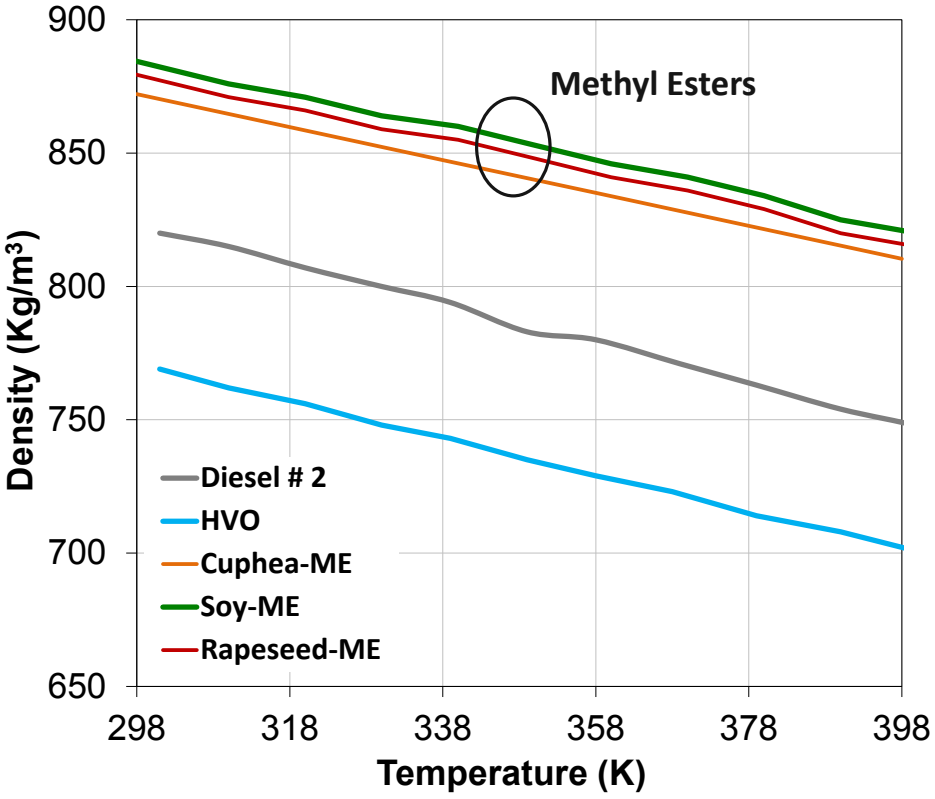
* A.K. Singhal et al., **Journal of Fluid Engineering, ASME 2002**

Fuels of Interest

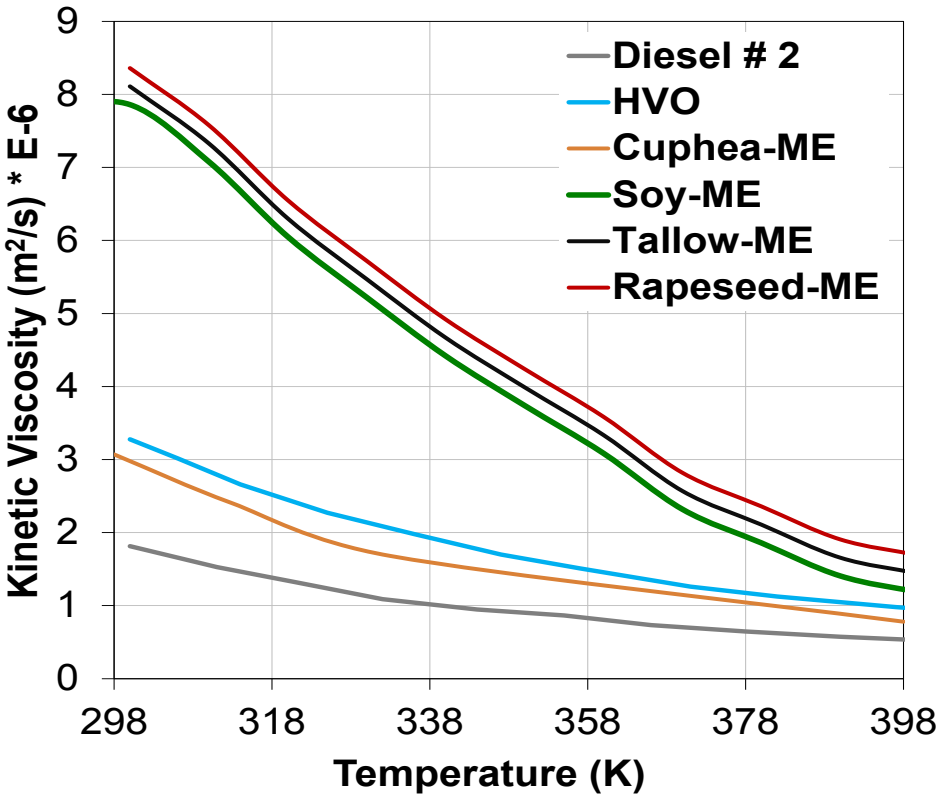
- Diesel # 2 properties obtained from literature
- Soy Methyl Ester (SME): prevalent in North America - Peter Cremer NA
- Rape-seed Methyl Ester (RME): prevalent in Europe – Properties obtained from Literature
- Cuphea Methyl Ester (CuME): explored by USDA - Knothe et al. Energy and Fuel 2009
- Hydro-treated Vegetable Oil (HVO): Helsinki University of Technology - Gong et al. SAE 2010-01-0739
- Jatropha and Karanja based biodiesel properties obtained from Dr. Avinash Agarwal at IIT, Kanpur (India)

Fuel Property	Diesel	SME	CuME	HVO
Carbon Content [wt %]	87	76.74	75.79	85
Hydrogen Content [wt %]	13	12.01	12.05	15
Oxygen Content [wt %]	0	11.25	12.16	0
Heat of Combustion [MJ/Kg]	42	37.4	34.8	44
Heat of Vaporization [KJ/Kg]	361	336	85	227
Cetane Number	40-45	46-55	56	80-89
Surface Tension @ 298 K [N/m]	0.0250	0.0315	0.0312	0.0125

