Integrated Nozzle Flow, Spray and Combustion Modeling Using KH-ACT Primary Breakup Model & Detailed Chemistry

Sibendu Som, Douglas E. Longman
Argonne National Laboratory

February 22nd 2011

AEC/HCCI Working Group Meeting at Sandia National Laboratory

Collaborators

Ms. Anita I. Ramirez, Prof. Suresh K. Aggarwal at **University of Illinois at Chicago**

Dr. Peter K. Senecal, Dr. Eric Pomraning at **CONVERGENT Science**

Prof. Tianfeng Lu, Mr. Zhaoyu Luo, Mr. Max Plomer at **University of Connecticut**

Acknowledgements

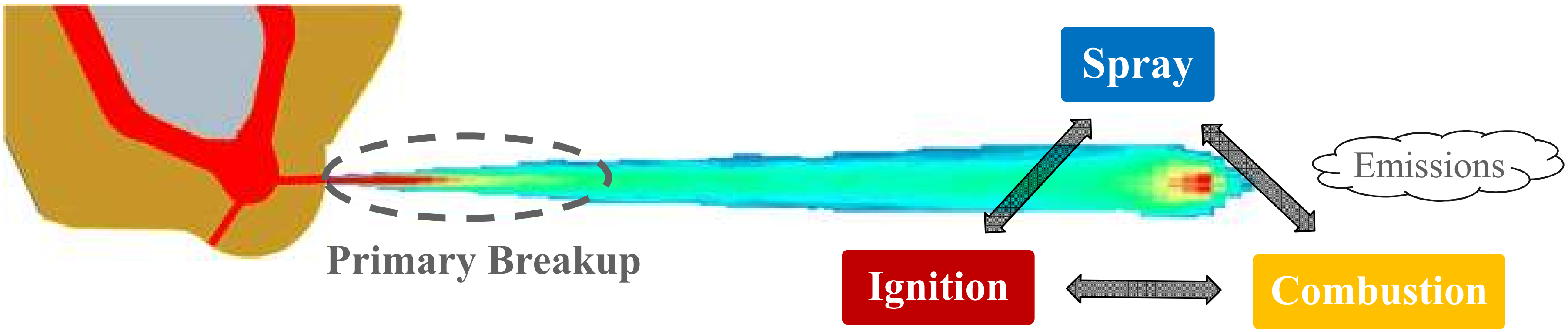
Sponsors: U.S. Department of Energy, Office of Vehicle Technology under the management of **Mr. Gurpreet Singh**

Caterpillar Inc. for hardware and engine support

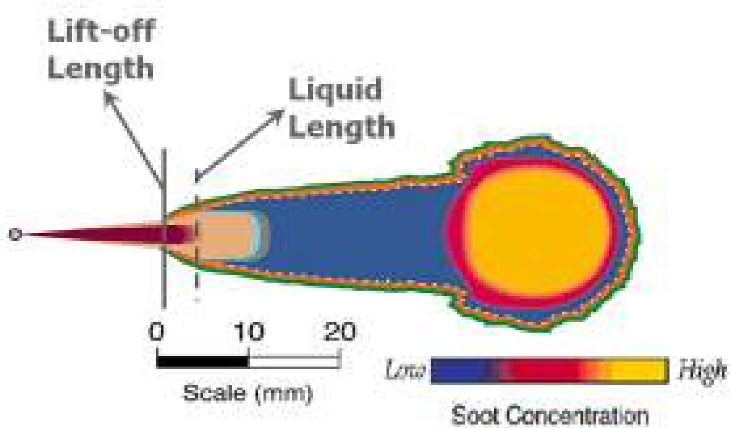
Dr. Lyle Pickett at Sandia National Laboratory for sharing biodiesel data

Integrated Modeling Approach

Influence of <u>fuel properties</u> on nozzle flow, spray, combustion and emission characteristics!!



Conceptual Combustion Model from Sandia National Laboratory

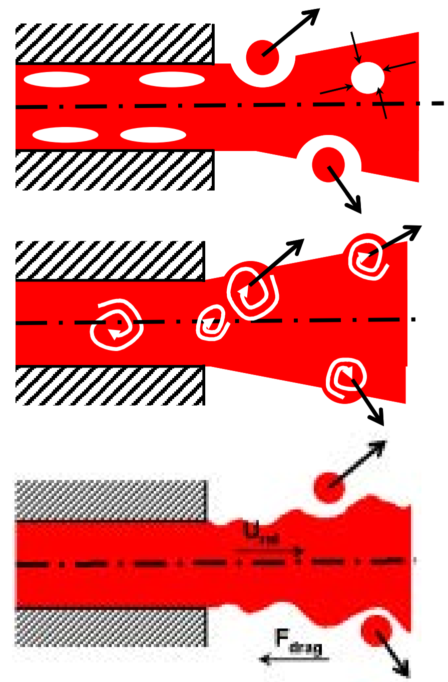


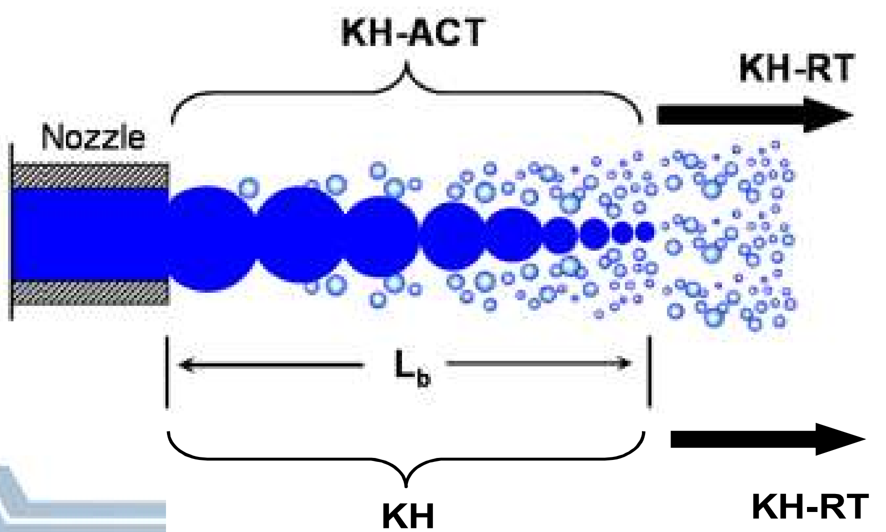
- ❑ Detailed inner-nozzle flow modeling with realistic fuel properties
- ❑ **KH-ACT** primary breakup model:
  Aerodynamics, Cavitation, Turbulence
- ❑ Spray Validation
  X-ray radiography data
- ❑ **Detailed Chemistry**:
  Methyl Butanoate
  Methyl Decanoate
  } **Biodiesel Surrogate**
- ❑ Validation against **flame lift-off** data

Primary Breakup Model

KH-ACT (Kelvin-Helmholtz-Aerodynamics Cavitation Turbulence) Model* "

- ❑ Length and time scales are calculated:
    - ○ Cavitation induced breakup: Based on bubble collapse and burst times
    - ○ Turbulence induced breakup : Based on k-ε model
    - ○ Aerodynamically induced breakup: Based on Kelvin-Helmholtz (KH) and Rayleigh Taylor (RT) instability
- ❑ Dominant ratio of length/time scale causes breakup
- ❑ Extensive model validation against **x-ray data** at Argonne





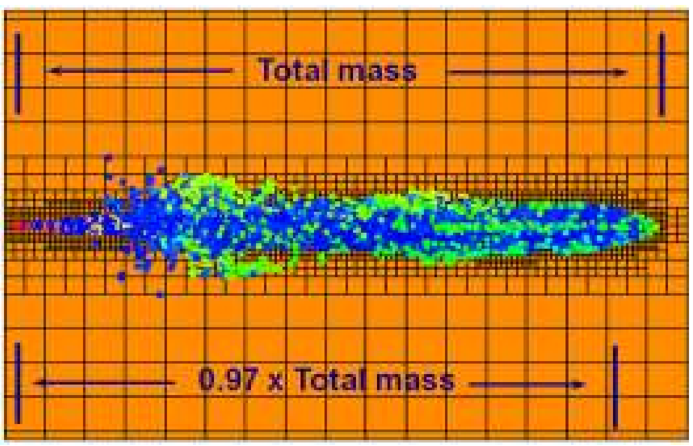
***Som et al., SAE 2009-01-0838**
Som and Aggarwal, Combustion and Flame 2010

Modeling Set-up in CONVERGE

- Liquid Injection using Blob model
- KH-RT model for secondary breakup
- Collision and coalescence model
- Multi-component Evaporation model
- Dynamic drag model on droplet
- Turbulent dispersion model
- Reynolds Average Navier-stokes turbulence model
- Detailed Chemistry Approach
- NOx and soot oxidation models

KH-ACT model implemented " in CONVERGE "

