Nozzle Flow Characterization of Alternate Fuels for Compression Ignition Engine Applications

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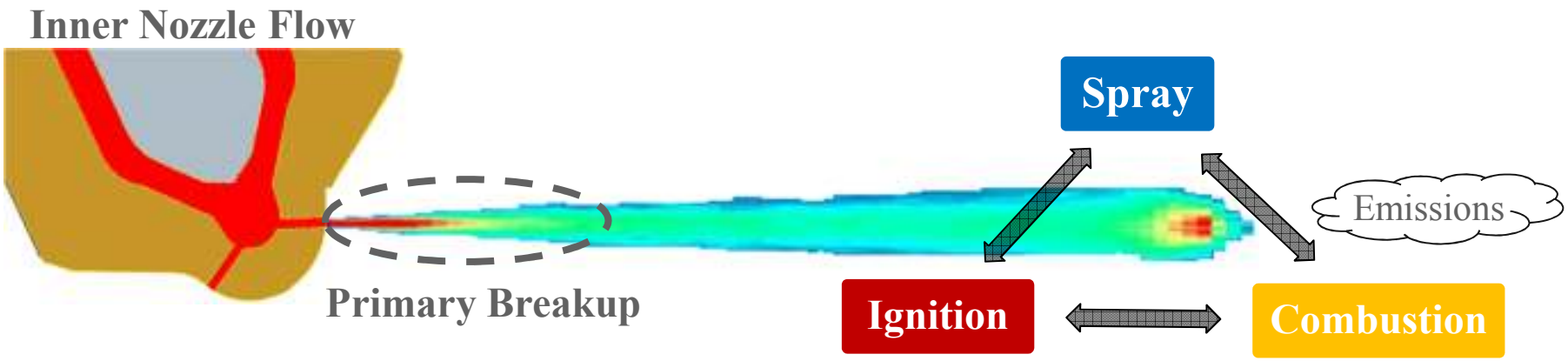
Fuel Injection and Sprays – Modeling (Part 2 of 2)

SAE 2011 World Congress

Modeling Approach

Influence of Physical and Chemical properties of fuel



- **KH-ACT** primary breakup model:
  Aerodynamics, Cavitation, Turbulence
- **Detailed Chemistry***:
  n-heptane : **Diesel surrogate**
  Methyl Decanoate: **Biodiesel surrogate**

* 9am Multi-dimensional Engine Modeling Session

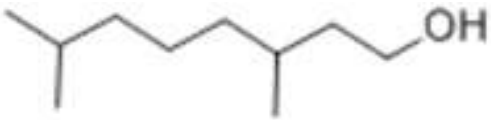
- Measure fuel properties such as density, viscosity, surface tension, vapor pressure, heat of combustion, heat of evaporation, distillation curve etc. for different alternate fuels
- Predict differences in inner-nozzle flow behavior of these fuels in terms of cavitation inception, turbulence levels, injection velocity, discharge coefficient etc.

Provide boundary conditions for spray and combustion simulations for different fuels !

Fuel of Interest

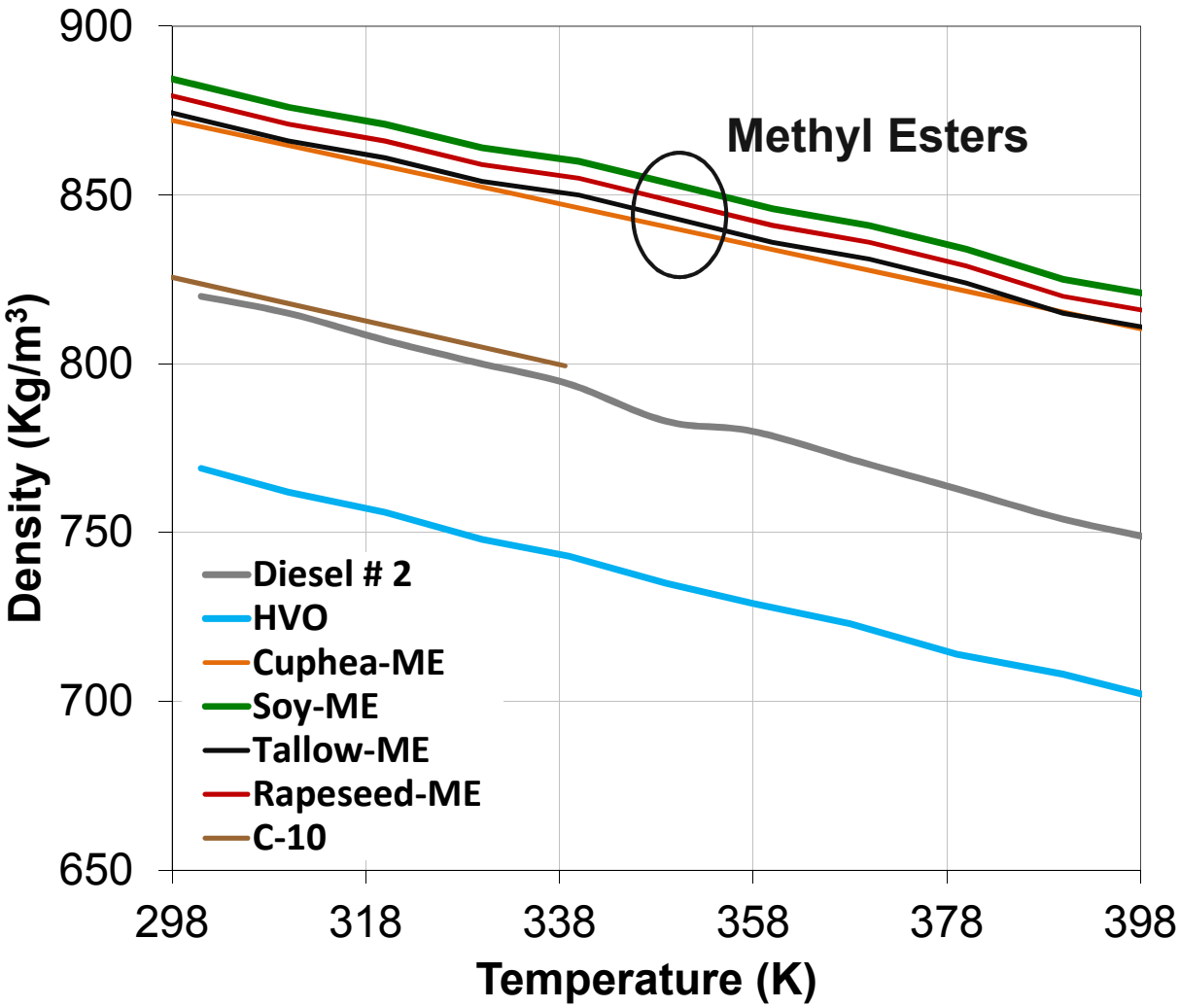
- Diesel # 2 properties obtained from literature
- Soy Methyl Ester (SME): prevalent in North America - Peter Cremer NA
- Rape-seed Methyl Ester (RME): prevalent in Europe – Properties obtained from Literature
- Cuphea Methyl Ester (CuME): explored by USDA - Knothe et al. Energy and Fuel 2009
- Hydro-treated Vegetable Oil (HVO): Helsinki University of Technology - Gong et al. SAE 2010-01-0739
- Geraniol is being explored at Argonne as an blending agent to diesel fuel

($C_{10}H_{22}O$) 3,7-DiMethyl-1-Octanol



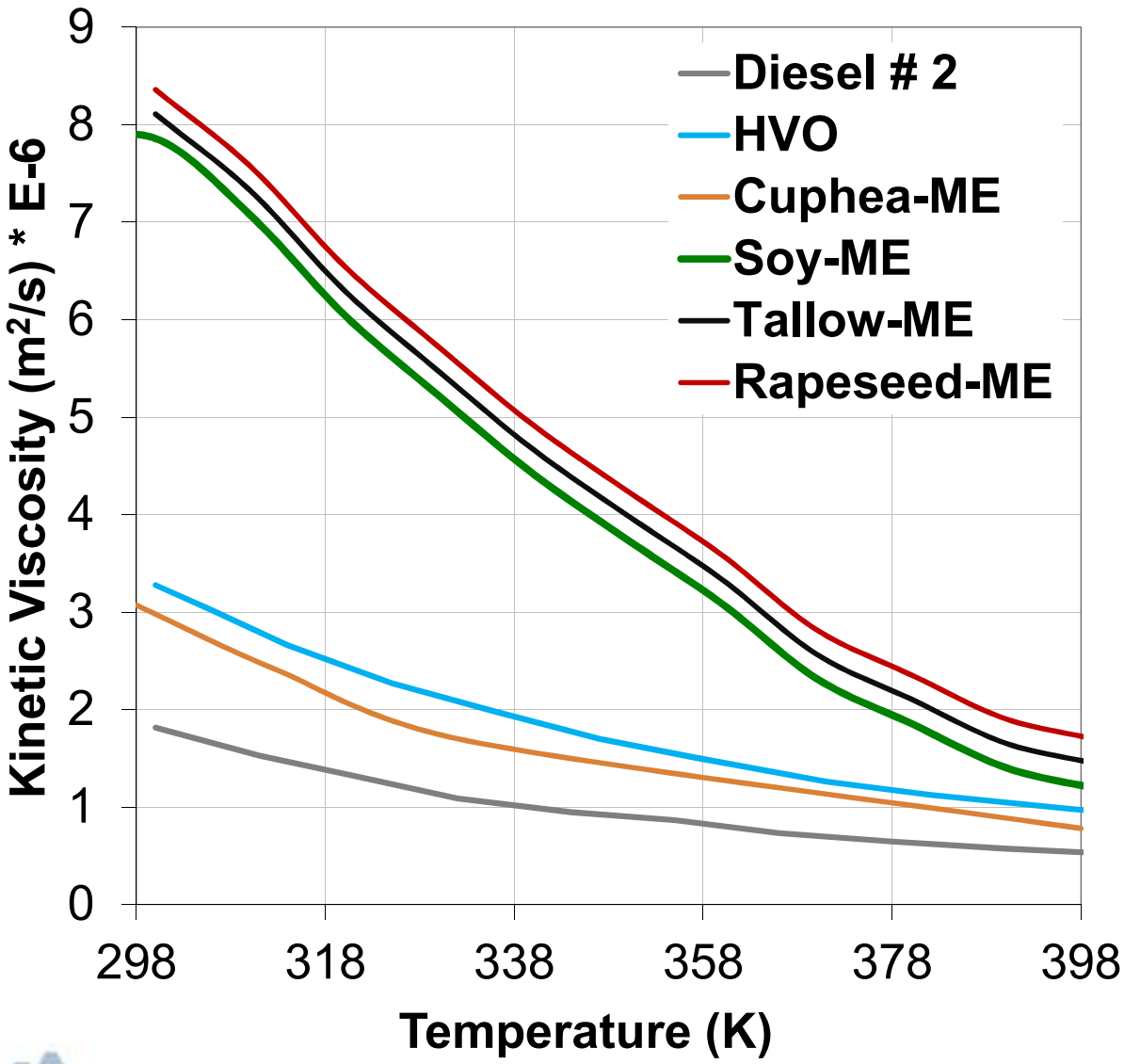
Fuel Property	Diesel	SME	RME	CuME	HVO	Geraniol
Carbon Content [wt %]	87	76.74		75.79	85	75.82
Hydrogen Content [wt %]	13	12.01		12.05	15	13.90
Oxygen Content [wt %]	0	11.25		12.16	0	10.28
Heat of Combustion [MJ/Kg]	42	37.4	39.7	34.8	44	41.4
Heat of Vaporization [KJ/Kg]	361	336		85	227	242
Cetane Number	40-45	46-55	54	56	80-89	28.05
Surface Tension @ 298 K [N/m]	0.0250	0.0315	0.0254	0.0312	0.0125	0.029