Fuel Properties vs. Temperature

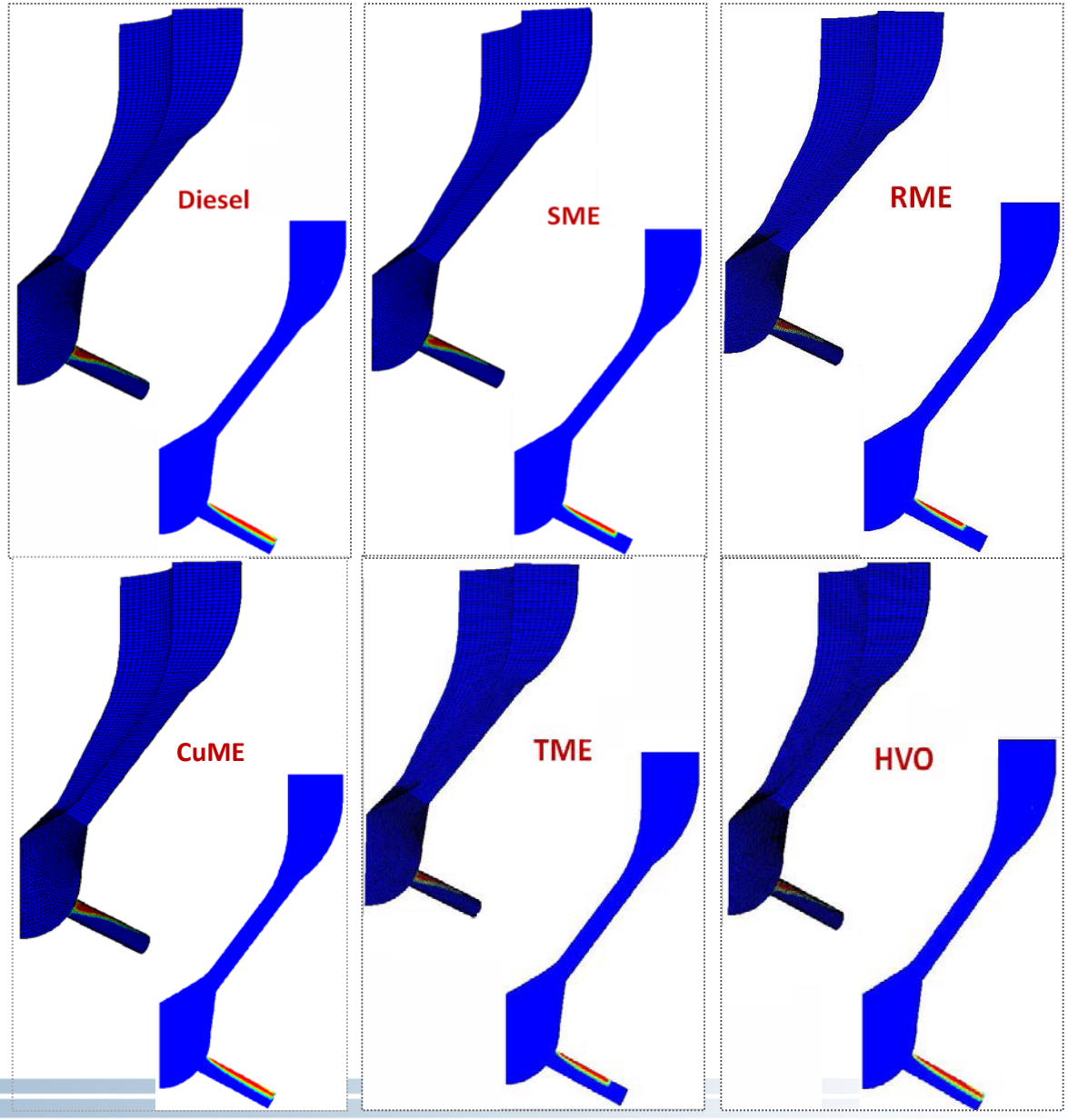


- Linear effect of temperature on density
- Methyl esters have similar densities



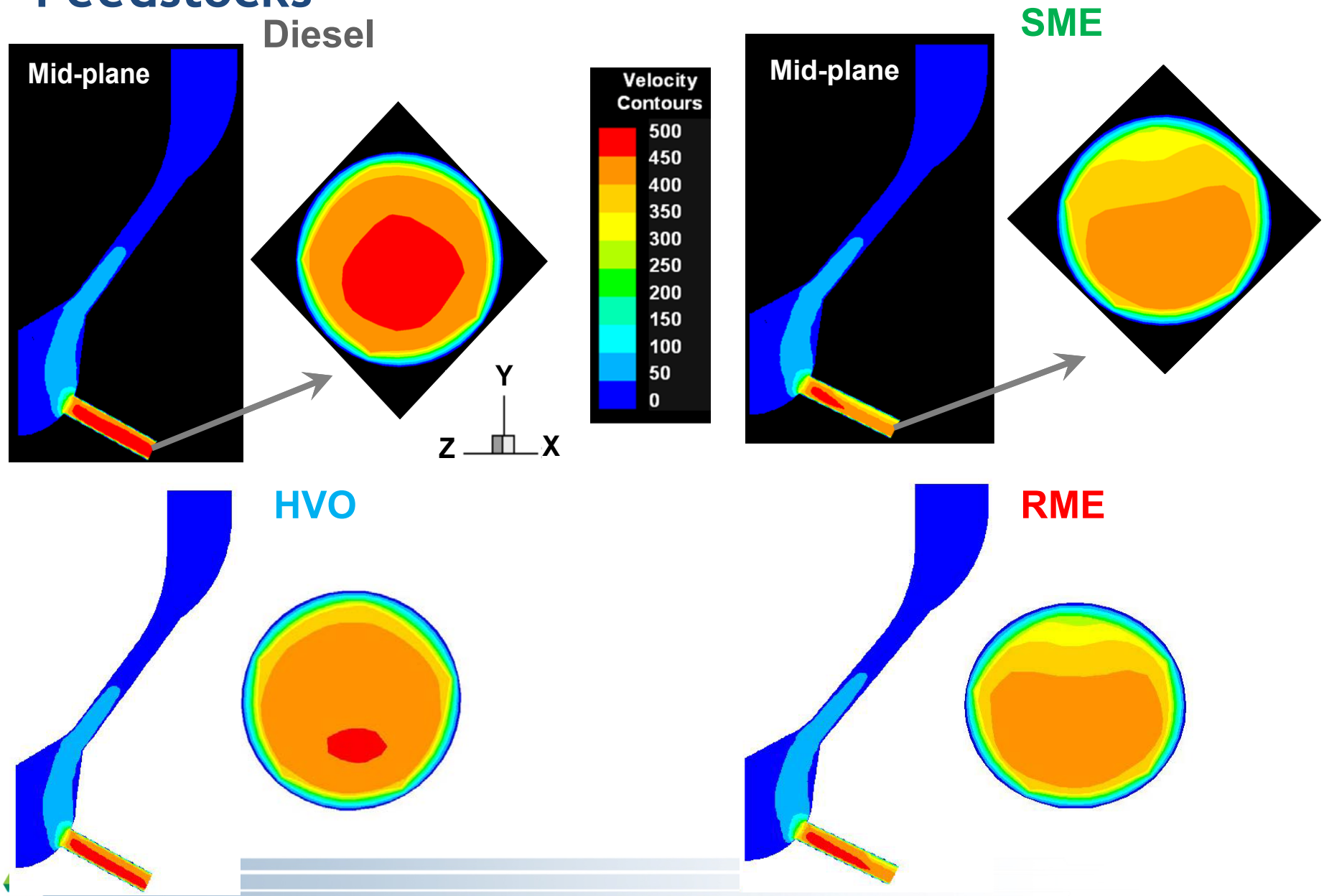
- Viscosity differences accentuated by accounting for fuel density (dynamic viscosity)
- Non-linear effect of temperature on viscosity
- Cuphea-ME behaves markedly different than other methyl esters
- Even at 398 K the viscosity of biodiesel is 2 times higher than that of diesel # 2

In-nozzle Cavitation with Biodiesel from different Feedstocks



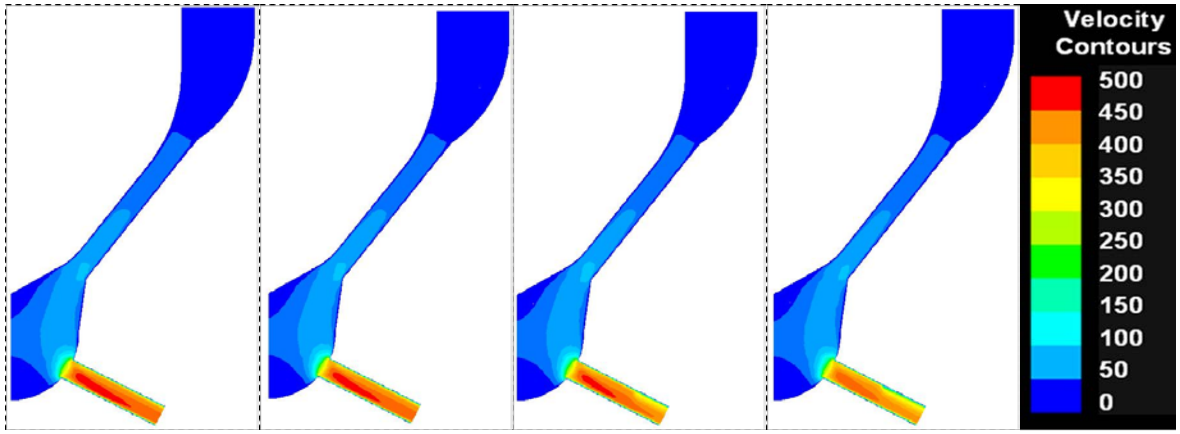
@ full needle open position (1 ms)