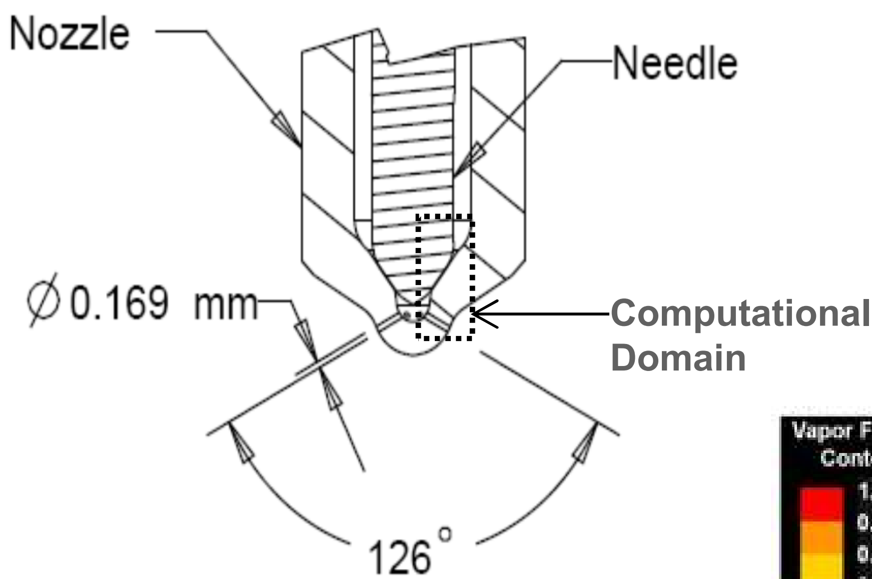
CONVERGE Manual
Senecal et al., SAE 2007-01-0159
S. Som, PhD thesis, UIC 2009



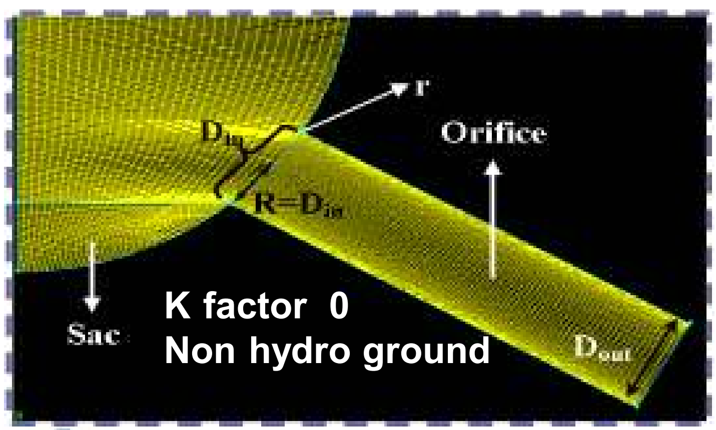
	RANS
Base grid size (mm)	4
Fixed embedding	3
AMR – Velocity field	3
AMR – Temperature field	3
Minimum grid size (mm)	0.25-0.5