Density vs. Temperature



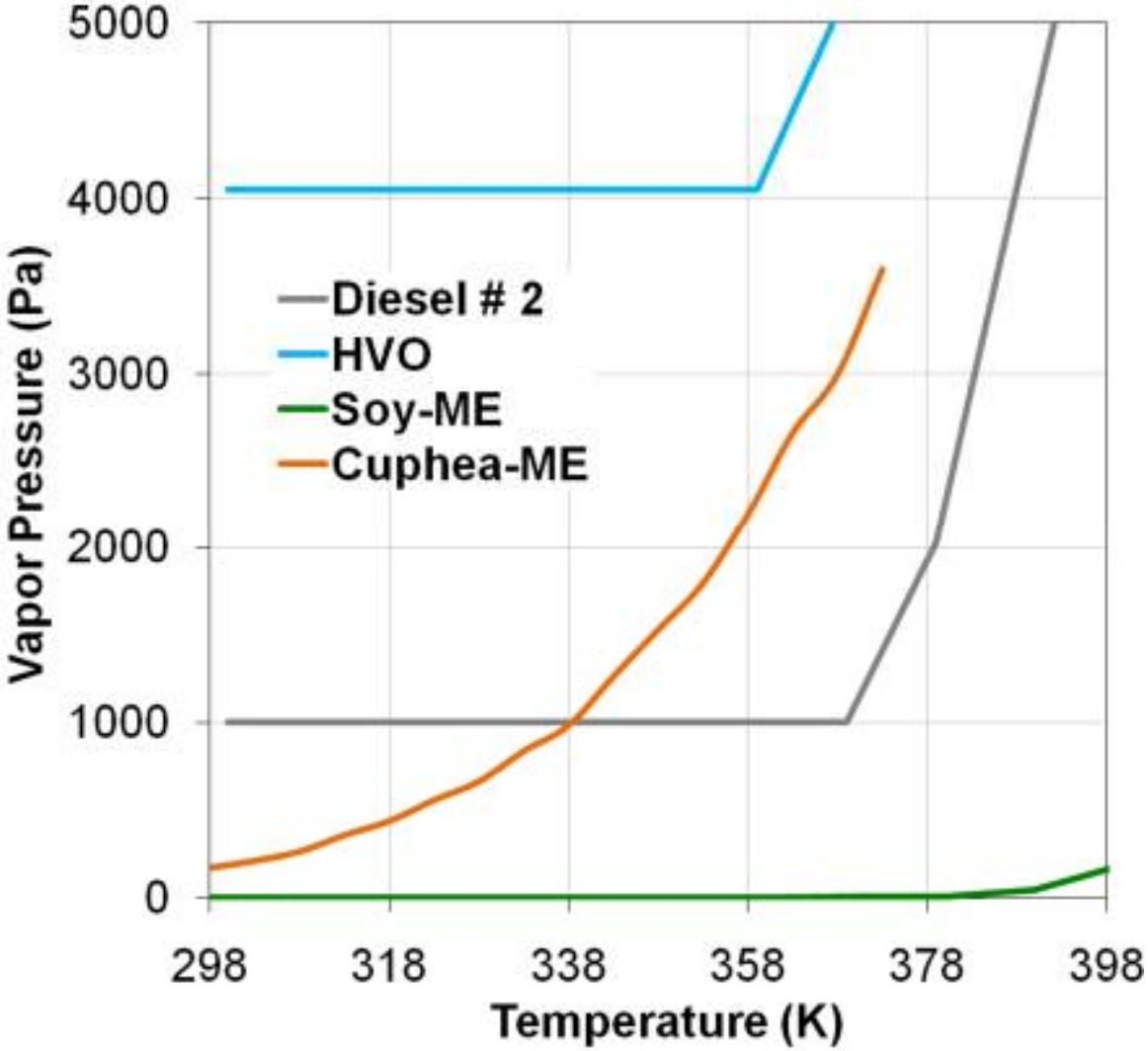
- Linear effect of temperature on density
- Methyl esters have similar densities