Velocity Distribution with Biodiesel from different Feedstocks



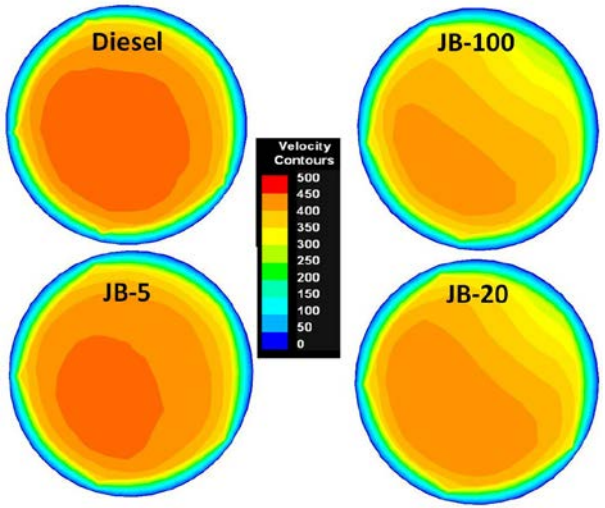
Jatropha, Karanja Characteristics vs. Diesel*

- Experimental spray work at IIT-Kanpur with Jatropha, Karanja and their blends with diesel fuel
- Nozzle flow simulations at Argonne to gain further insights into the influence of fuel properties on spray behavior
- Experimentally observed spray characteristics can be explained by the in-nozzle flow behavior



*Journal paper submitted to "Applied Energy"

Fuel	Spray tip penetration (mm)	Spray area (mm^2)	Cone angle (degree)
Diesel	12.02	27.82	15.86
JB5	12.55	30.52	17.35
JB20	13.06	33.82	18.79
JB100	13.88	35.41	19.41



Spray Combustion Modeling Set-up

Modeling Tool	CONVERGE
Dimensionality and type of grid	3D, structured with Adaptive Mesh Resolution
Spatial discretization approach	2nd order finite volume
Smallest and largest characteristic grid size(s)	Base grid size: 2mm Finest grid size: 0.125mm Gradient based AMR on the velocity and temperature fields. Fixed embedding in the near nozzle region to ensure the finest grid sizes
Total grid number	1.5 million for 0.125mm
Parallelizability	Good scalability up to 128 processors

Turbulence and scalar transport model(s)	**RNG k-ε**
Spray models	Breakup: KH-RT with breakup length concept Collision model: NTC, O'Rourke Coalescence model: Post Collision outcomes Drag-law: Dynamic model Dispersion: Stochastic Heat-transfer: Ranz and Marshall
Time step	Variable based on spray, evaporation, combustion processes

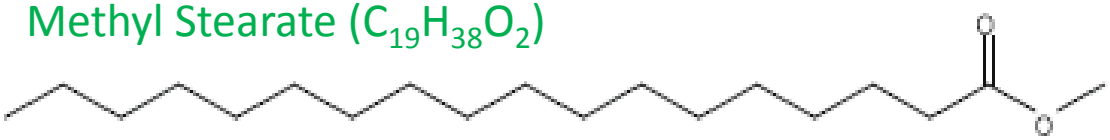
Turbulence-chemistry interactions model	**Direct Integration of detailed chemistry well-mixed (no sub-grid model)**
Time discretization scheme	PISO (Pressure Implicit with Splitting of Operators)
Chemistry acceleration	Analytical Jacobian

*** S. Som et al., Combustion and Flame 2010, Fuel 2010 & 2011, Energy and Fuels 2010 & 2011**

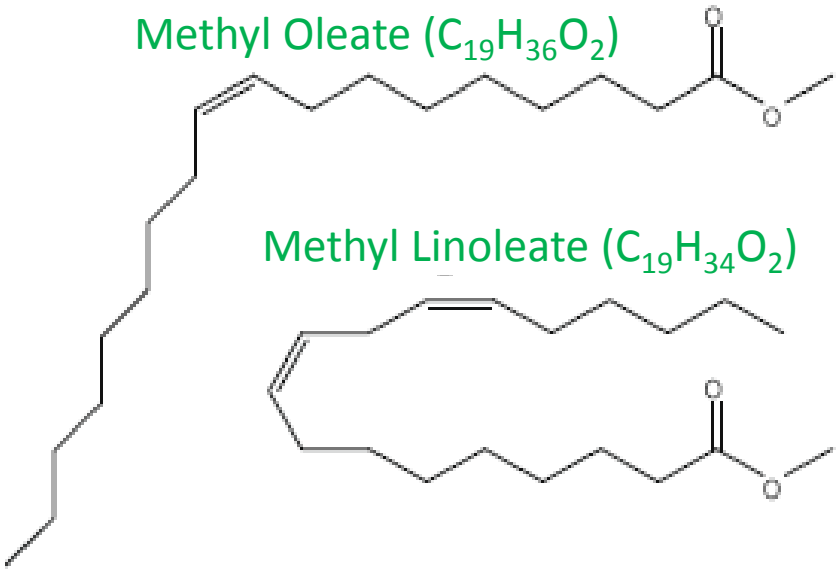
Approach to Biodiesel Surrogate Selection

Methyl Palmitate ($C_{17}H_{34}O_2$)

Methyl Stearate ($C_{19}H_{38}O_2$)

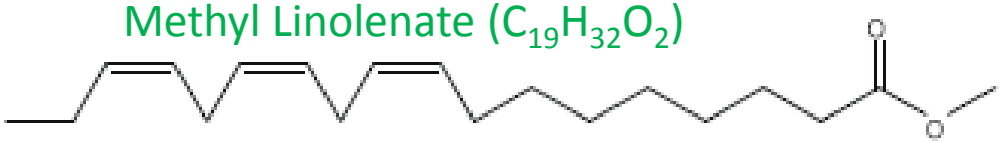


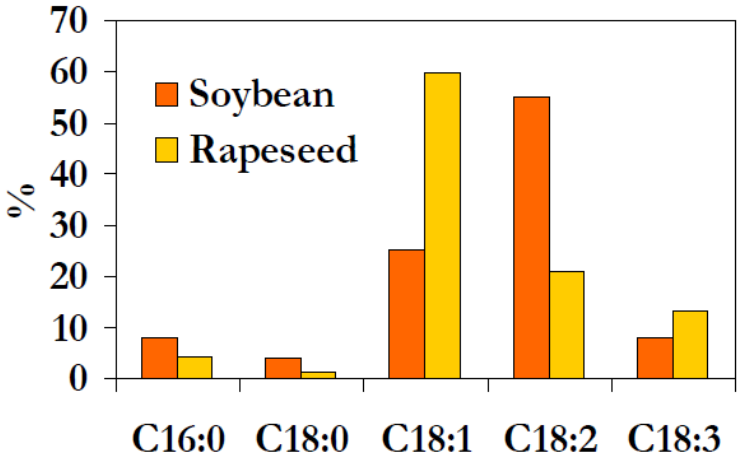
Methyl Oleate ($C_{19}H_{36}O_2$)



Methyl Linoleate ($C_{19}H_{34}O_2$)

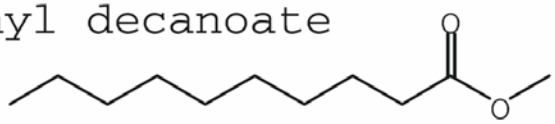
Methyl Linolenate ($C_{19}H_{32}O_2$)