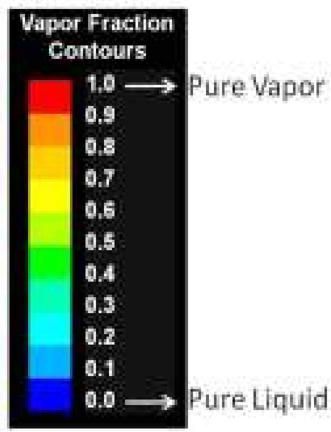
Injector Geometry and Grid Generated

6-hole production Injector

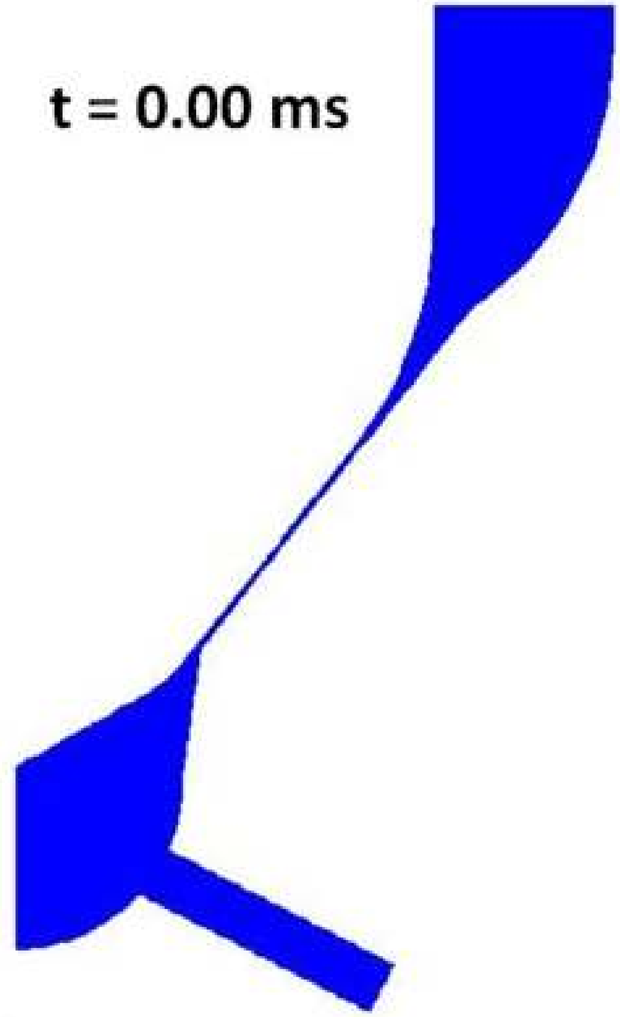


Nozzle Orifice



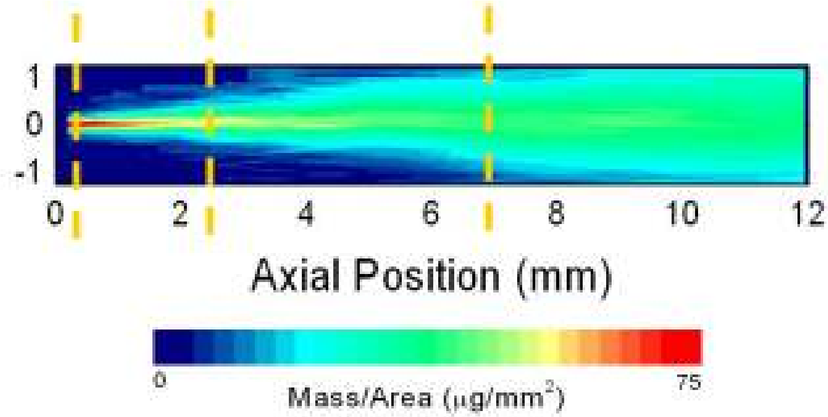


D=169μm
Cylindrical
Non-hydroground
L/D=4.2

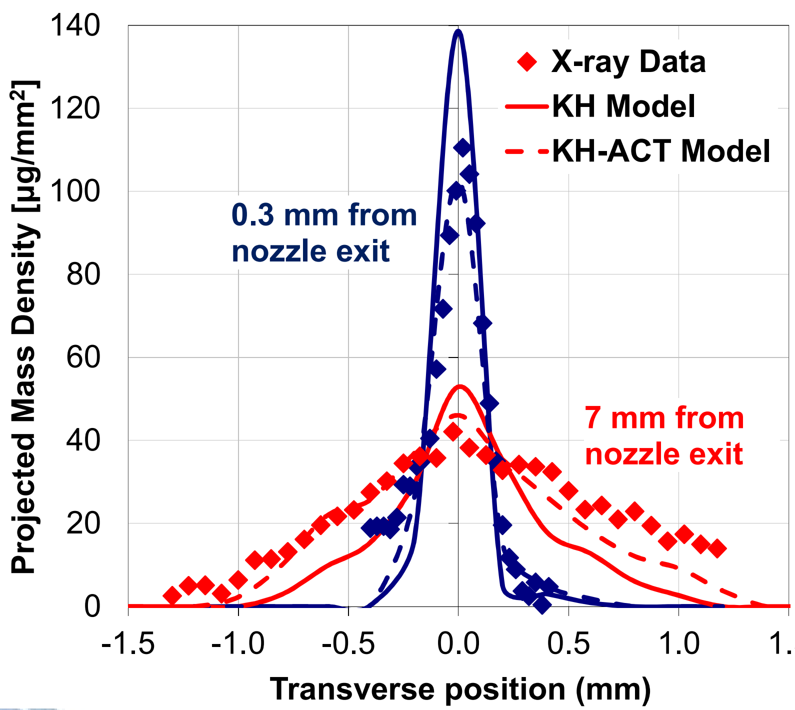


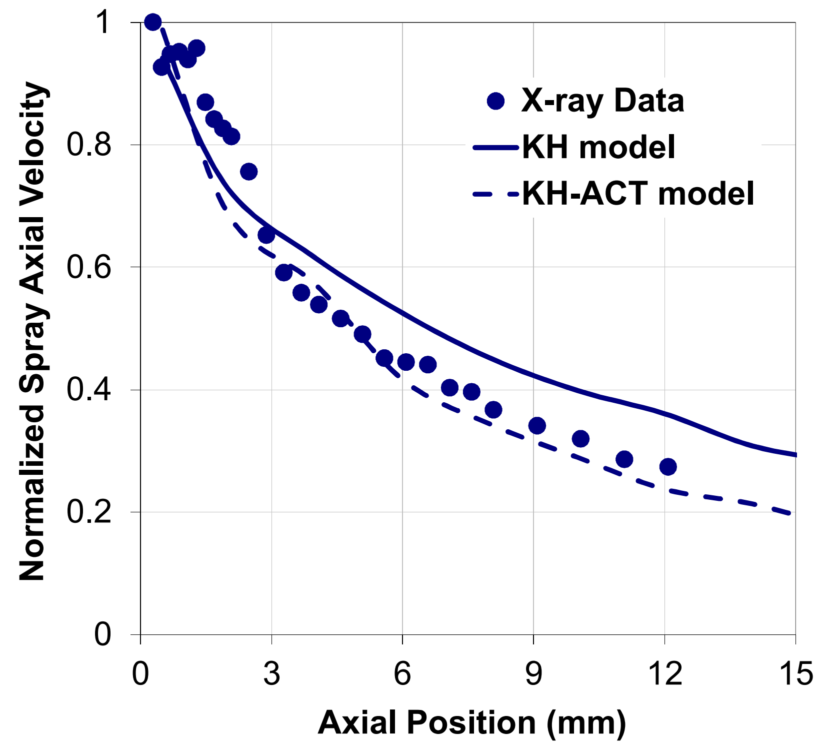
*Som et al., *FUEL* (2010)
Som et al., *JEGTP* (2010)

Spray Validation against X-ray Data



X-ray radiography Data: Ramirez et al., JEF 2009



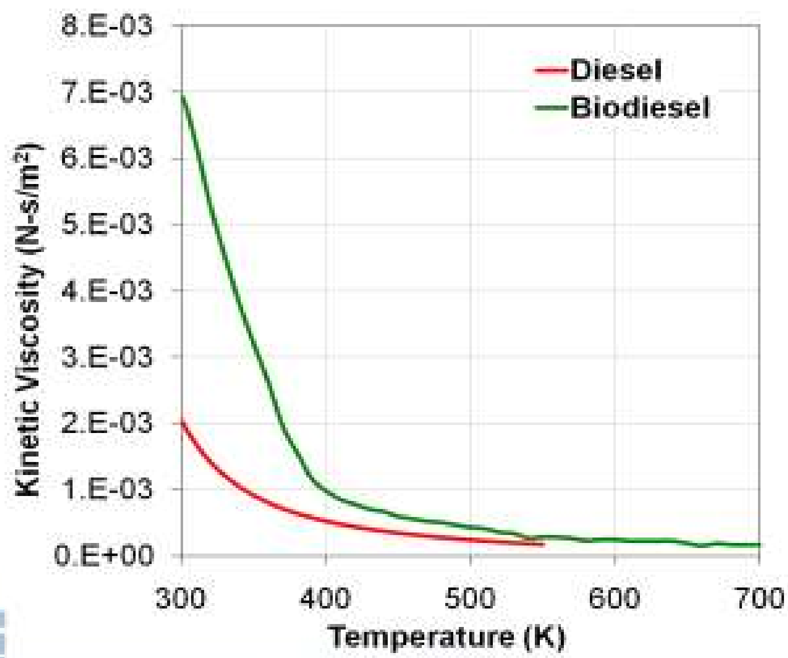


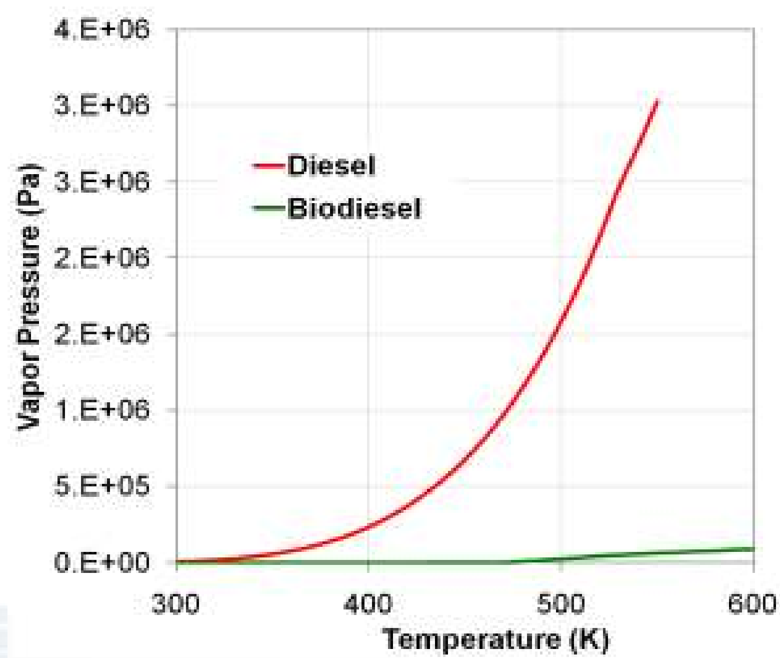
- The spray loses half of its initial velocity within the first 6 mm
- Simulation capture the Gaussian mass distributions from x-ray data well
- Spray Dispersion accurately captured by only the KH-ACT model. KH model under-predicts spray spreading

Differences in Fuel Properties*

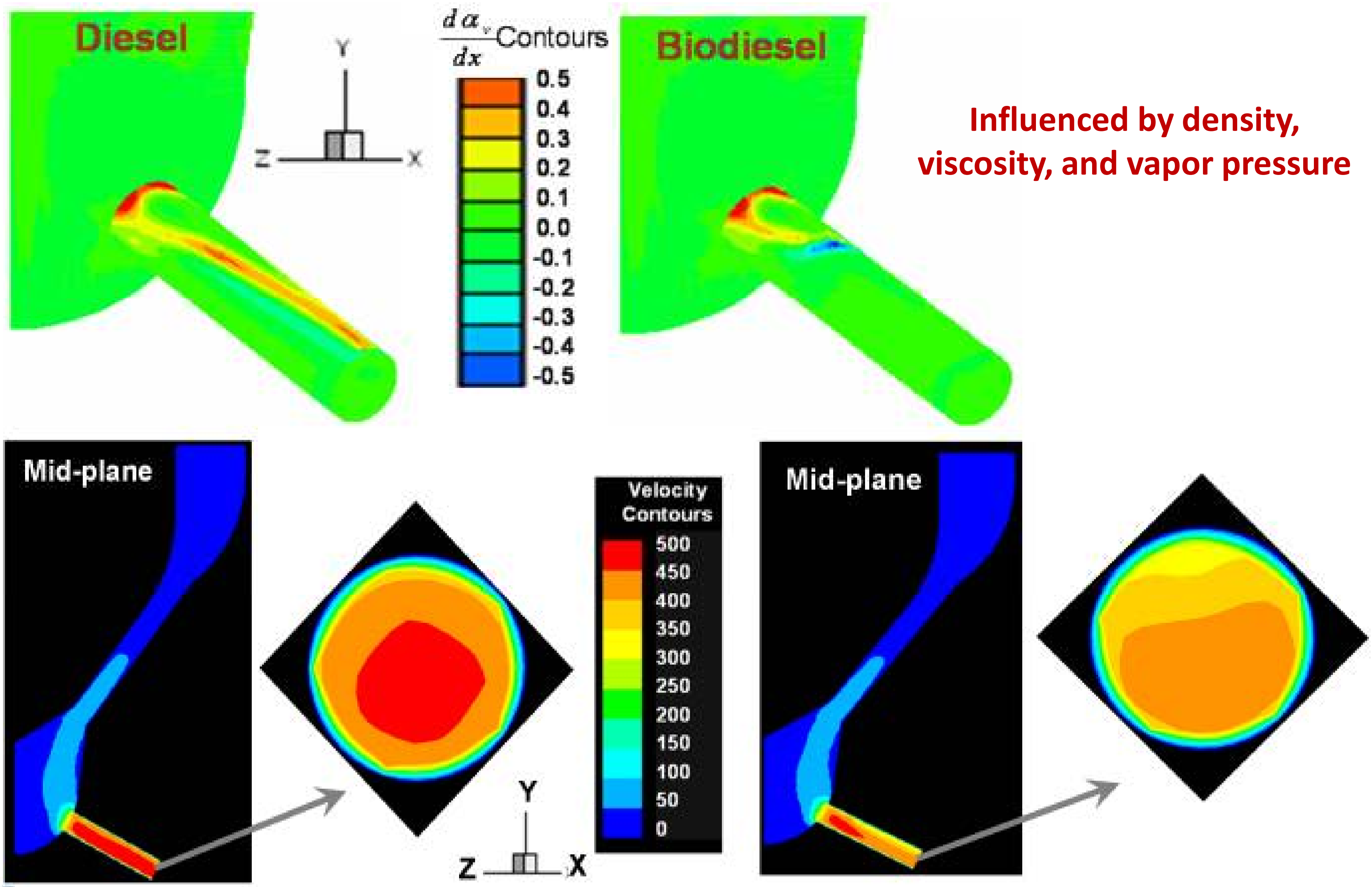
Fuel Property	Diesel	Biodiesel (SME)
Carbon Content [wt %]	87	76.74
Hydrogen Content [wt %]	13	12.01
Oxygen Content [wt %]	0	11.25
Density @ 15^{o}C (kg/m3)	**820**	**877.2**
Surface Tension @ 25^{o}C (N/m)	**0.020**	**0.0296**
Heat of Combustion (MJ/Kg)	**42.0**	**37.4**
Heat of Vaporization (KJ/Kg)	**361.0**	**336.0**