Kinematic Viscosity vs. Temperature



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

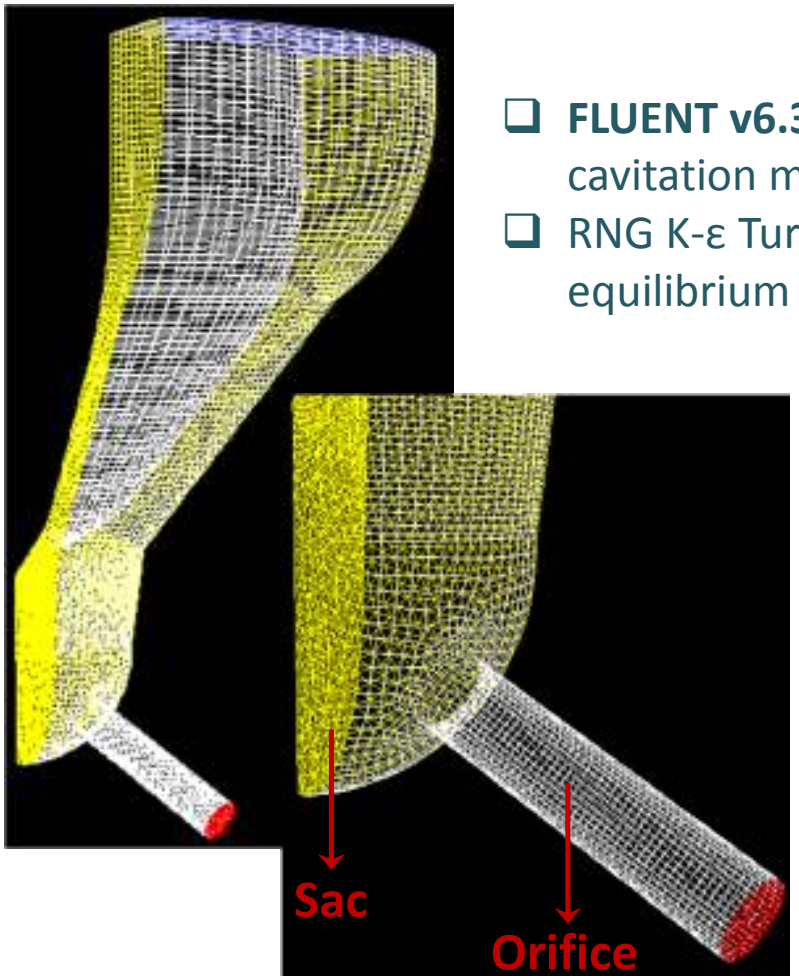
Vapor Pressure vs. Temperature



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

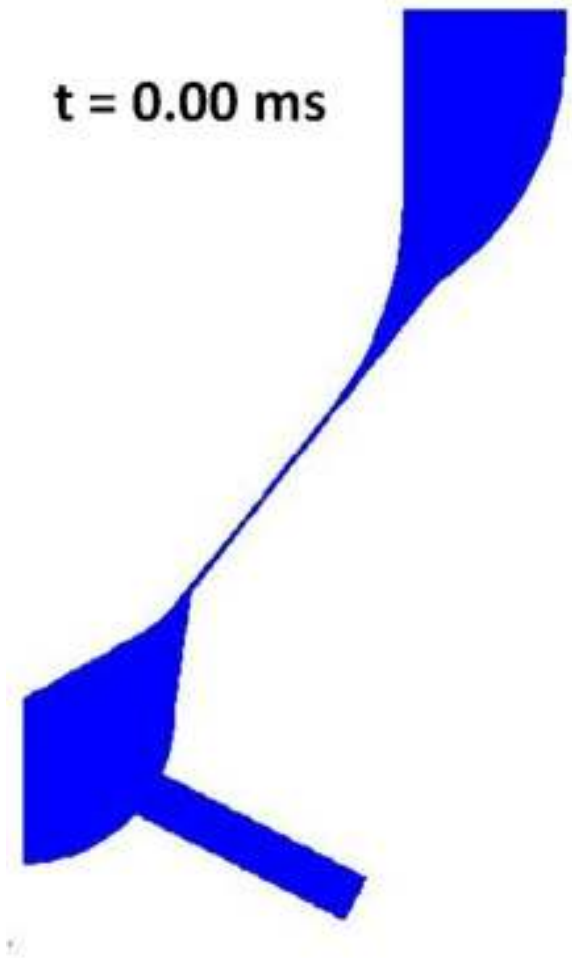
Mini-Sac Nozzle Grid Generated

Front View



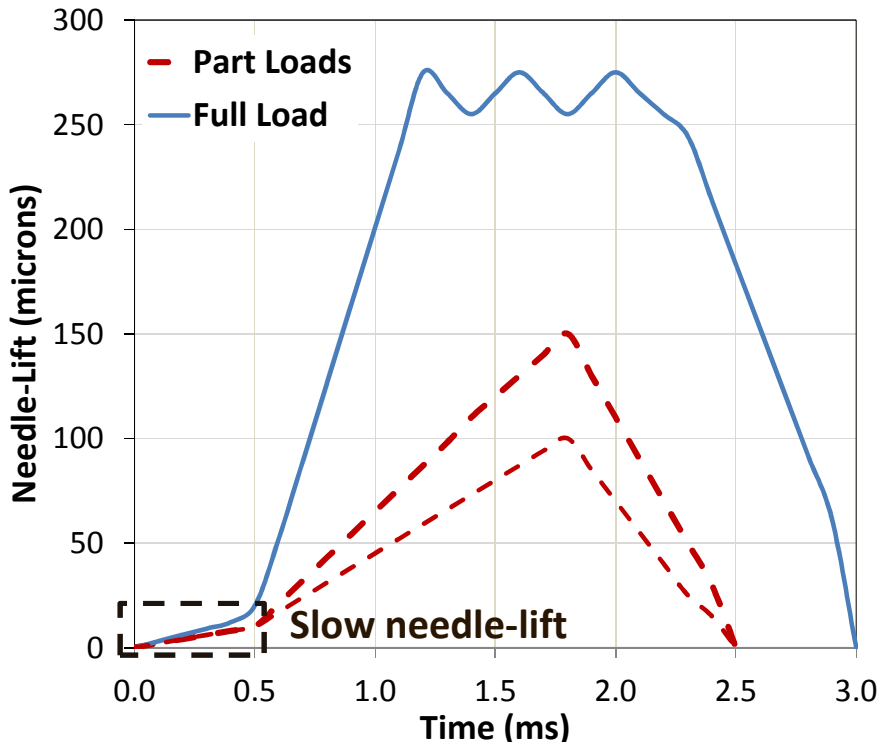
- **FLUENT v6.3**: Mixture based cavitation model
- RNG K-ε Turbulence model, non-equilibrium wall-functions

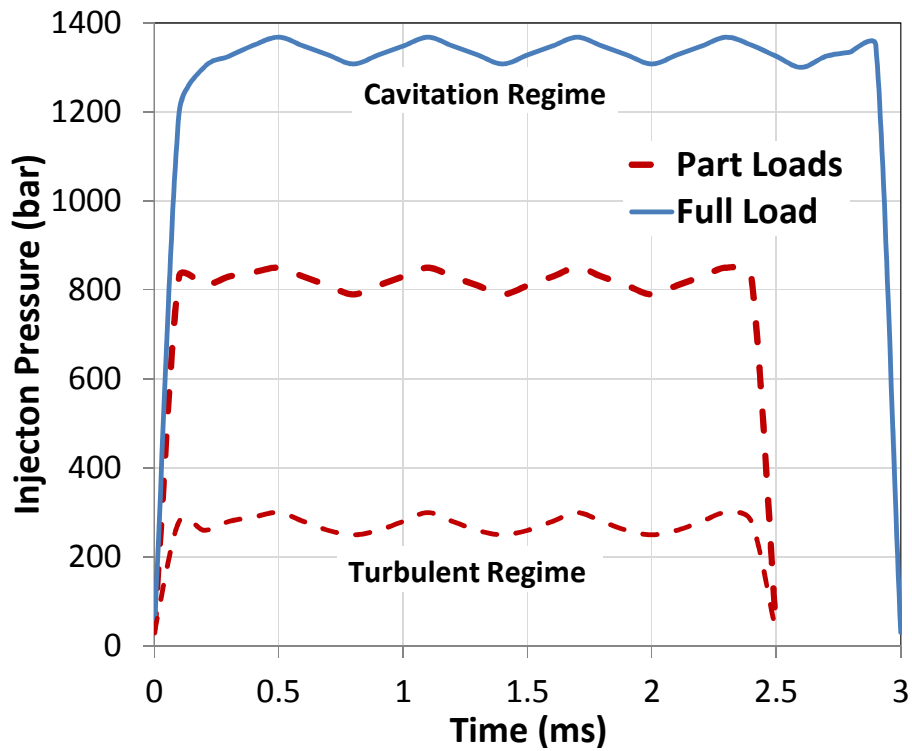
D = 169 µm
Cylindrical
Non-hydroground
L/D=4.2



1) S. Som, A.I. Ramirez, D.E. Longman, S.K. Aggarwal, ***Fuel*** **90: 1267-1276, 2011**
2) S. Som, D.E. Longman, A.I. Ramirez, S.K. Aggarwal, ***Fuel*** **89: 4014-4024, 2010**