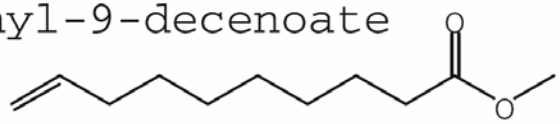


Biodiesel is a mixture of long-chain, oxygenated, unsaturated components

methyl decanoate

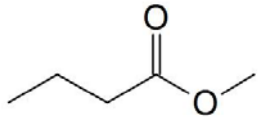


methyl-9-decenoate



n-heptane, n-C_7H_{16}

methyl butanoate



n-heptane, n-C_7H_{16}

Approach: Mechanism Reduction Methodology

Detailed Biodiesel Mechanism (from LLNL)
3329 species, 10806 reactions

~ 30 times reduction

DRG

Isomer lumping

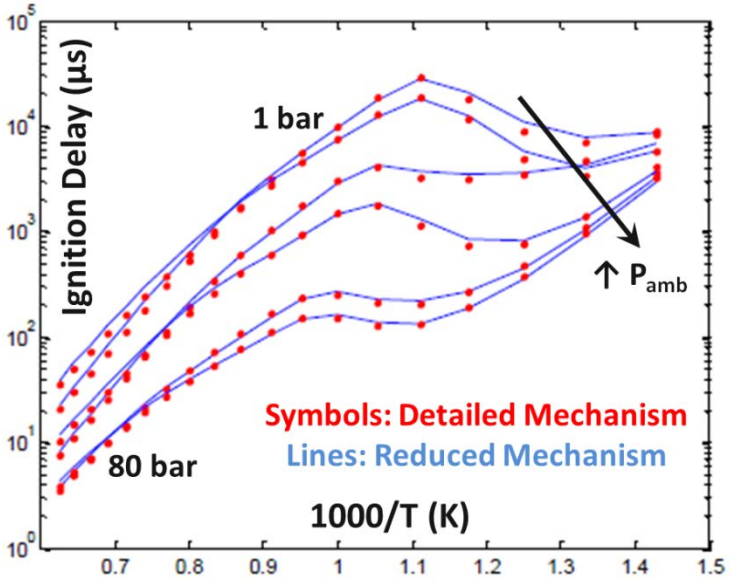
DRGASA & Error Cancelation

115 species, 460 reactions[1]

Computational times scales with N^2 ~ N^3

- Directed Relation Graph (DRG) and Directed Relation Graph Aided with Sensitivity Analysis (DRGASA) tools applied for mechanism reduction in collaboration with Prof. Tianfeng Lu et al. at University of Connecticut

Download mechanism
www.transportation.anl.gov/engines/multi_dim_model_combustion.html



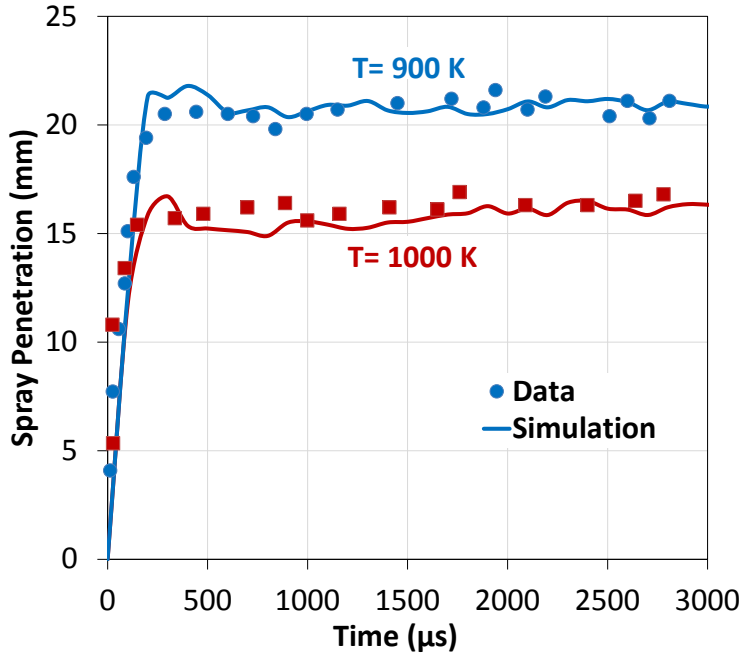
Range of operation:
- ✓ Pressure: 1-100 atm
- ✓ Equivalence ratio: 0.5-2.0
- ✓ Initial temperature: 700 – 1800 K

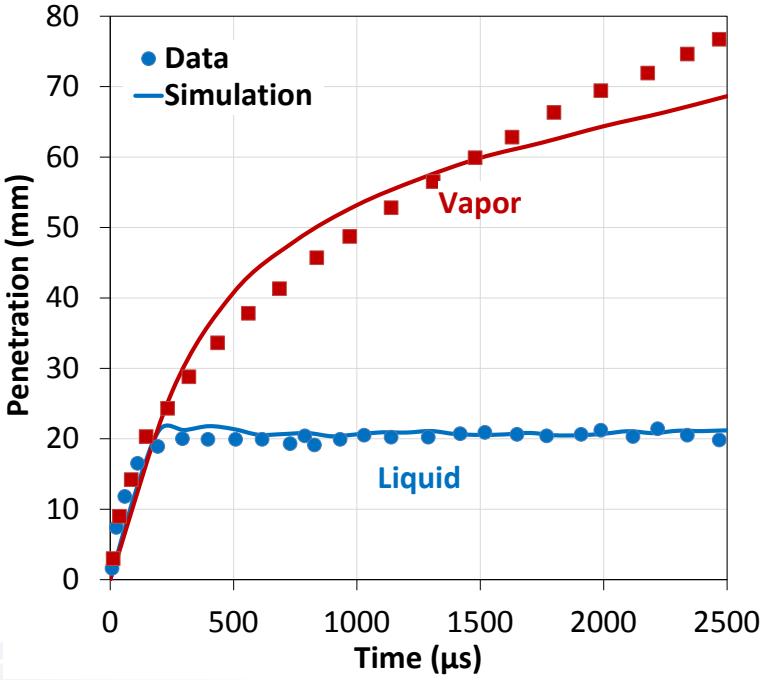
Soy-Biodiesel Spray Simulations

Injection & Ambient conditions for Biodiesel studies at Sandia*

Parameter	Quantity
Injection System	Bosch Common Rail
Nozzle Description	Single-hole, mini-sac
Duration of Injection [ms]	7.5
Orifice Diameter [µm]	90
Injection Pressure [Bar]	1400
Fill Gas Composition (mole-fraction)	N_2=0.7515, O_2=0.15, CO_2=0.0622, H_2O=0.0363
Chamber Density [kg/m³]	22.8
Chamber Temperature [K]	900, 1000
Fuel Density [kg/m³]	877
Fuel Type	Soy-Methyl Ester
Fuel Injection Temperature [K]	363

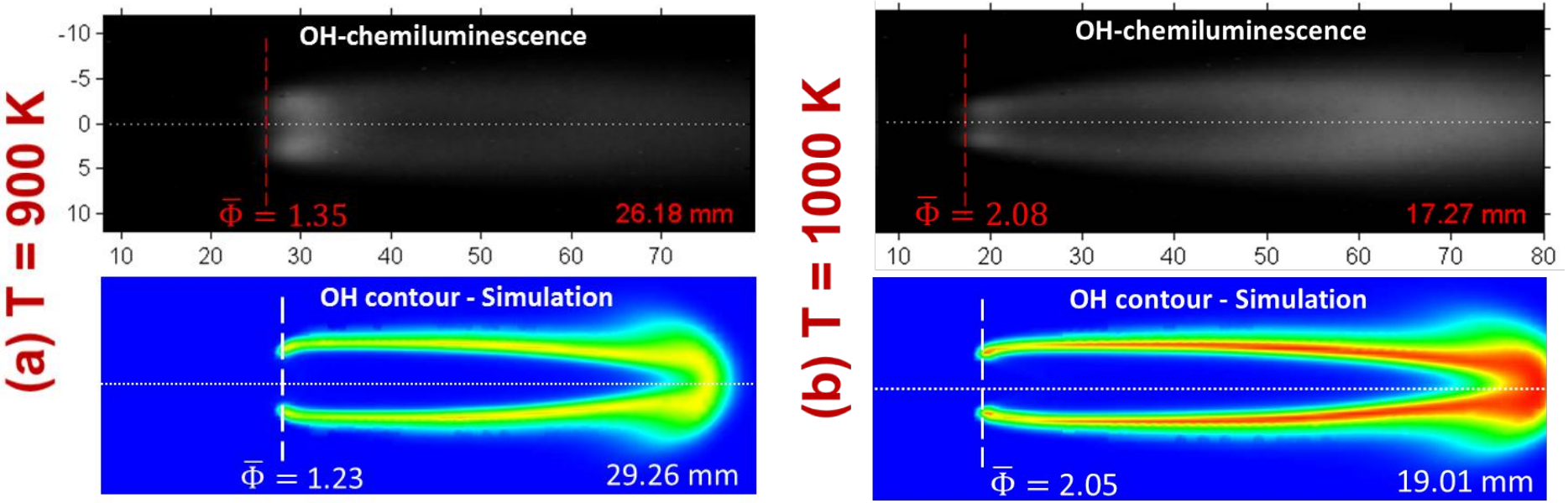
Experimental data*: JG Nerva, CL Genzale, S Kook, JMG Oliver, LM Pickett. International J. of Engine Research 2012