***S. Som et al., FUEL 2010 "**





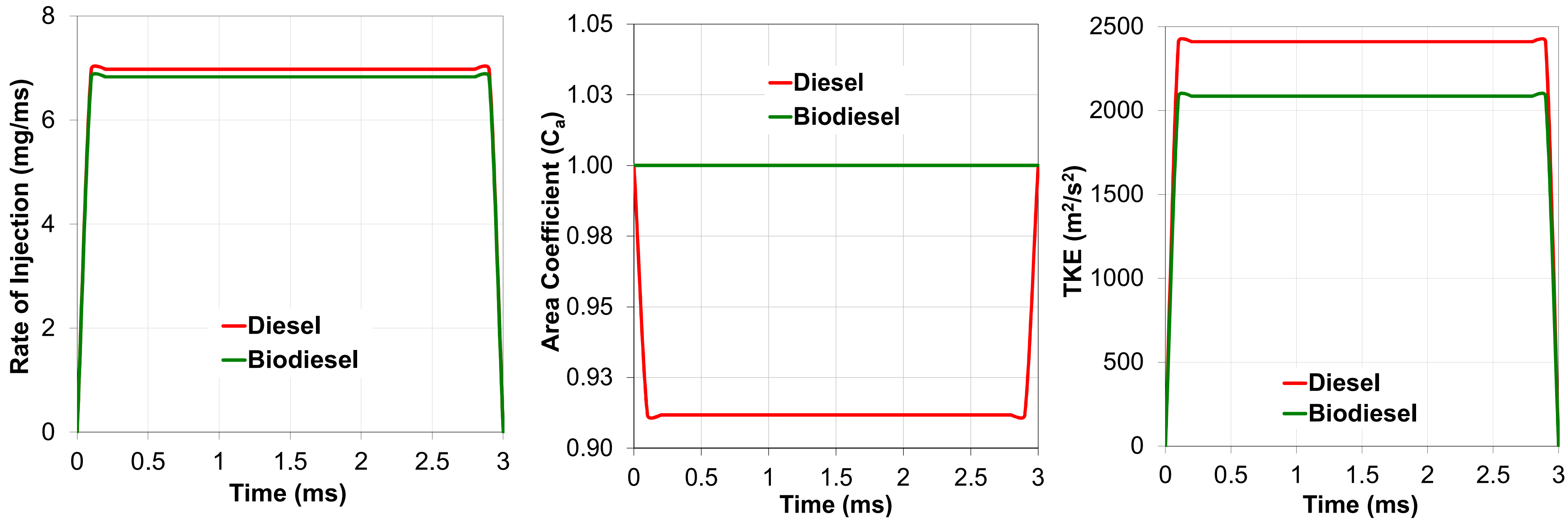
Vapor Volume Fraction & Velocity Distribution



Influenced by density, viscosity, and vapor pressure

Quasi Dynamic Coupling Strategy*

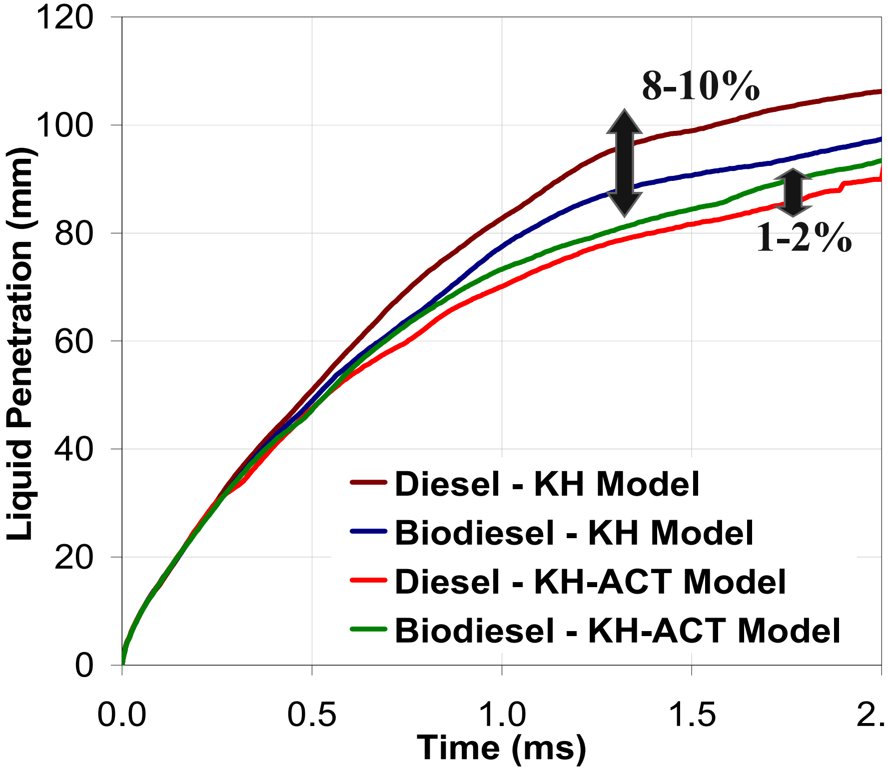
Boundary condition for KH-ACT model



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

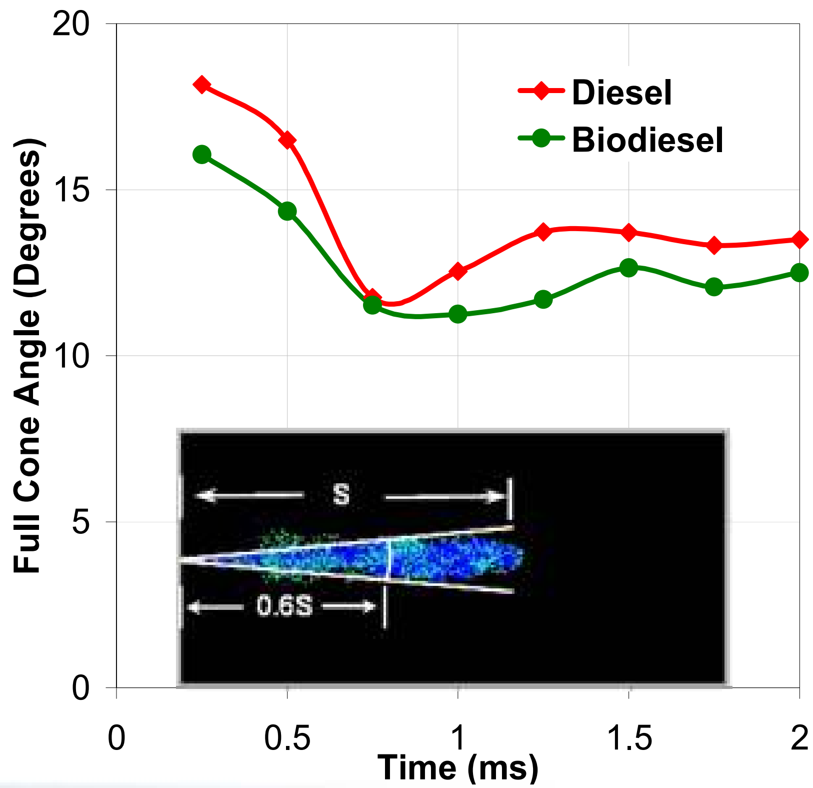
Property	Diesel	Biodiesel
Injection Pressure (bar)	1100 | 1300	1100 | 1300
Total Mass Injected (mg)	17.54 | 20.94	17.18 | 20.50
Discharge Coefficient (C_d)	0.64 | 0.64	0.61 | 0.62
Area Coefficient (C_a)	0.92 | 0.92	1 | 1
TKE (m^2/s^2)	1409 | 2410	1356 | 2135
Injection Duration (ms)	3	3
Ambient Density (Kg/m^3)	34	34
Ambient Temperature (K)	300	300

Spray Penetration & Cone-angle



- Experimental trend: Biodiesel penetrates more than diesel
- KH-ACT model accurately captures the experimental trend i.e., biodiesel penetrates marginally more than Diesel