Boundary Conditions

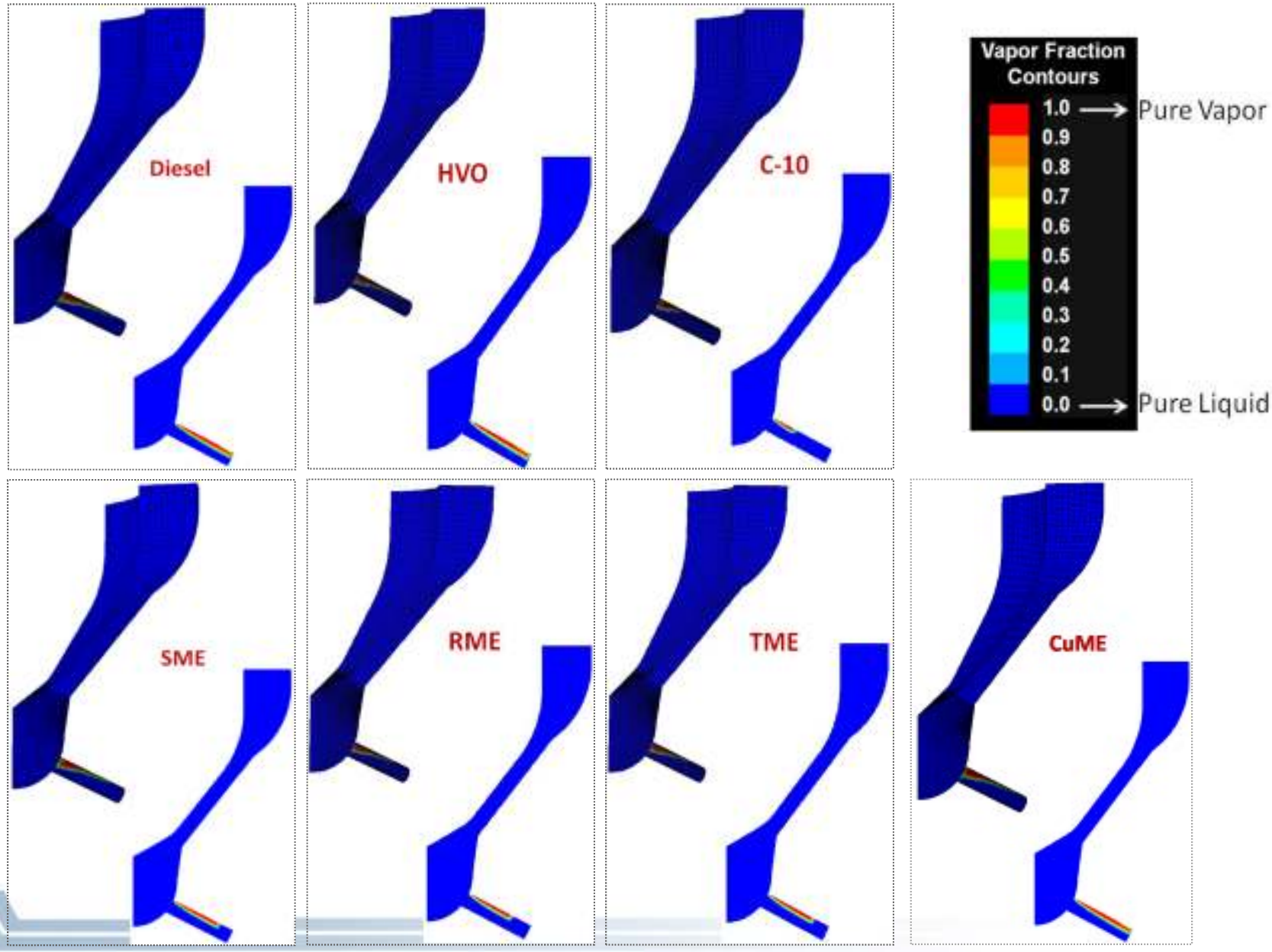




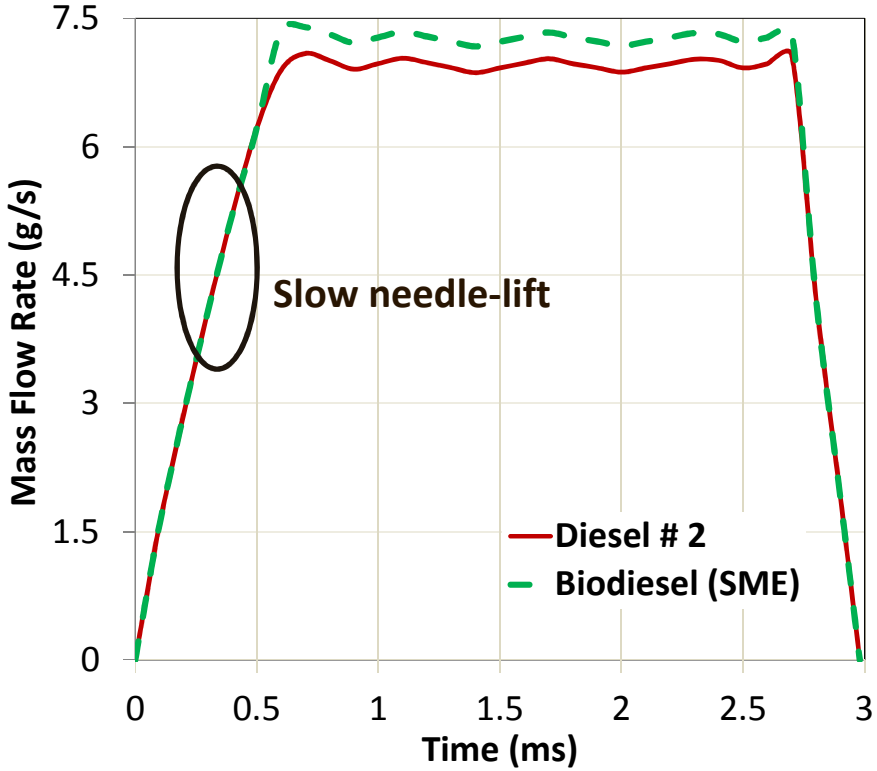
Kastengren et al. ASME-ICES2009-76302

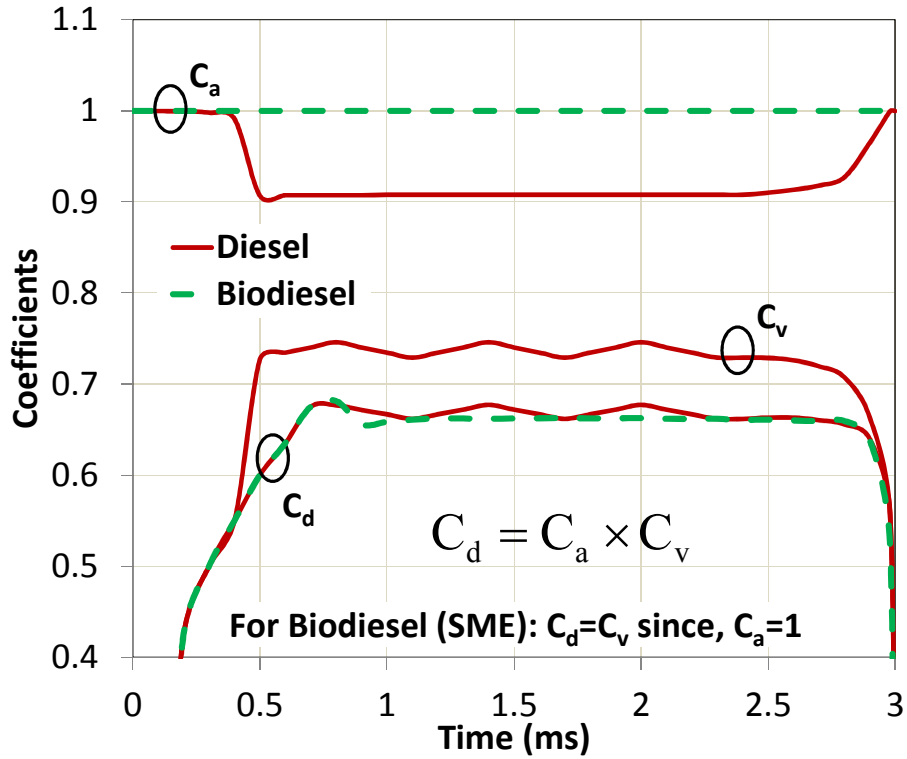
- Full needle opening (275 µm) is characteristics of long injection durations and higher load conditions
- Part load conditions, characterized by smaller durations of injection, needle does not open completely
- Needle opens very slowly for the first part of injection i.e., t < 0.5 ms
- Injection pressures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

Vapor Distribution under Cavitation Regime



Transient Profiles under Cavitation Regime



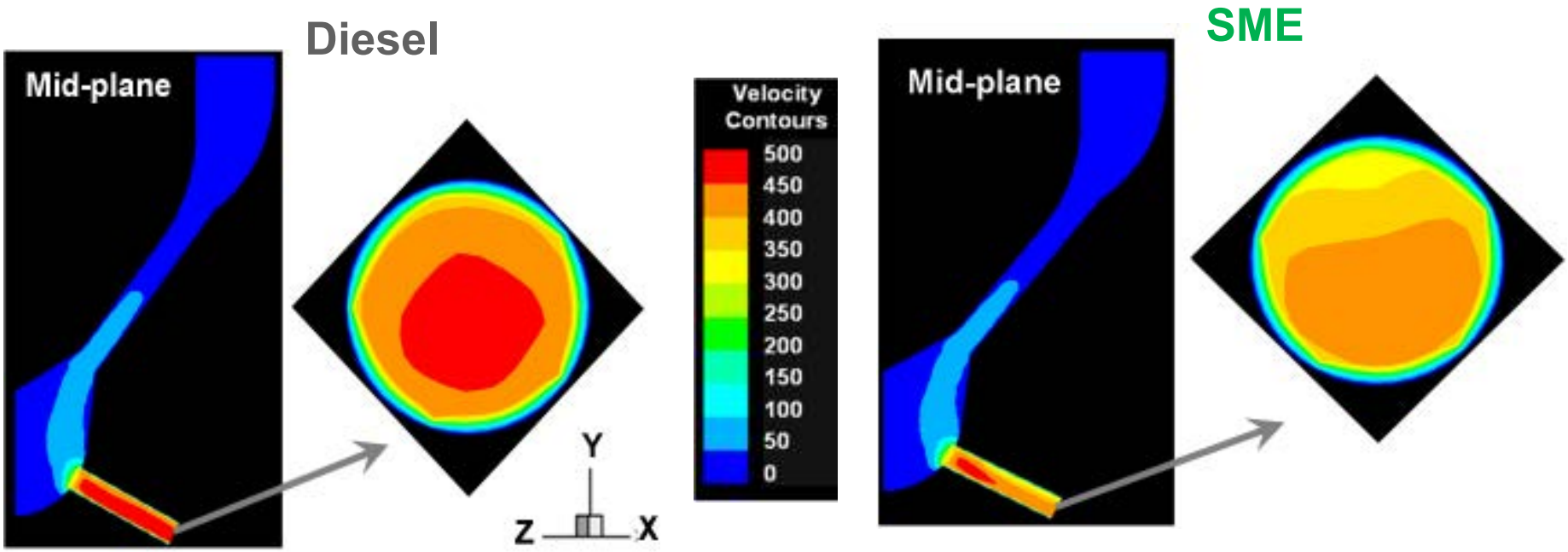


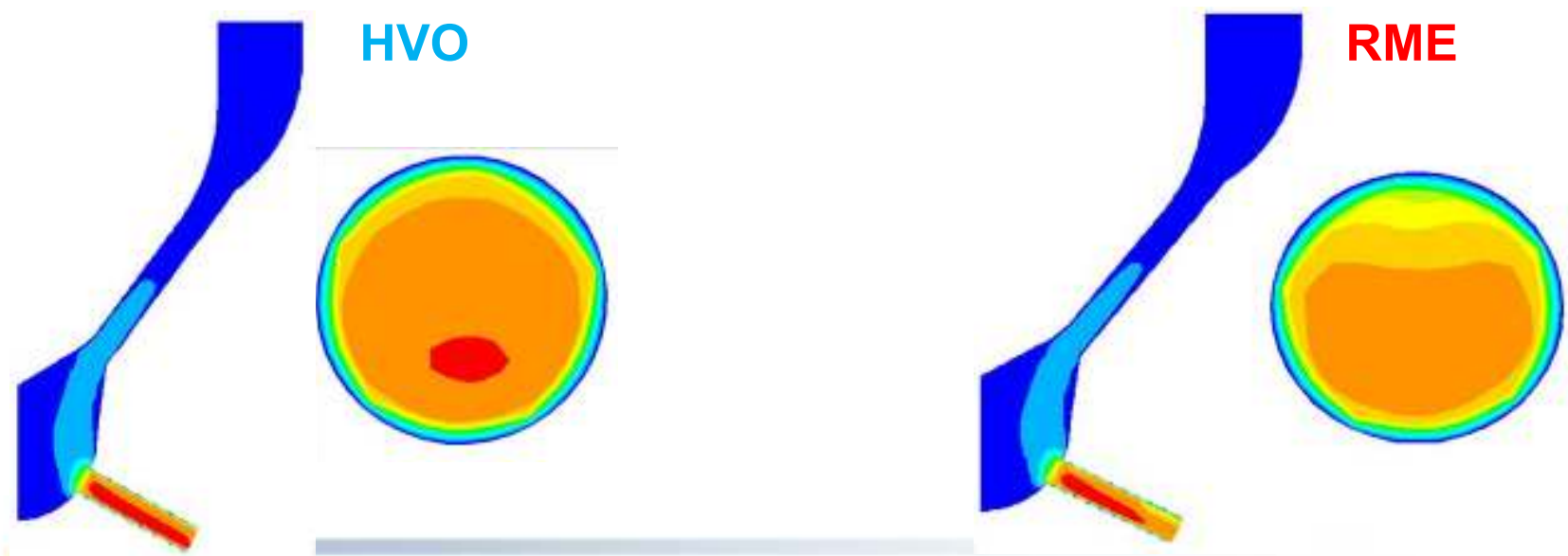
- **Mass flow rate depends on the competition between:**
  a) Extent of cavitation at the nozzle exit
  b) Nozzle exit velocity
  c) Liquid density of fuel
- **Mass flow rate of biodiesel (SME) is marginally higher**
- **Discharge coefficient is similar for both fuels** due to higher theoretical mass flow rates for SME

$$\left(\dot{m}_{fuel}\right)_{cal} = \rho_{fuel} A_{exit} V_{cal}$$

$$\left(\frac{\dot{m}_{SME}}{\dot{m}_{Diesel}}\right)_{th} \propto \sqrt{\frac{\rho_{SME}}{\rho_{Diesel}}}$$