Non-reacting spray characteristics well predicted by the simulations!

Validation of Biodiesel Spray Combustion Simulations

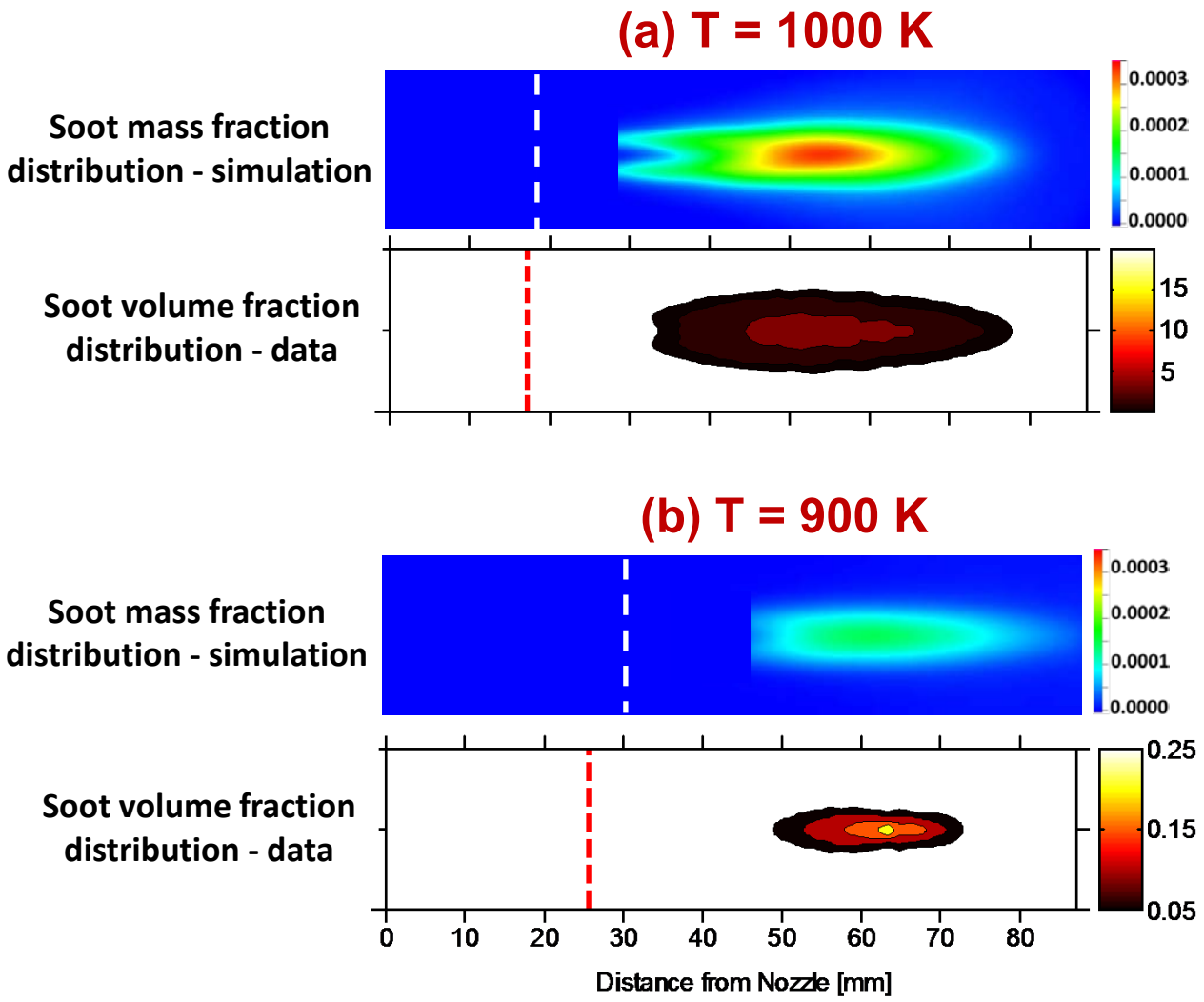


	Ignition Delay (ms)	Lift-off length (mm)	Equivalence Ratio	
Sandia Data	0.683	26.18	1.35	T = 900 K
115 species Mechanism	0.711	29.26	1.23	
Sandia Data	0.396	17.27	2.08	T = 1000 K
115 species Mechanism	0.411	19.01	2.05	

The 115 species reduced mechanism can capture the combustion characteristics very well

Prediction of Soot Distribution

115 species mechanism



C_2H_2 is used as a soot pre-cursor

Biodiesel Chemical Kinetic Mechanisms of Interest

Mechanisms	1 [1] (MD,MD9D,NHPT)	2 [2] (MD,MD9D,NHPT)	3 [3] (MB,NHPT)	4 [4] (MB,NHPT)
Reduction procedures	directed relation graph (DRG) + DRG-aided sensitivity analysis (DRGASA) w/ error cancellation + isomer lumping + 2nd round DRGASA	DRG w/error propagation (DRGEP) + isomer lumping + 2nd round DRGEP; for MD and MD9D separately, then combined	directed relation graph (DRG) + DRG-aided sensitivity analysis (DRGASA) + isomer lumping	removal of unimportant species in 0D sim.; combined w/ a skeletal NHPT mech. + rate parameters adjustments
Sample space	P: 1 to 100atm; φ: 0.5 to 2.0; T: 700 to 1800K	φ=0.5; T=800K	P: 1 to 100atm; φ: 0.5 to 2.0; T: 700 to 1800K	P:40 to 60 bar; φ: 0.4 to 1.5; T:650 to 1350 K;
# of species	115	77	145	41
# of reactions	460	209	869	150
Surrogate mixture composition	25% MD + 25% MD9D + 50% NHPT	25% MD + 25% MD9D + 50% NHPT	20% MB + 80% NHPT	33% MB + 67% NHPT

[1] Z. Luo, et al. Fuel 99 (2012) 143–153 {115 species mechanism, developed in the current study}

[2] J.L. Brakora, et al. SAE 2011-01-0831

[3] W. Liu, et al. Proc. Combust. Inst., 34 (2013) 401-409

[4] J.L. Brakora, et al. SAE 2008-01-1378

3-D Turbulent Spray Combustion Simulations

	Ignition Delay (ms)	Lift-off length (mm)	Equivalence Ratio at lift-off location	
Sandia Data*	0.683	26.18	1.35	
Mechanism 1	0.711	29.26	1.23	T = 900 K
Mechanism 2	0.280	14.18	2.86	
Mechanism 3	0.835	32.82	1.19	
Mechanism 4	0.580	22.1	1.53	
Sandia Data*	0.396	17.27	2.08	
Mechanism 1	0.405	19.01	2.05	
Mechanism 2	0.150	10.12	3.12	T = 1000 K
Mechanism 3	0.630	22.76	1.98	
Mechanism 4	0.225	12.66	2.67	

Ignition delay: the time from actual start of injection to the time when temperatures above 2000 K are first observed in any computational cell.