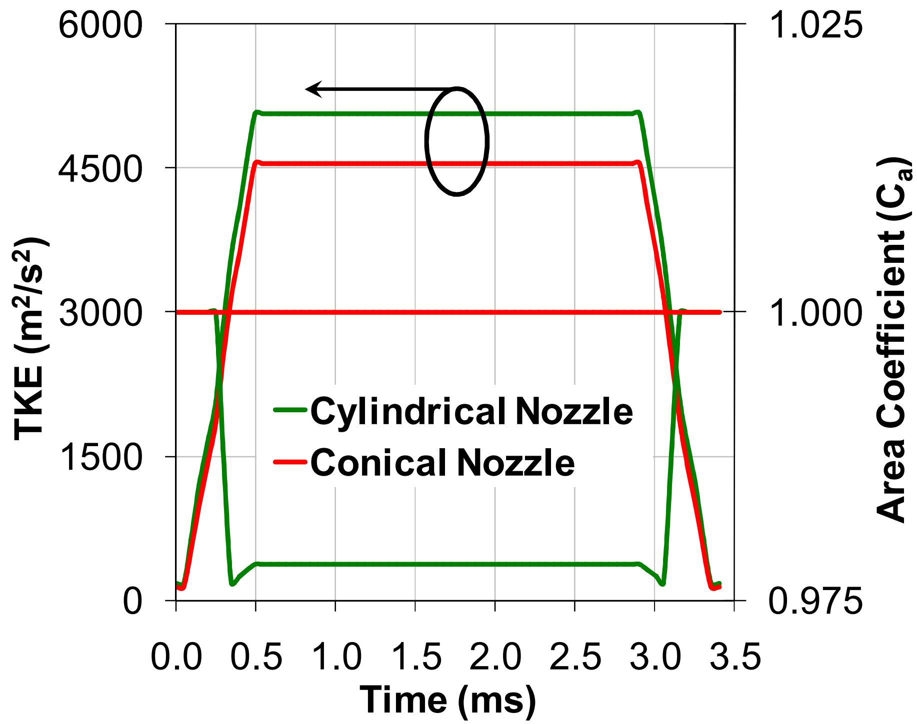
- Spray dispersion is lower for biodiesel in the far field region
- Poorer atomization characteristics for biodiesel due to its higher viscosity, surface tension, lower cavitation and turbulence

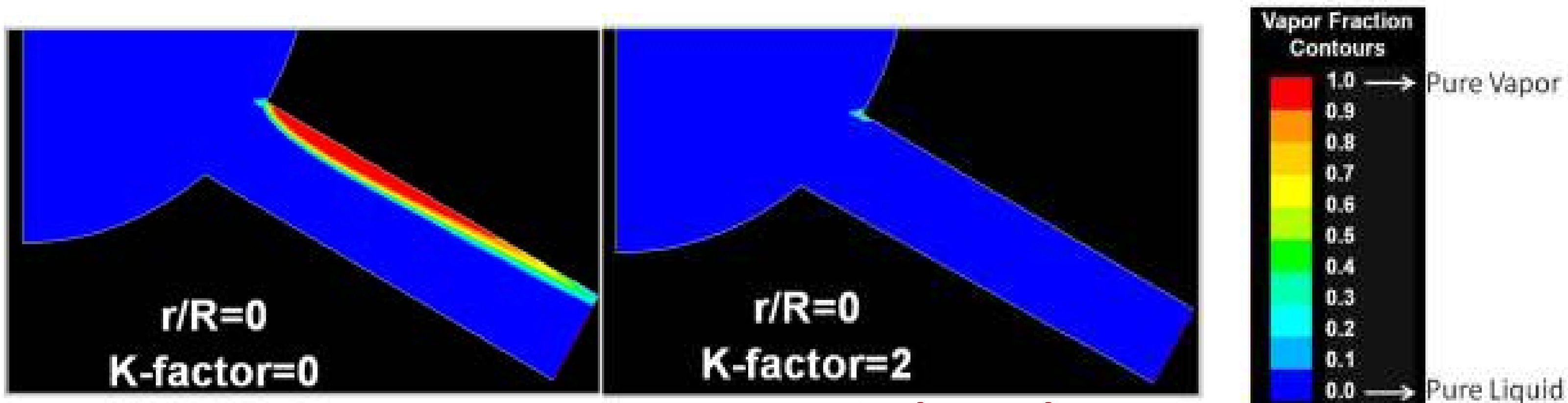


Effect of Conicity on Inner Nozzle Flow

Geometrical Characteristics	Cylindrical Nozzle	Conical Nozzle
D_{in} (µm)	169	169
D_{out} (µm)	169	149
K_{factor}	0	2
L/D	4.2	4.7

$$K_{factor} = \left(\frac{D_{in} - D_{out}}{10} \right) \mu m$$

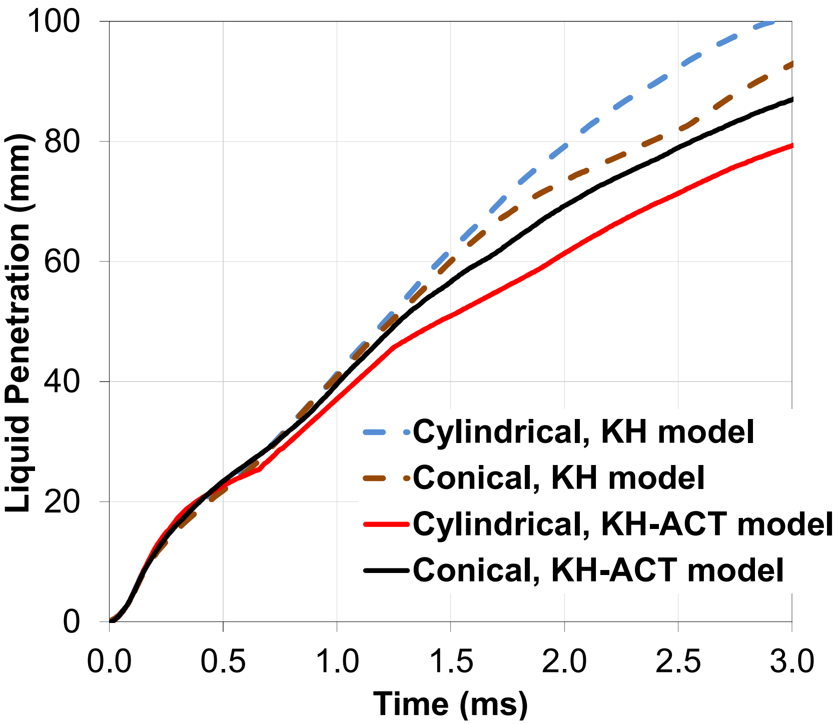




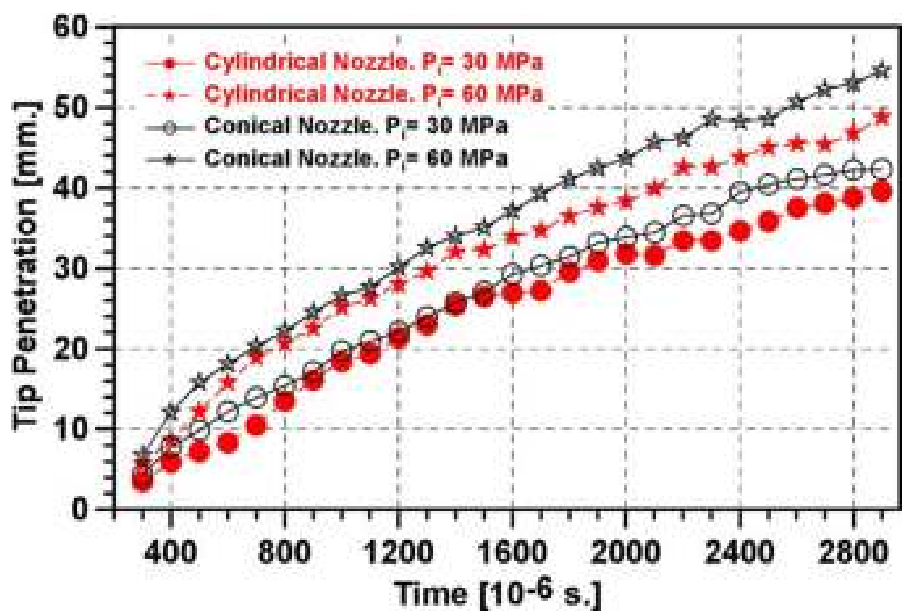
Cylindrical Nozzle

Conical Nozzle

Influence of Nozzle Geometry on Spray Penetration



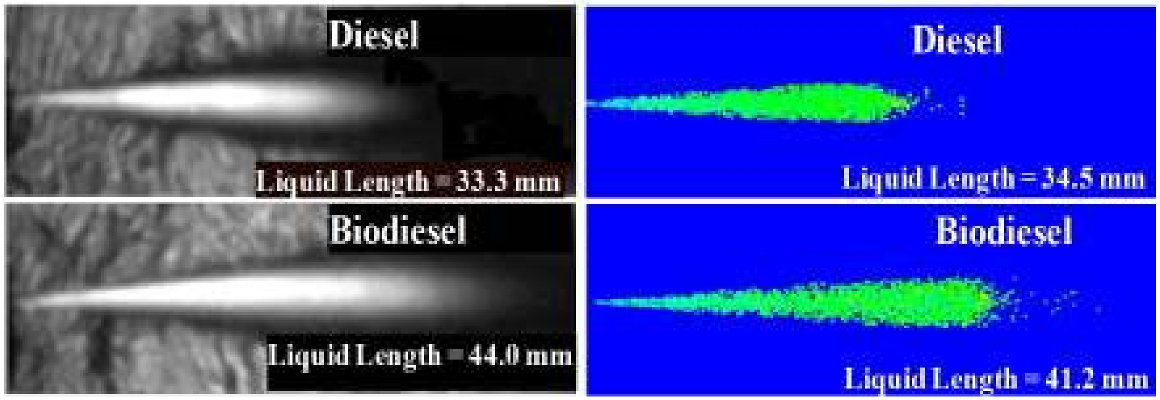
F Payri, V Bermudez, R Payri, FJ Salvador: FUEL (2004)