Velocity Distribution under Cavitation Regime



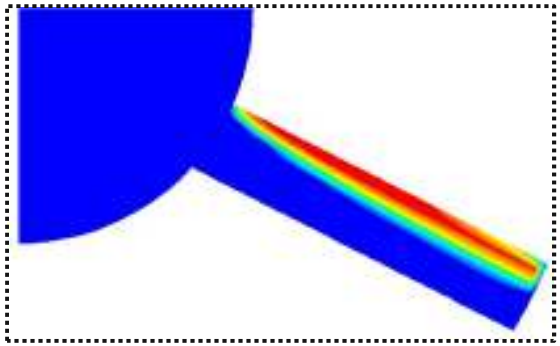


Flow Characteristics under Cavitation Regime

Fuel Property	Diesel	HVO	CuME	SME	C-10
Quasi-steady mass flow rate (g/s)	7.09	6.84	7.02	7.49	7.74
Exit Velocity (m/s)	480	472.4	458	434.9	432.4
Reynolds Number @ 298K	52,105	29,835	29,910	11,609	6,500
Turbulent Kinetic Energy (m^2/s^2)	2463	2904	2814	3404	3735
Turbulence Dissipation Rate (m^2/s^3)	4.1E+9	4.9E+9	4.4E+9	4.8E+9	5.2E+9
T (s) [TKE/TDR]	6.05E-7	5.92E-7	6.44E-7	7.08E-7	7.18E-7
Discharge Coefficient (C_d)	0.688	0.685	0.689	0.686	0.750
Area Coefficient (C_a)	0.90	0.92	0.91	1	1

$P_{inj} \approx 1300$ bar $\quad P_{back} = 30$ bar $\quad$ Orifice Diameter $= 169\ \mu m$

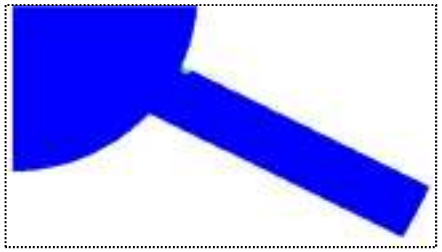
- Exit velocity is higher for fluids with lower viscosity
- Mass flow rate is higher for fuels without cavitation at the nozzle exit
- Shorter time-scale for turbulent eddies => faster breakup

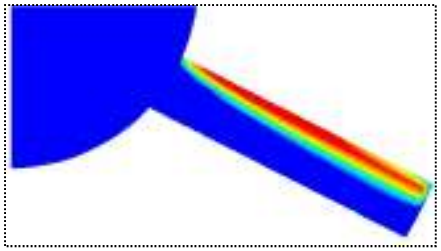


Cavitation Number for Inception

Fuel	@ Inception (Turbulent Regime)		@ nozzle exit (Cavitation Regime)	
	Pressure (bar)	Cavitation Number	Pressure (bar)	Cavitation Number
Diesel	100	2.33	500	15.67
HVO	120	3.01	600	19.02
CuME	125	3.17	1000	32.33
SME	160	4.33		
TME	170	4.67		
RME	180	5.00		
C-10	250	7.34		

Does not transition to cavitation regime even at P_{inj} = 2000 bar!

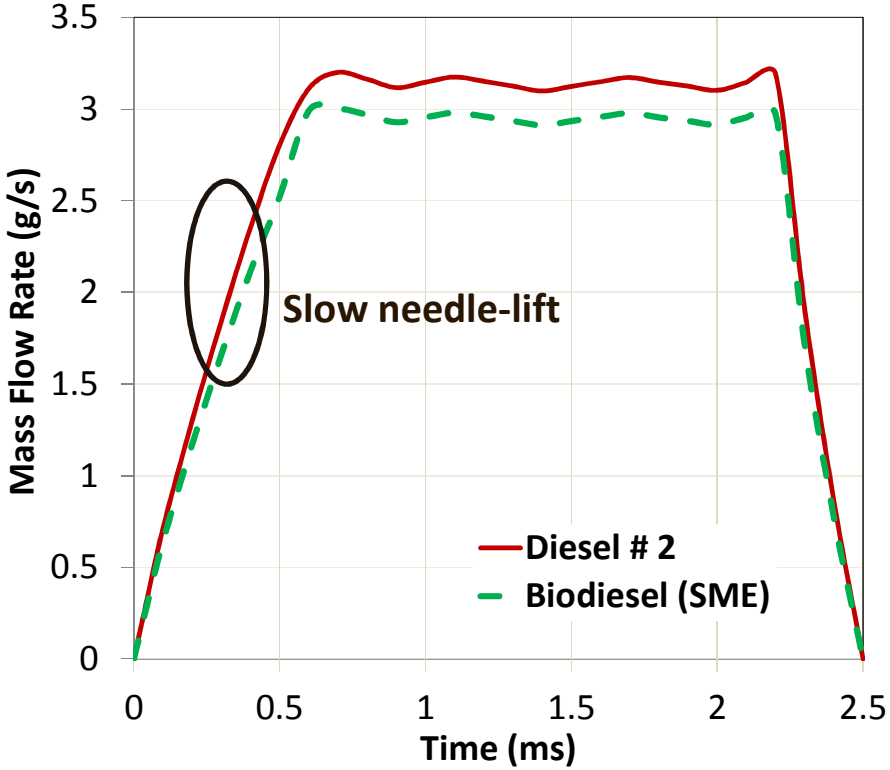


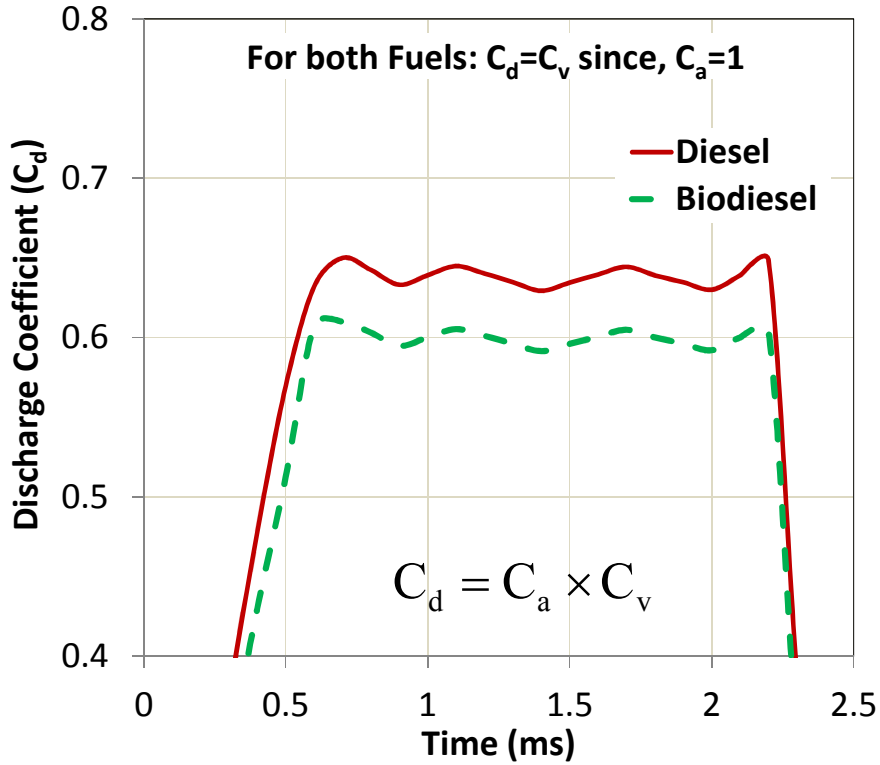


High viscosity, low vapor pressure => less propensity to cavitate
Low viscosity, high vapor pressure => high propensity to cavitate

$$CN = \frac{P_{inj} - P_{back}}{P_{back} - P_{vapor}}$$

Transient Profiles under Turbulent Regime





- **Mass flow rate depends on the competition between:**
  a) Liquid density of fuel
  b) Extent of cavitation at the nozzle exit
  c) Nozzle exit velocity
- **Mass flow rate and discharge coefficient of diesel is higher**
- Fluctuations in the mass flow rate and discharge coefficient profiles are due to the injection pressure profile

$$\left(\dot{m}_{fuel}\right)_{cal} = \rho_{fuel} A_{exit} V_{cal}$$

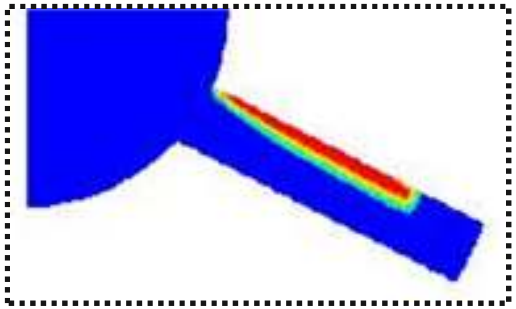
$$\left(\frac{\dot{m}_{SME}}{\dot{m}_{Diesel}}\right)_{th} \propto \sqrt{\frac{\rho_{SME}}{\rho_{Diesel}}}$$