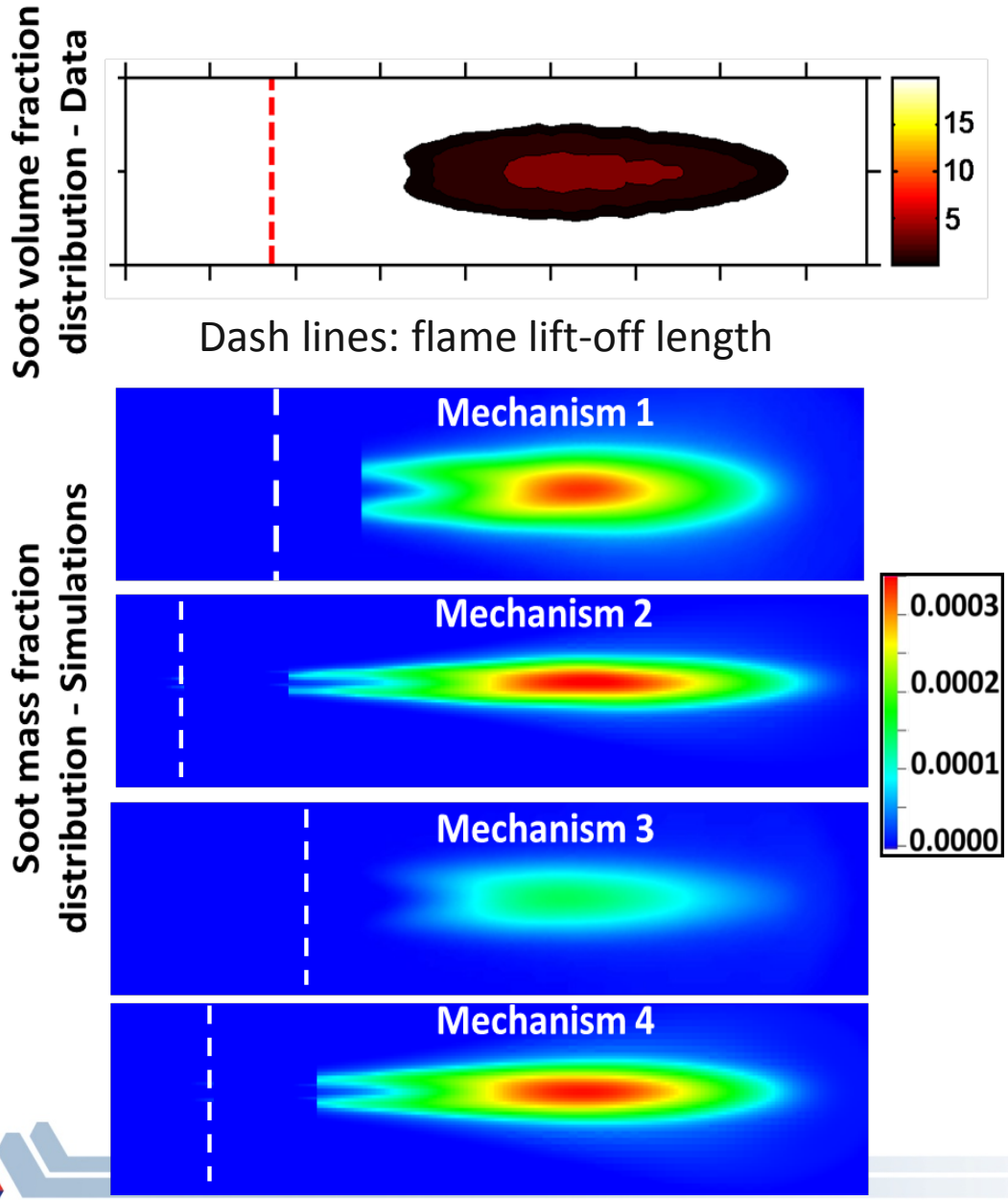
Flame lift-off length: distance from the tip the injector to the nearest upstream location of Y_{OH} = 0.05% contour.

φ @ lift-off : averaged over a transverse line @ lift-off location

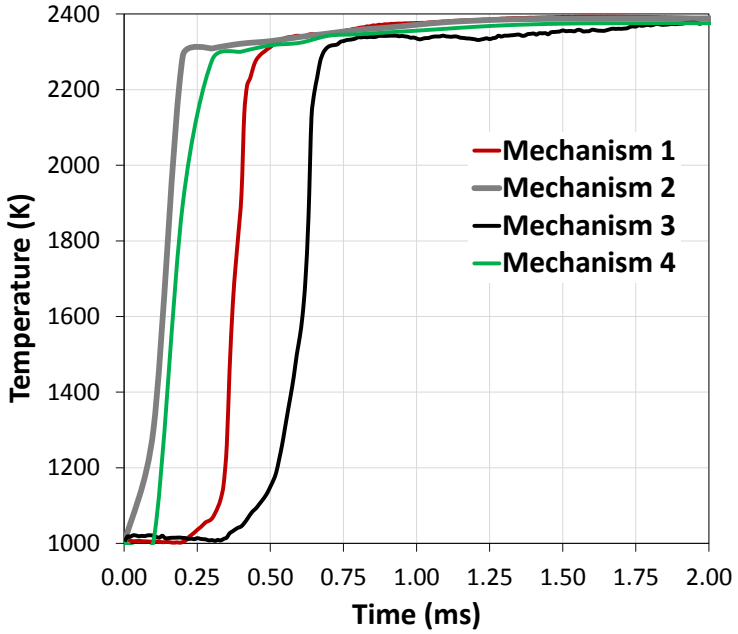
Based on reduction procedure and mechanism size better prediction with mechanism 1 is expected.

* C.L. Nerva, et al. *International Journal of Engine Research* (2012)

Comparison of Combustion and Soot Characteristics



- C_2H_2 is used as a precursor for soot formation in simulations
- Qualitative comparison as soot density unknown
- Equilibrium flame temperatures predicted are very similar between different mechanisms although ignition characteristics were significantly different



Collaborations

Argonne National Laboratory

Engine and Emissions Group: (Provide data for model validation)

Convergent Science Inc. (Algorithm and code development in CONVERGE)

Sandia National Laboratory (Provide experimental data for biodiesel fuel)

Lawrence Livermore National Laboratory (Mechanism development)

University of Connecticut (Mechanism Reduction)

National Renewable Energy Laboratory (Experimental data with IQT for different biodiesel surrogates of interest)

US Department of Agriculture (Cuphea Methyl Ester samples for engine testing)

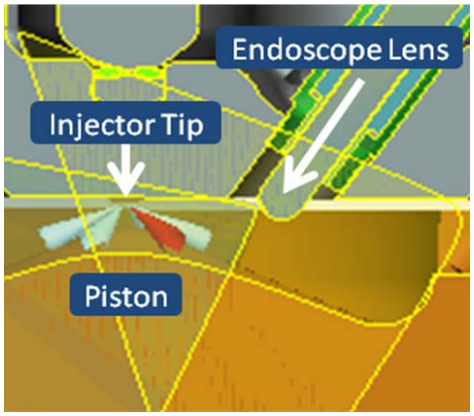
Indian Institute of Technology (Jatropha and Karanja biodiesel fuels for engine testing)

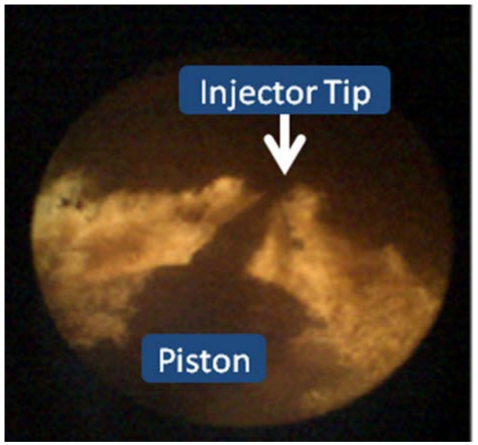
Response to Previous Year Reviewer Comments