- Penetration characteristics of cylindrical and conical nozzles predicted by KH-ACT model (only) are consistent with experimental trends observed by Payri et al.
- Cylindrical nozzle predicts fastest breakup. This is due to enhanced cavitation and turbulence thus: 1) SMD, 2) Spray penetration are lowest

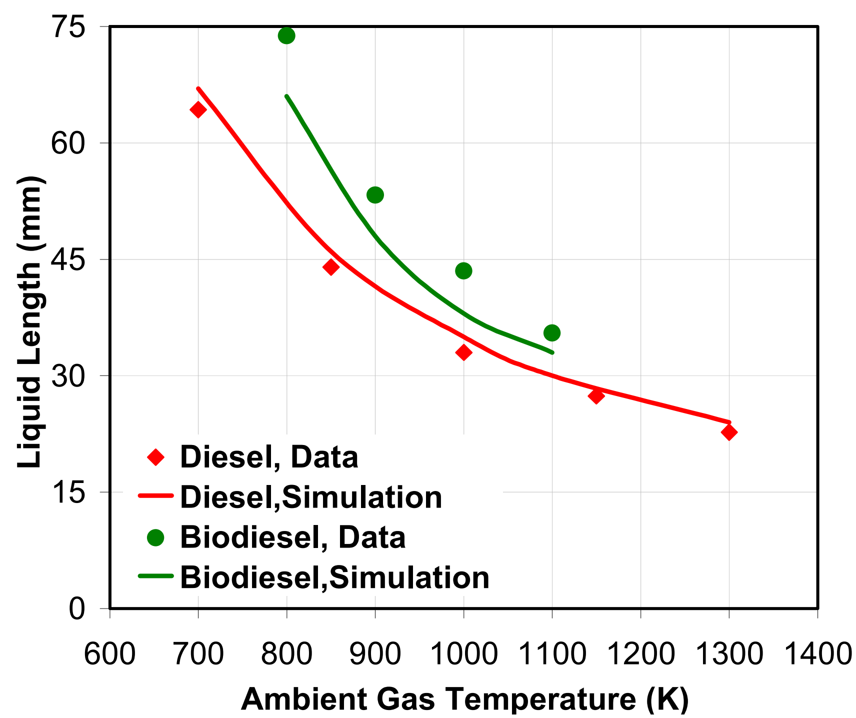
*S Som, DE Longman, AI Ramirez, SK Aggarwal. *FUEL* 2011

Evaporating Sprays: Liquid Length

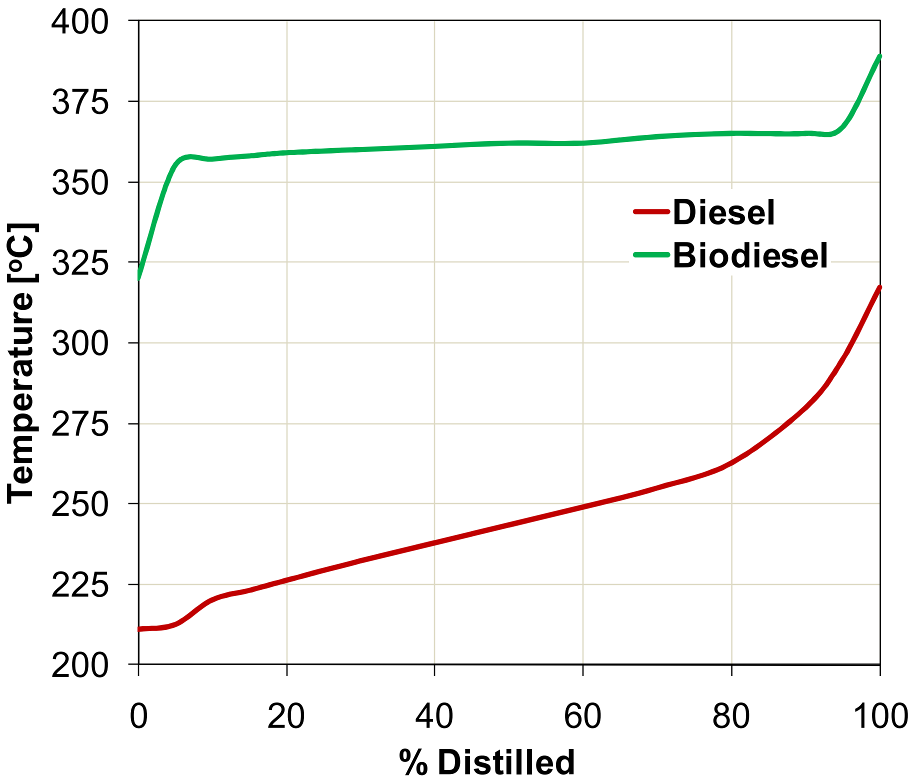


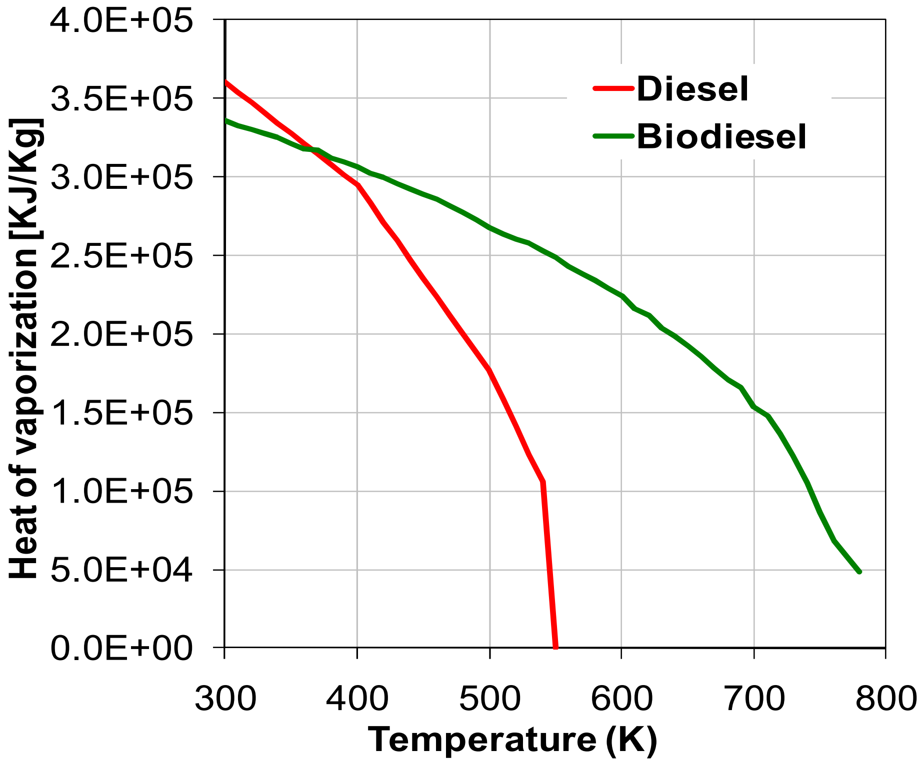
Data from:
1) DL Siebers: SAE 980809
2) BS Higgins, CJ Mueller, DL Siebers: SAE 1999-01-0519

Injection System	Detroit Diesel, Common Rail
Number of Orifices	1-Cylindrical and Non-hydroground
Orifice Diameter [μm]	100 to 500 L/D = 4.2
Injection Pressure [MPa]	40 to 180
Ambient Temperature [K]	700 to 1300
Ambient Gas Composition	N_2, H_2O, O_2, CO_2
Ambient Density [kg/m^3]	3.3 to 60
Oxygen concentration	15-21 %
Fuel Density [kg/m^3]	832
Fuel Temperature [K]	400
Discharge Coefficient	0.78 to 0.84



Why is the liquid length higher for Biodiesel?