Flow Characteristics under Turbulent Regime

Fuel Property	Diesel	HVO	CuME	SME	C-10
Quasi-steady mass flow rate (g/s)	3.3	3.0	3.2	3.1	2.86
Exit Velocity (m/s)	178	172	172	165	167
Reynolds Number @ 298K	24025	13750	13790	5400	3000
Turbulent Kinetic Energy (m^2/s^2)	661	714	648	648	673
Turbulence Dissipation Rate (m^2/s^3)	3.9E+8	4.4E+8	3.4E+8	3.4E+8	5.2E+9
T (s) [TKE/TDR]	1.7E-6	1.6E-6	1.9E-6	1.9E-6	1.8E-6
Discharge Coefficient (C_d)	0.75	0.72	0.75	0.70	0.67
Area Coefficient (C_a)	1	1	1	1	1

$P_{inj} \approx 300$ bar $\quad P_{back} = 30$ bar $\quad$ Orifice Diameter $= 169\ \mu m$

- SME, TME, RME predict similar nozzle flow characteristics (not shown here)
- In the absence of cavitation at nozzle exit, fuels with lower viscosity have higher mass flow rates
- Shorter time-scale for turbulent eddies => faster breakup



Account for Losses in Injected Energy

Turbulent Regime

Orifice Diameter (microns)	169
Back Pressure (bar)	30
Duration of Injection (ms)	3
Discharge coefficients	0.67-0.75

$M_{diesel} > M_{biodiesel}$ (5-8%)

$IE_{diesel} > IE_{biodiesel}$ (15-18%)

Mass flow rate of biodiesel needs to be increased by about 20-25 % to account for this loss in injected energy with biodiesel

@ P_{inj} = 300 bar, a 20% increase in total mass flow rate of biodiesel corresponds to an injection pressure of 415 bar. Hence, the P_{inj} needs to be increased by about 35-40%!

Cavitation Regime

	Diesel	SME
Density (Kg/m^3)	820	870
Heat of Combustion (MJ/Kg)	42.0	37.4

$M_{biodiesel} > M_{diesel}$ (3-5%)

$IE_{diesel} > IE_{biodiesel}$ (7-10%)

Mass flow rate of biodiesel needs to be increased by about 8-12 % to account for this loss in injected energy with biodiesel

@ P_{inj} = 1300 bar, a 10% increase in total mass flow rate of biodiesel corresponds to an injection pressure of 1570 bar. Hence, the P_{inj} needs to be increased by about 18-20%!

Summary & Future Work

- Physical and chemical properties of different fuels measured
- Detailed nozzle flow modeling performed:
  - ✓ Differences in physical properties resulted in significant differences in nozzle flow characteristics
  - ✓ Different trends in cavitation and turbulent regimes observed
  - ✓ Initial and boundary conditions for spray modeling are determined
- Comparison of different alternate fuels:
  - ✓ Difference in flow characteristics between SME, RME, TME are minimal
  - ✓ Inner nozzle flow characteristics of CuME are similar to diesel fuel
  - × Geraniol behaves markedly different than diesel fuel. Also due to its low Cetane number value, it is perhaps not a good blending agent for diesel fuel
  - ✓ HVO behaves similar to diesel fuel. Its high cetane number value is desirable as a diesel fuel blend

- **CAT single-cylinder engine studies with these alternate fuels to understand the performance and emission characteristics**
- **Characterize Jatropha and Karanja biodiesel**

Collaborators

Prof. Avinash K. Agarwal at **Indian Institute of Technology,** Kanpur, India

Acknowledgements

Sponsors: U.S. Department of Energy, Office of Vehicle Technology under the management of **Mr. Kevin Stork**

Dr. Gerhard Knothe, US Department of Agriculture, for Cuphea based biodiesel samples

Dr. O. Kaario, Dr. M. Larmi, Helsinki University of Technology, for Hydro-treated Vegetable Oil properties

Thank You!

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dlongman@anl.gov

Background & Objectives

- During the past decade, the possibility of using Biodiesel has received significant attention since, it fits well with the existing infrastructure and is environmentally friendlier than Petrodiesel

- Biodiesel is a lucrative alternate for compression ignition engines. However, differences in physical & chemical properties of biodiesel and petrodiesel are not insignificant

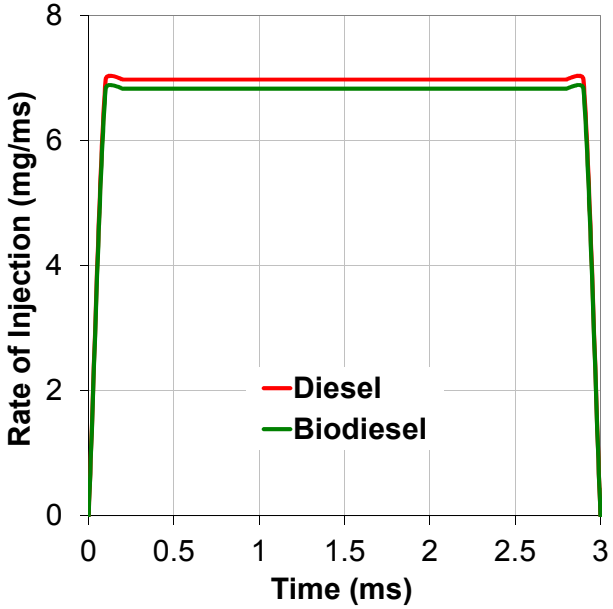
- The physical and chemical properties of biodiesel from different feedstocks also vary significantly. Of specific interest:
  - (1) Soy methyl ester
  - (2) Tallow methyl ester
  - (3) Cuphea methyl ester
  - (4) Rape-seed methyl ester

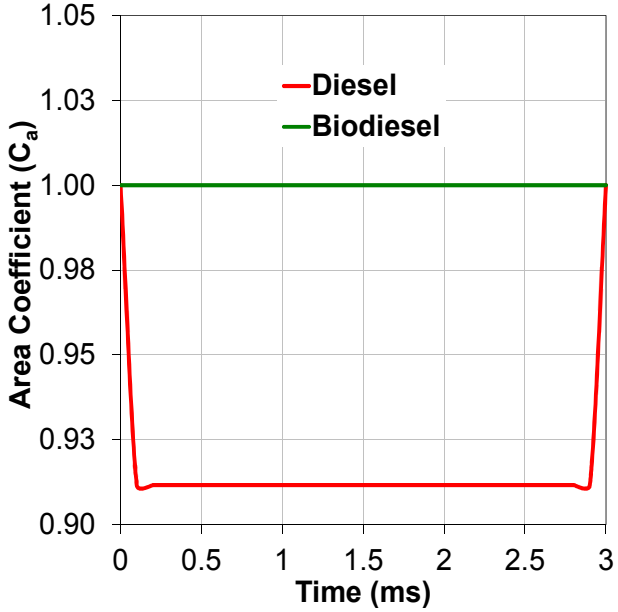
- Measure fuel properties such as density, viscosity, surface tension, vapor pressure, heat of combustion, heat of evaporation, distillation curve etc. for different alternate fuels

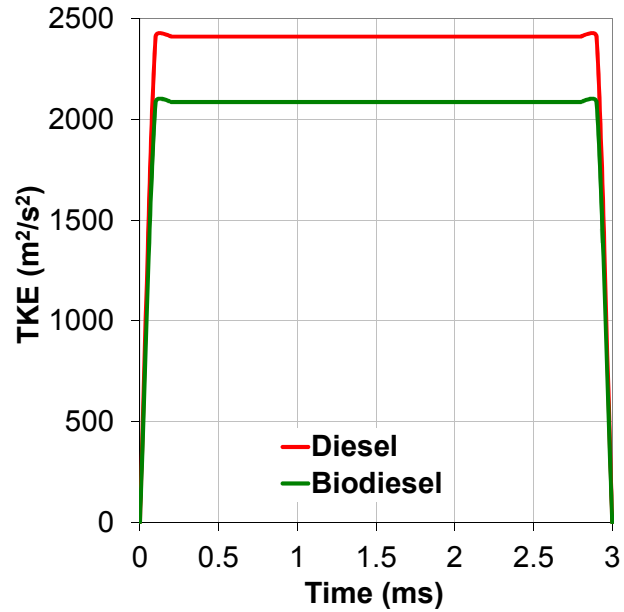
- Predict differences in inner-nozzle flow behavior of these fuels in terms of cavitation inception, turbulence levels, injection velocity, discharge coefficient etc.