Not applicable

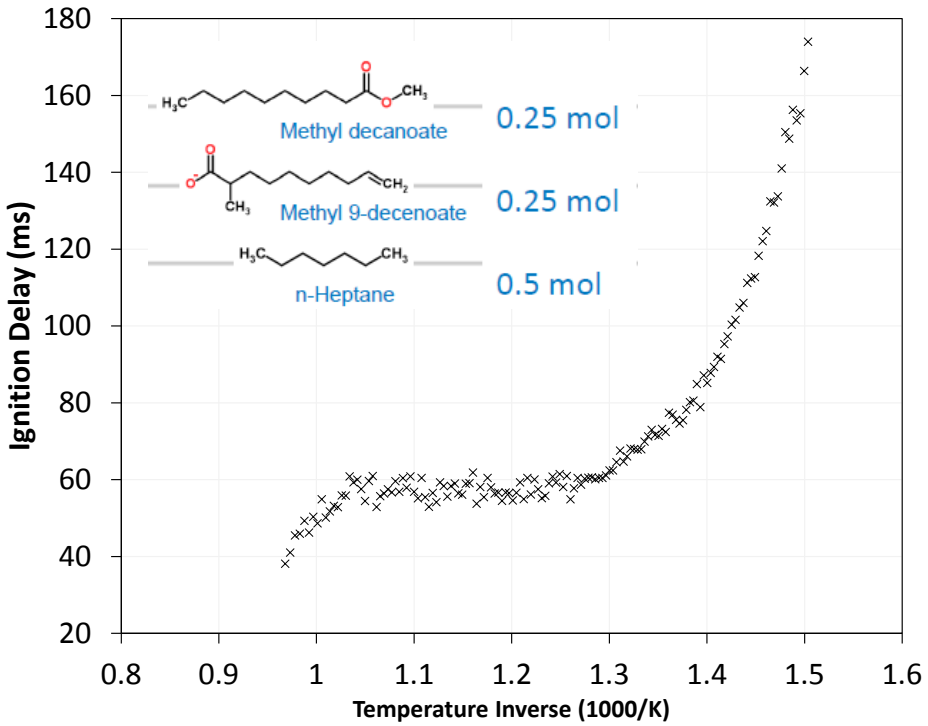
Future Work: Exploring Cuphea Derived Biodiesel with USDA

- Cuphea biodiesel is derived from ornamental plants and has good characteristics for transportation applications
- USDA provided with 5 gallons of Cuphea biodiesel for engine testing
- Planned experimental Work
  - Compare combustion characteristics of Cuphea and diesel fuels
  - Start of injection sweep to characterize the ignition and combustion characteristics
  - 2-color optical pyrometry for in-cylinder visualization
- Planned simulation work
  - Develop a reduced chemical kinetic mechanism for Cuphea methyl ester in collaboration with Lawrence Livermore National Laboratory
  - Validate engine simulations against the experimental test matrix for diesel and Cuphea fuels



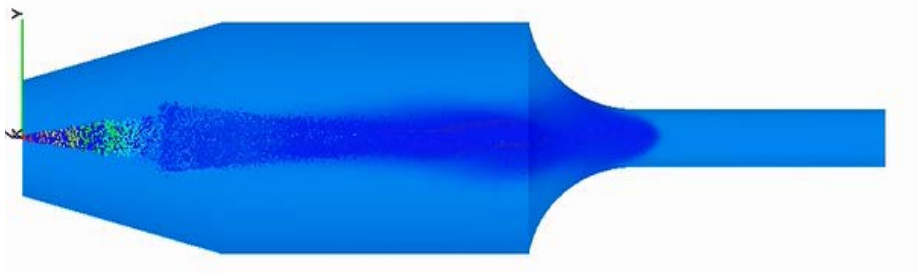


Future Work: Simulating the Ignition Quality Tester

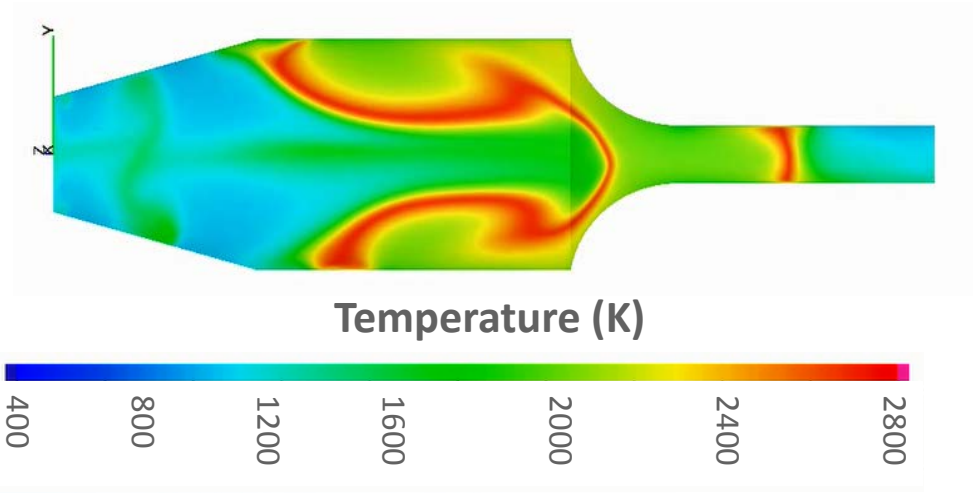


Project Details

- NREL (Brad Zigler et al.) has provided us measurements of the ignition characteristics of the individual biodiesel surrogates in the **Ignition quality tester (IQT) device**
- Argonne will perform **high-fidelity HPC simulation of the IQT to validate the biodiesel component sub-mechanisms**
- Sample simulation results are shown