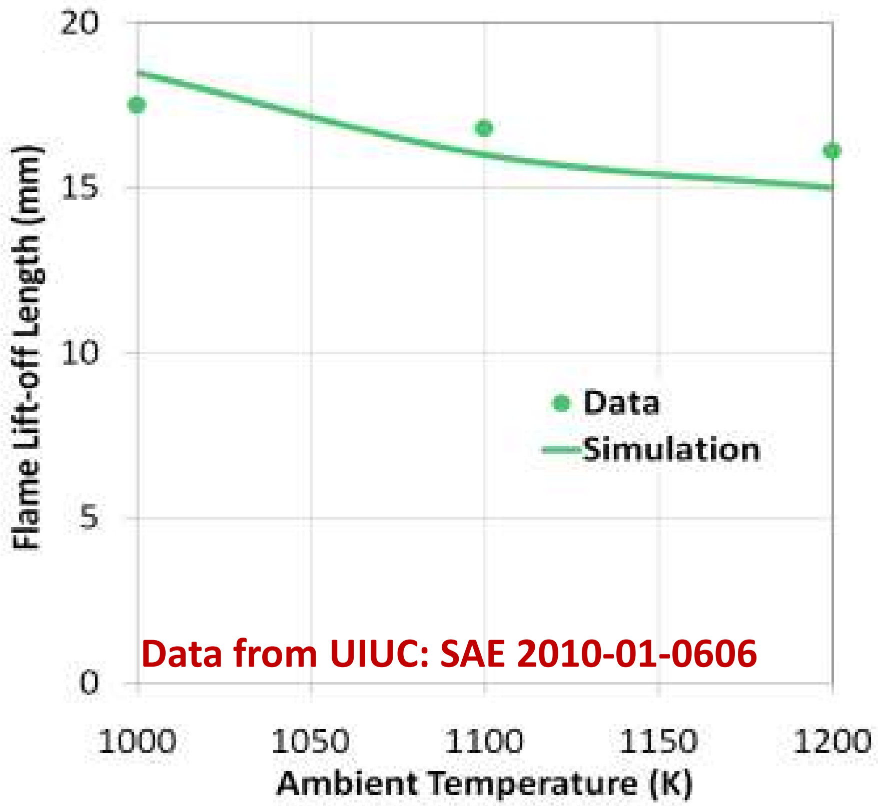


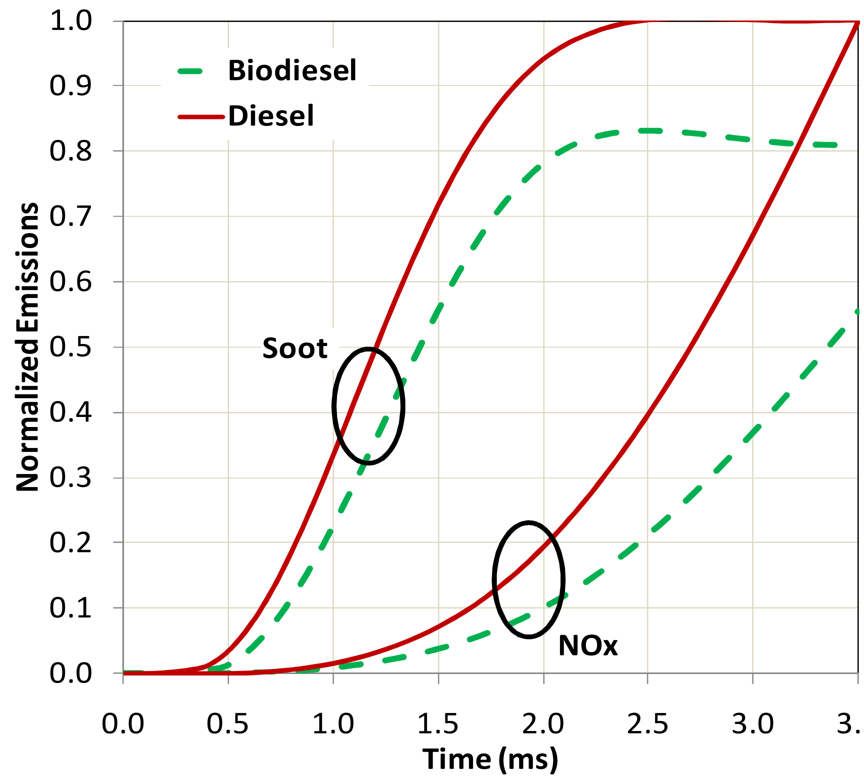


Slower breakup for biodiesel* is due to lesser amount of inner nozzle turbulence and cavitation. This results is increased spray penetration and reduction in spray cone-angle!

***S Som, DE Longman, AI Ramirez, SK Aggarwal. *FUEL* 2010**

Combustion Modeling with Detailed Chemistry





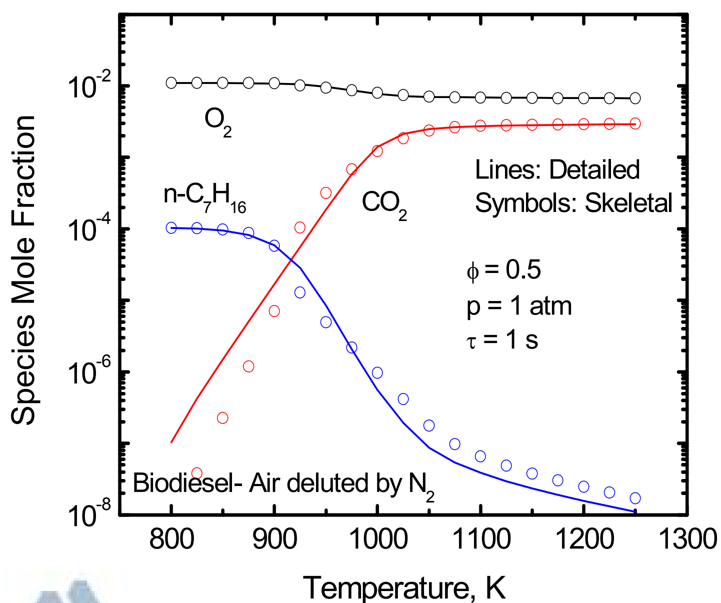
- Diesel surrogate (n-heptane): 42 species, 168 reaction mechanism from Chalmers University
- Biodiesel surrogate (methyl butanoate): 41 species, 150 reaction mechanism {Brakora et al. SAE 2008-01-1378}
- Lower soot emission trends with biodiesel well captured
- Biodiesel surrogate not able to capture the accurate NOx trends!

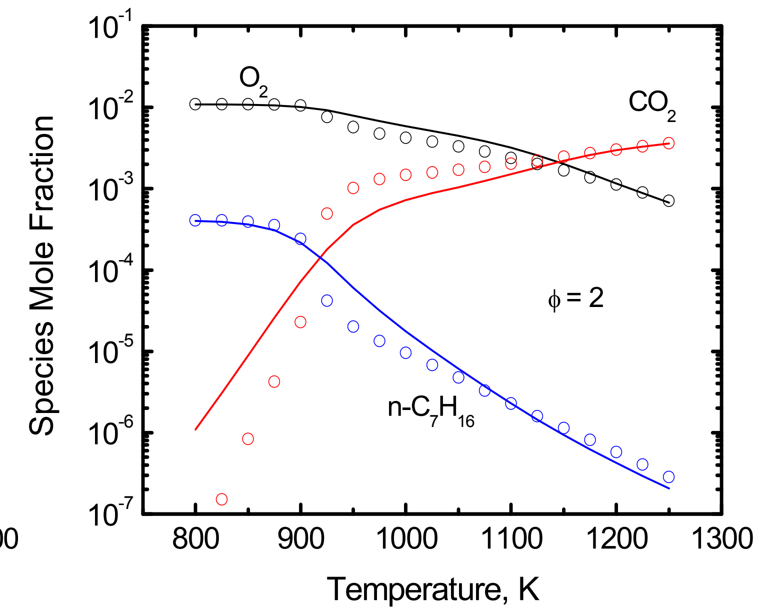
Biodiesel Kinetic Model* for ICE Applications

- Detailed Mechanism (Methyl Decanoate + Methyl Decenoate + N-heptane) from LLNL 2010: 3329 species, 10806 reactions
- Directed Relation Graph (DRG) reduction: 664 species, 2672 reactions
- Isomer lumping : 641 species, 2670 reactions
- Sensitivity analysis aided DRG and error cancellation:
- Range of operation:
  - Pressure: 1-100 atm
  - Equivalence ratio: 0.5-2.0
  - Initial temperature: 700 – 1800 K

123 species, 394 reactions
89 species, 364 reactions

***Z. Luo, M. Plomer, T. Lu, S. Som, D.E. Longman, IC#18.**
US National Combustion Institute meeting, March 2011



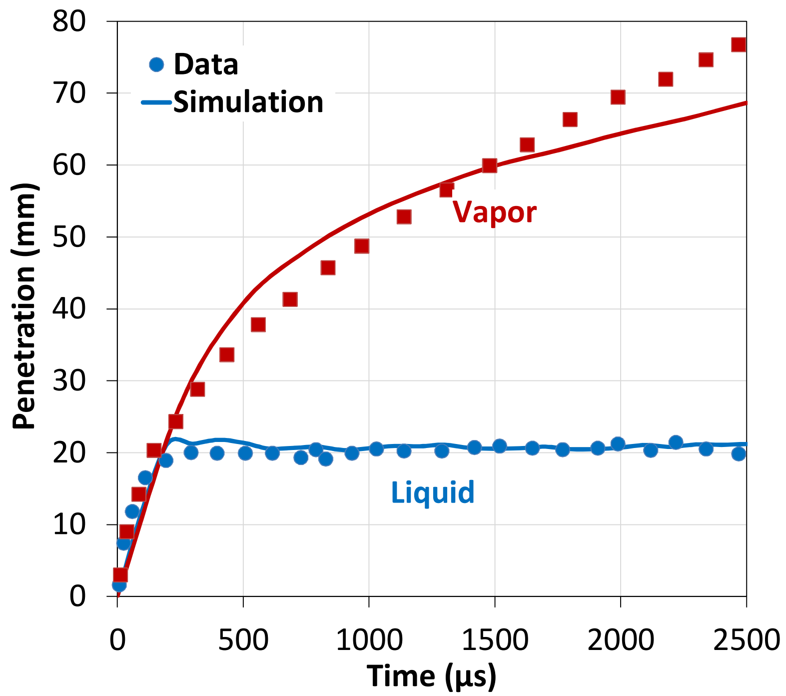


JSR Data:
Dagaut et al. PCI 31 (2007)