Coupled Nozzle Flow and Spray Modeling

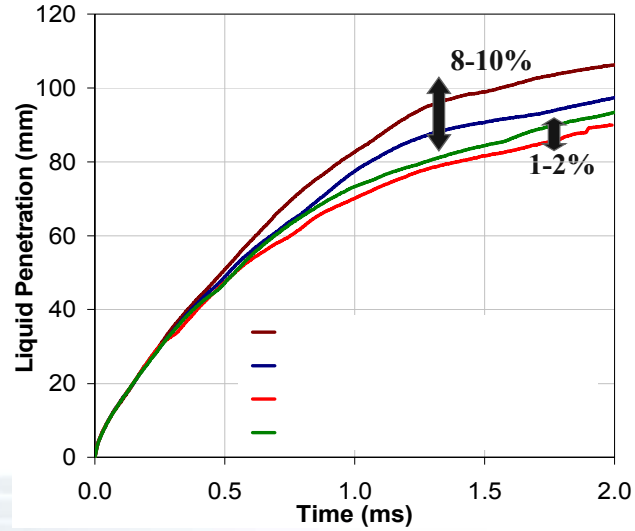
Boundary condition for KH-ACT model







1) S Som et al. SAE 2009-01-0838
2) Ramirez et al. JEF 2009
3) S Som et al. Combustion and Flame 2010

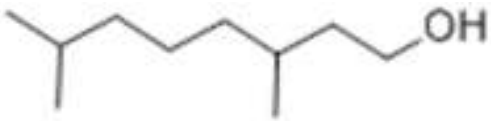


Alternate Fuels of Interest

- Diesel # 2: Properties obtained from Literature
- Soy Methyl Ester (SME): Peter Cremer NA
- Rapeseed (RME) and Tallow (TME) Methyl Esters: Properties obtained from (Graboski et al. Progress in Energy and Combustion Science 1998)
- Cuphea based biodiesel (CuME): USDA (Knothe et al. Energy and Fuel 2009)

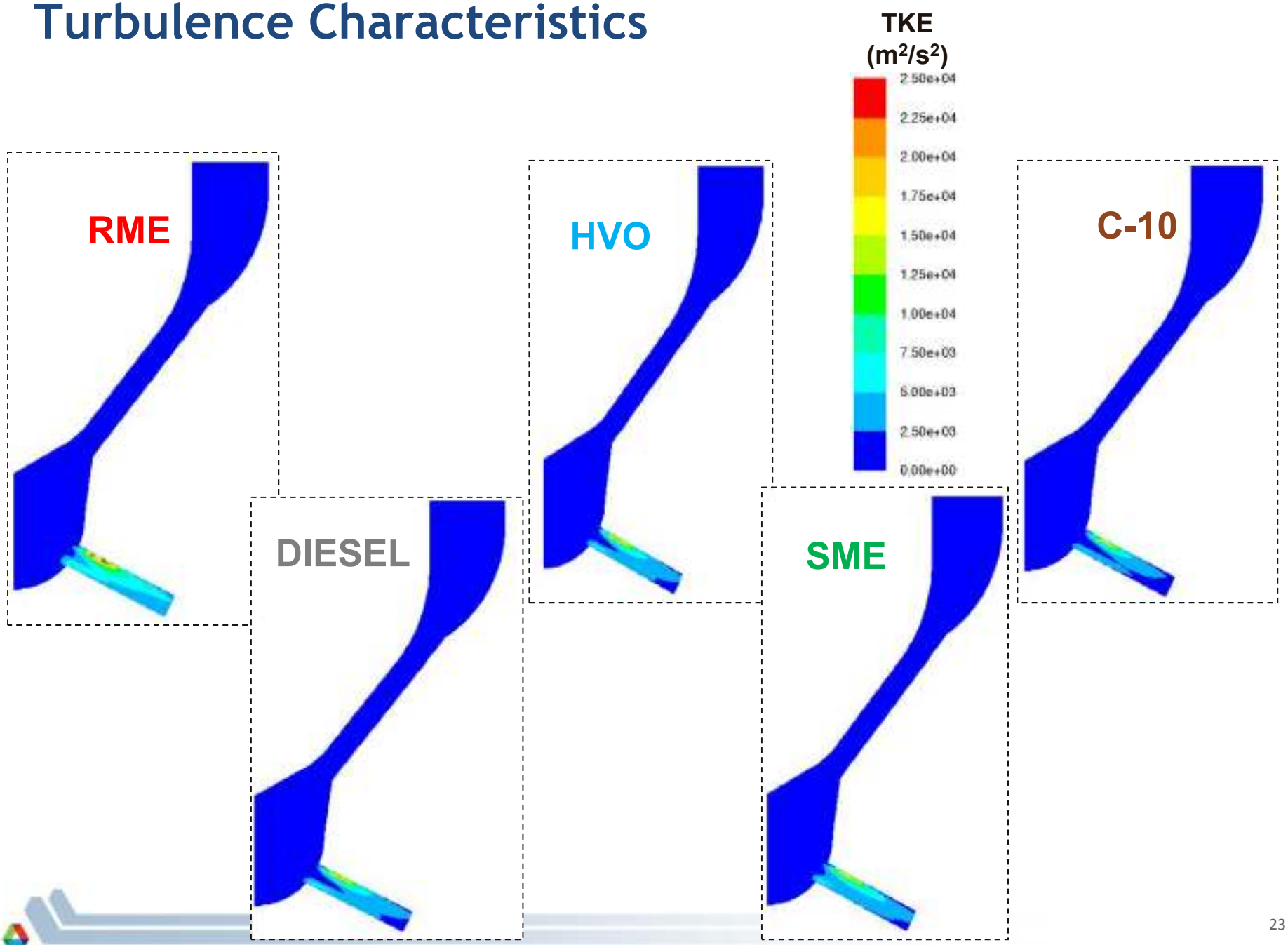
Cuphea Ignea: Ornamental plants

- Geraniol **($C_{10}H_{22}O$)** 3,7-DiMethyl-1-Octanol



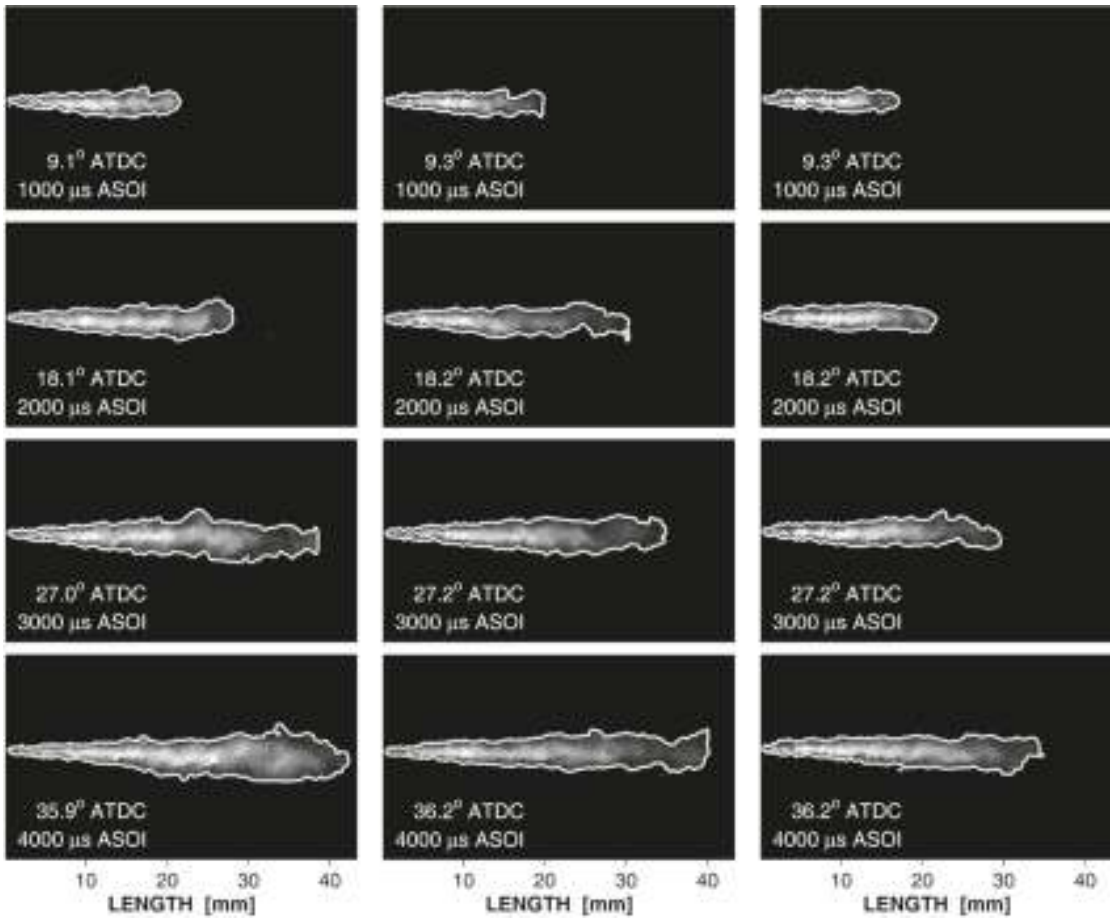
- Hydro-treated vegetable oil (HVO): Helsinki University of Technology (Gong et al. SAE 2010-01-0739)

Turbulence Characteristics

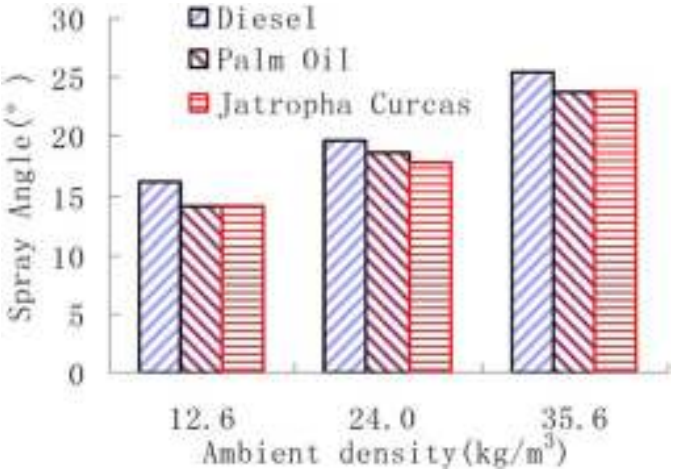


Penetration Characteristics of Biodiesel from Different Feedstocks: Experimental results