Spray Droplet Distribution inside the IQT



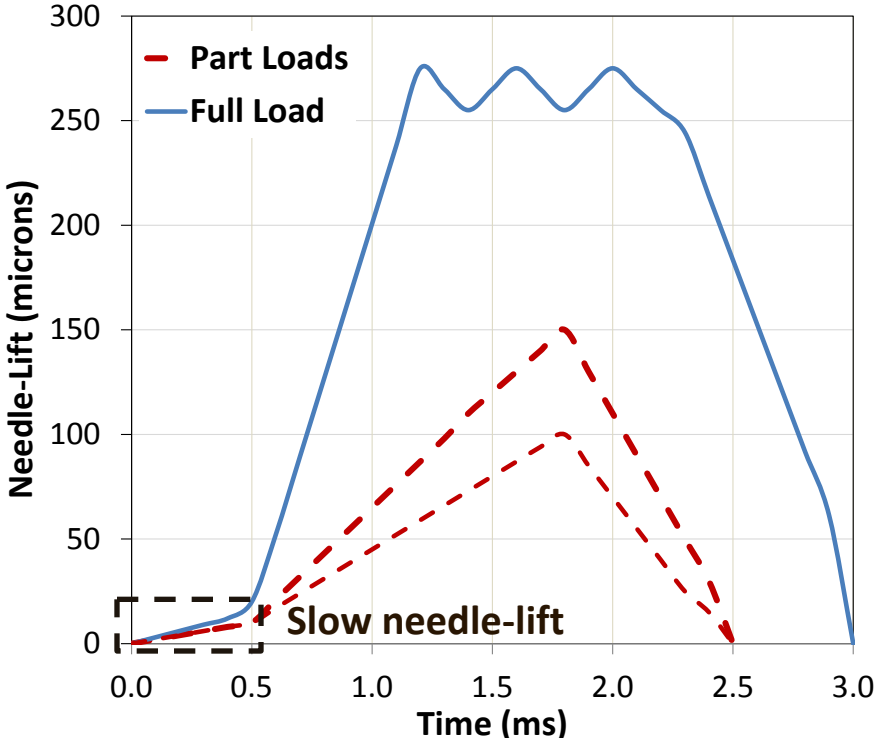
Summary

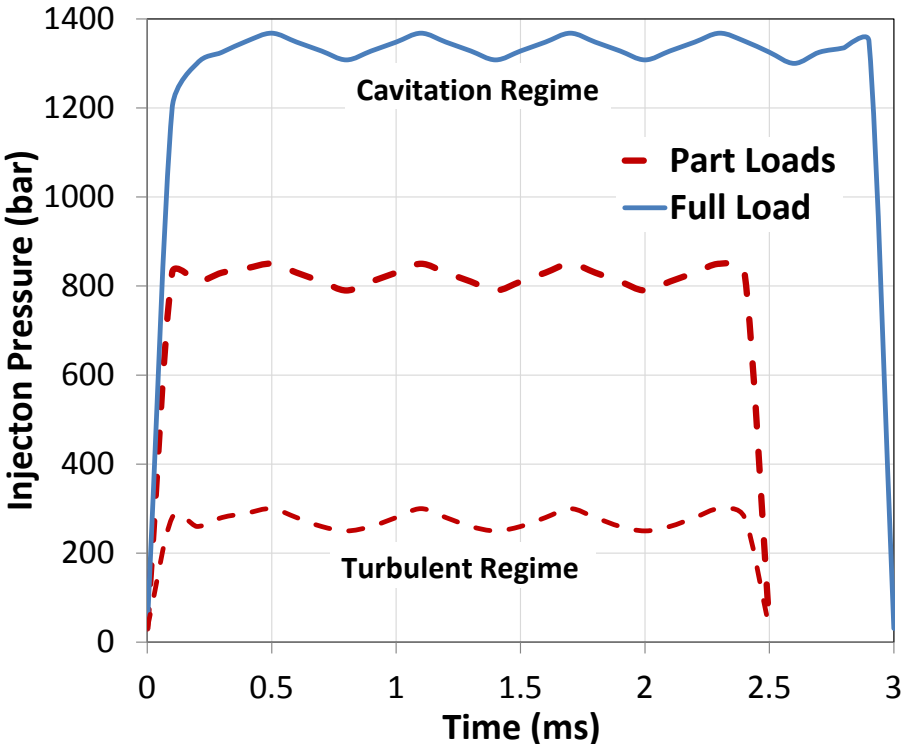
- **Objective**
  - Development of predictive nozzle flow, spray, and combustion modeling approaches aided by comprehensive validation for biodiesel fuels of interest
- **Approach**
  - Development and validation of reduced chemical kinetic models for CFD simulations with biodiesel fuels
- **Technical Accomplishment**
  - Differences in nozzle flow characteristics were observed between biodiesel from different feedstocks and diesel fuel. These differences may have a profound influence on the spray and combustion characteristics
  - Reduced chemical kinetic model (for a three component surrogate) developed and extensively validated against experimental data
  - Different mechanisms available in literature for biodiesel combustion are compared against the new reduced mechanism and against experimental data
- **Collaborations and coordination**
  - Experimental data from in-house, NREL, and Sandia National Laboratory
  - Simulation collaboration with Lawrence Livermore National Laboratory and University of Connecticut
  - Different biodiesel fuels from USDA and IIT-K
- **Future Work - FY14**
  - Experimental and simulation studies with Cuphea Methyl Ester as a suitable “drop-in” fuel
  - Simulating the IQT from NREL for further validating reduced reaction mechanism for biodiesel fuels

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.)

Boundary Conditions

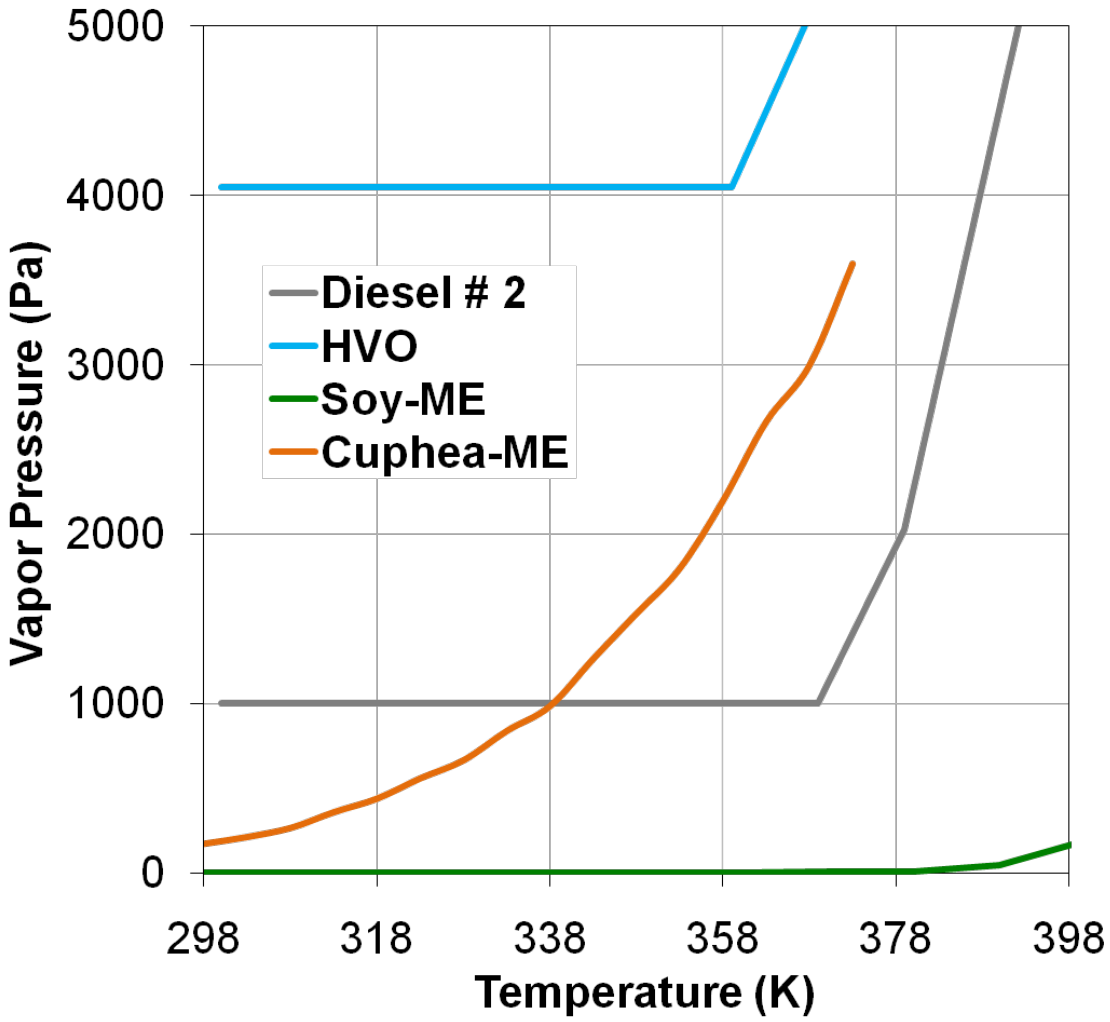




Kastengren et al. ASME-ICES2009-76302

- Full needle opening (275 µm) is characteristics of long injection durations and higher load conditions
- Part load conditions, characterized by smaller durations of injection, needle does not open completely
- Needle opens very slowly for the first part of injection i.e., t < 0.5 ms
- Injection pressures for **cavitation and turbulent regimes** based on diesel # 2 (Som et al. Fuel 2010)

Fuel Properties: Vapor Pressure vs. Temperature



Cavitation (phase-change) occurs when local pressure inside the injector nozzle orifice is below the vapor pressure of fuel!

Fuel Properties Boiling/Distillation Curves