Soy-ME **Cuphea-ME** **Diesel # 2**



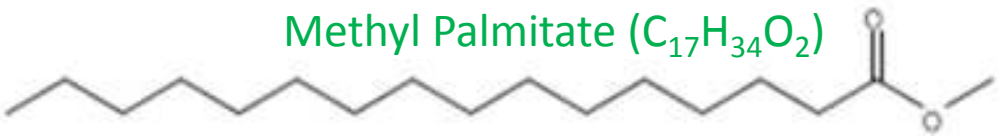
Fisher et al. Energy and Fuel 2010



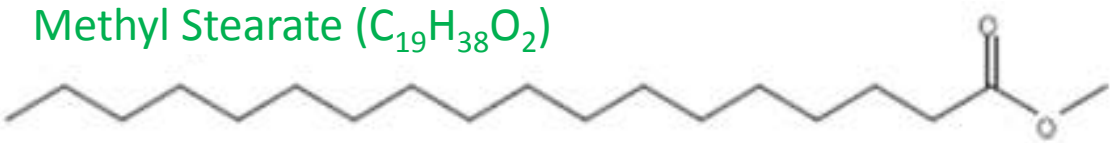
Deng et al. SAE 2010-01-2268

Composition of Biodiesels

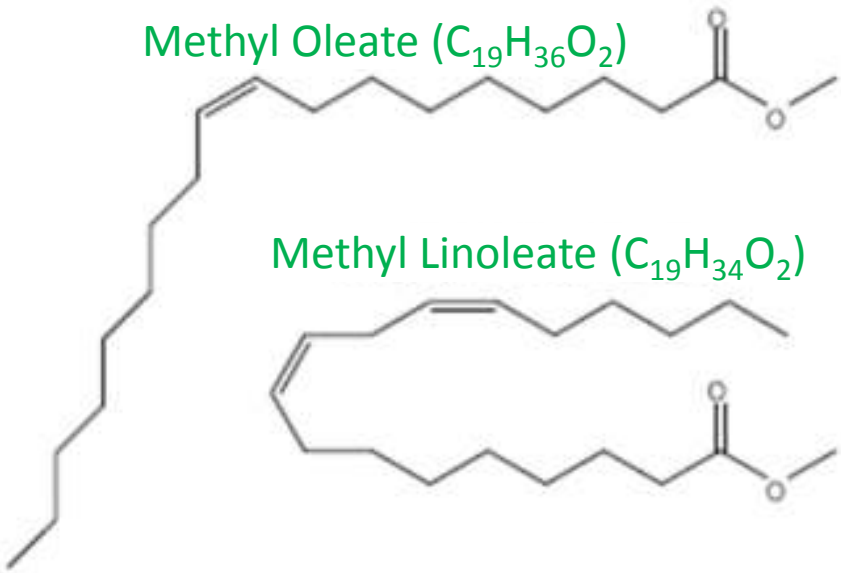
Methyl Palmitate ($C_{17}H_{34}O_2$)



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

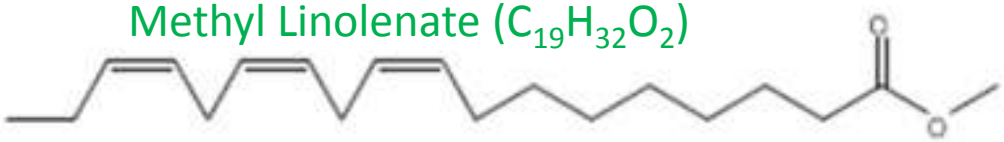


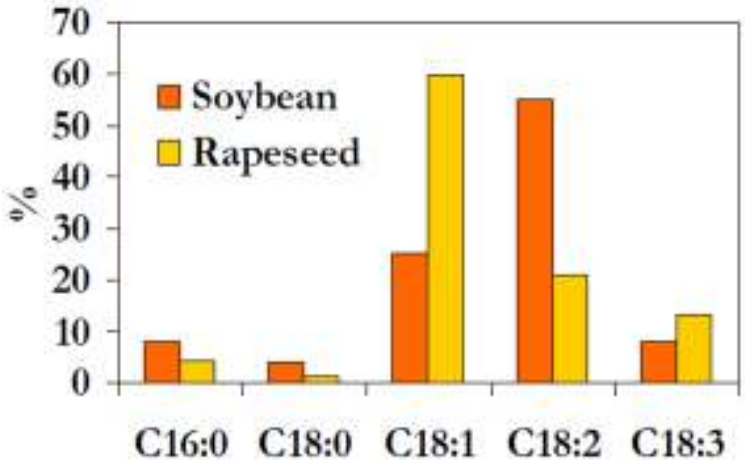
Methyl Oleate ($C_{19}H_{36}O_2$)



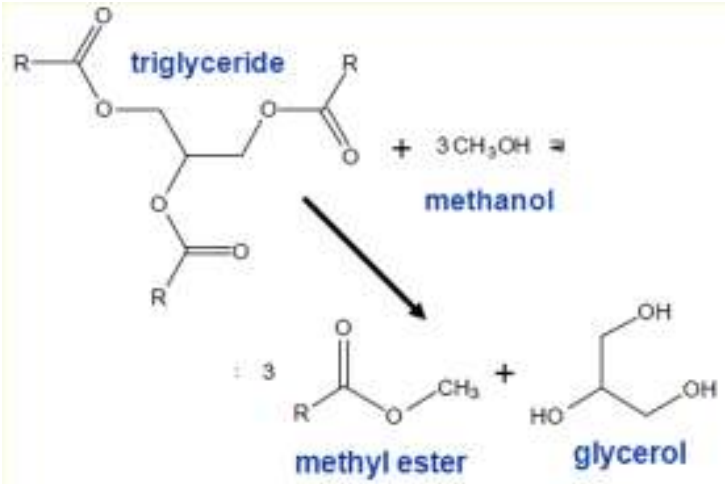
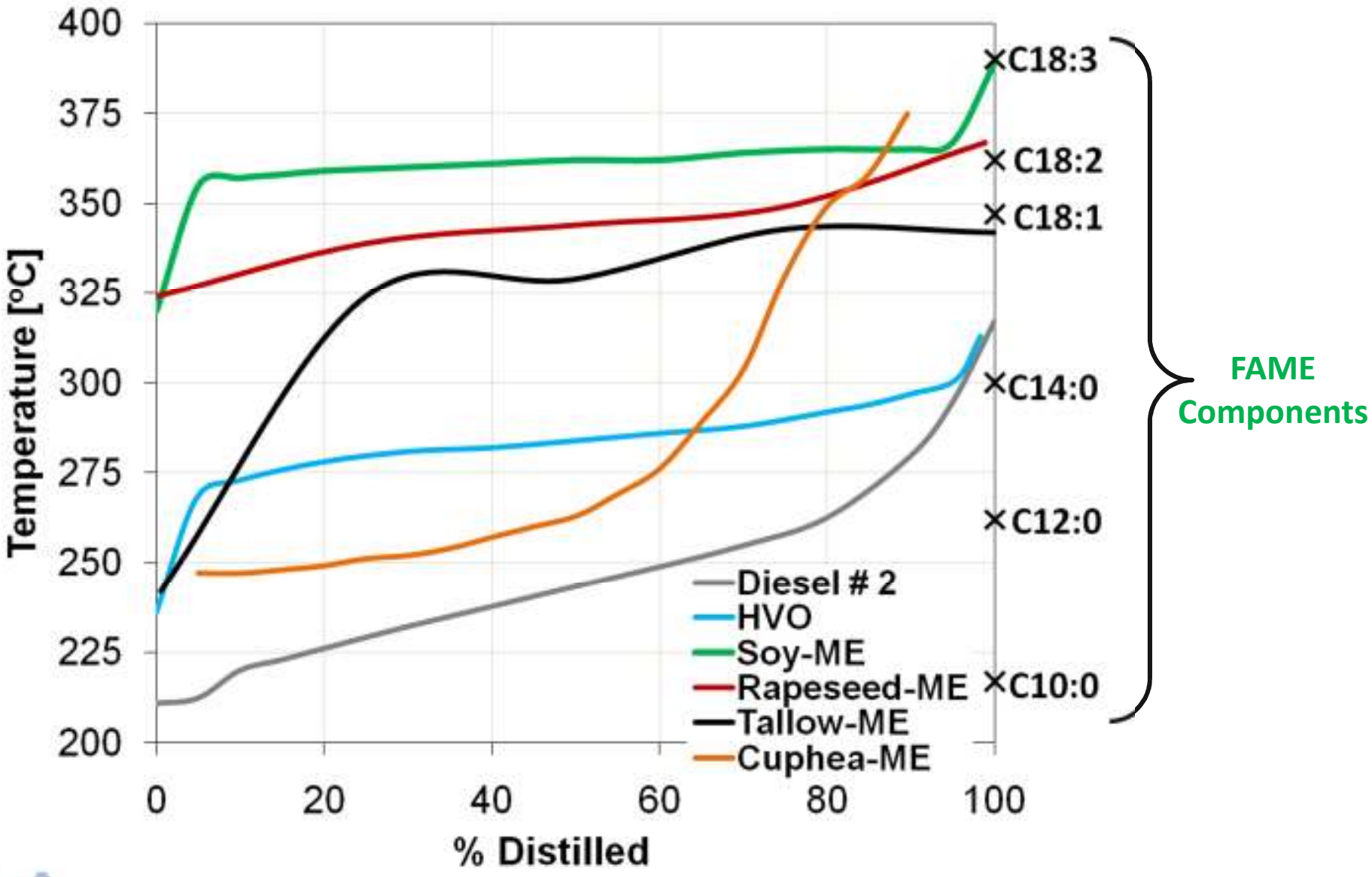
Methyl Linoleate ($C_{19}H_{34}O_2$)

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





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



Boiling/Distillation Curves