Biodiesel: Case set-up

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/m^3]	22.8
Chamber Temperature [K]	1000
Fuel Density [kg/m^3]	877
Fuel Injection Temperature [K]	363

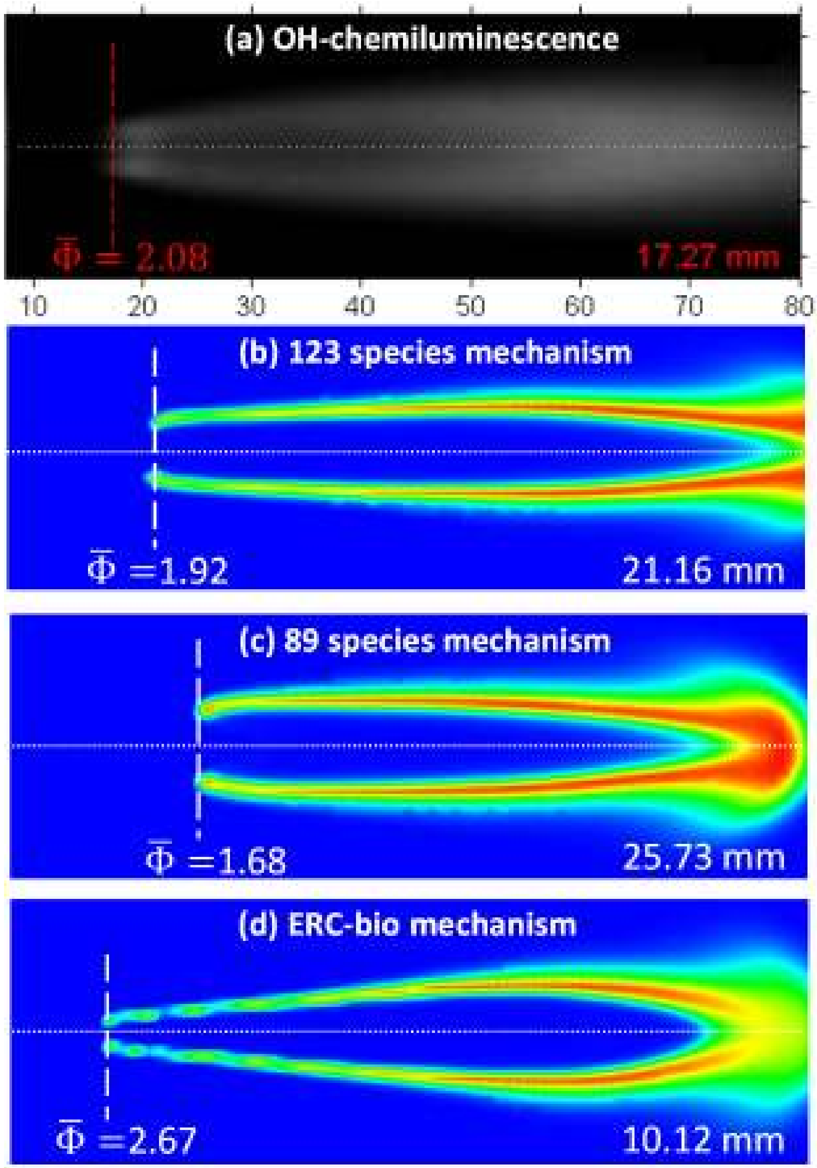


*Pickett & Co-workers (2011) *Personal Communication*

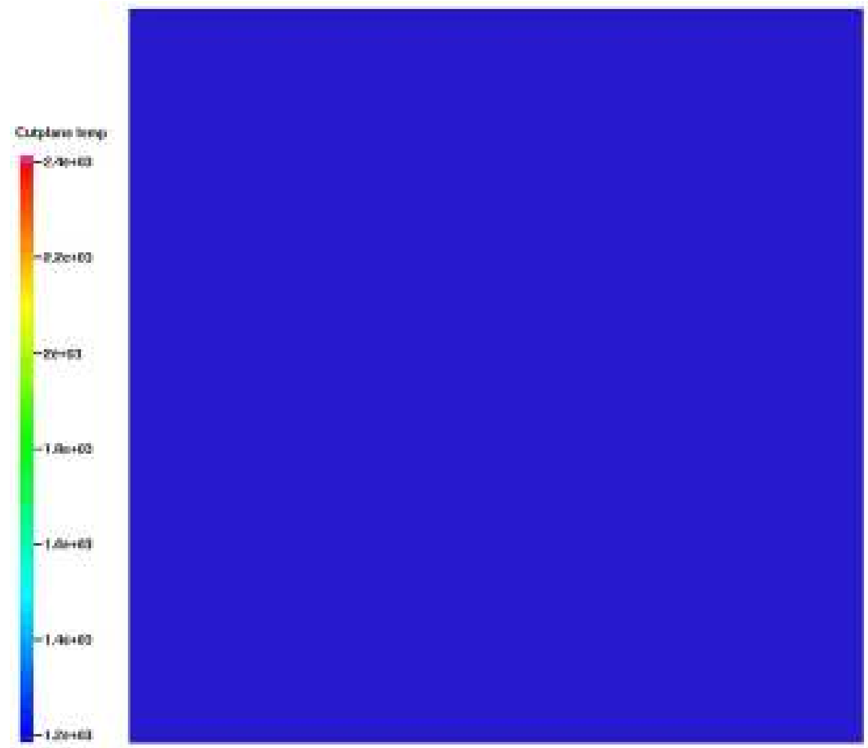
JG Nerva, CL Genzale, JMG Oliver, LM Pickett. Fundamental Spray and Combustion Measurements of Biodiesel under Diesel steady conditions. *Under preparation*

- Lu – 123: 123 species, 394 reactions. Paper # IC18. US National Combustion Meeting, March 2011
- Lu – 89 : 89 species, 364 reactions. Paper # IC18. US National Combustion Meeting, March 2011
- ERC-bio mechanism: 41 species, 150 reactions. SAE Paper No. 2008-01-1378

Validation of Different Reaction Mechanisms



	Ignition Delay (ms)
Sandia Data	0.396
Lu - 123 species	0.510
Lu - 89 species	0.580
ERC-Bio mechanism	0.220



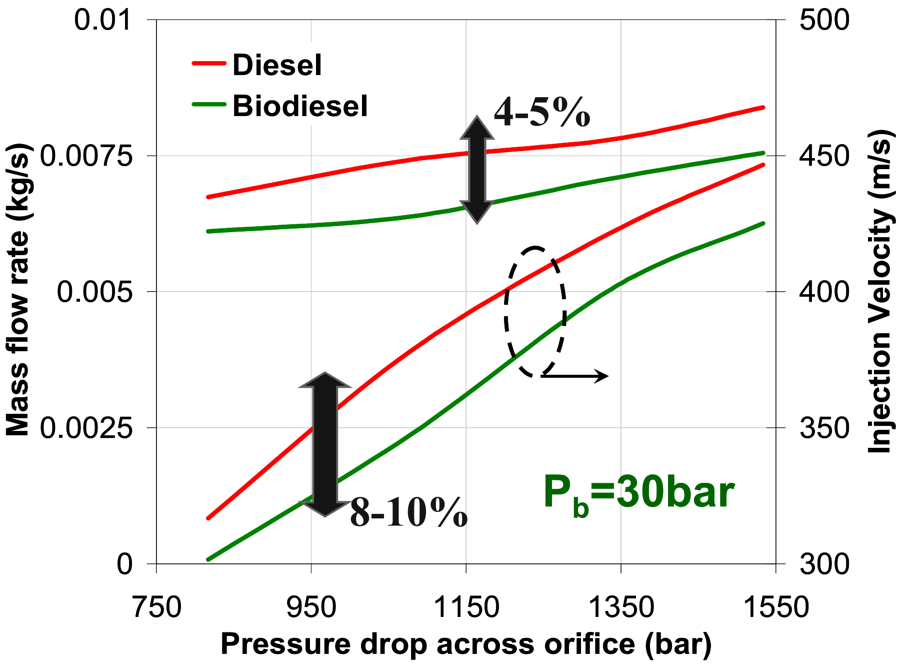
Summary & Future Work

- ❑ Developed **KH-ACT primary breakup** model:
  - ✓ Captures biodiesel spray characteristics accurately
  - ✓ Predicts influence of nozzle orifice geometry
- ❑ Integrated Modeling Approach:
  - ✓ Coupled nozzle-flow, spray, and combustion modeling
  - ✓ Robust **validation against x-ray radiography data**
- ❑ Combustion modeling with detailed chemistry:
  - ✓ MD+MD9D+NHPT as a surrogate for biodiesel
  - ✓ **123 species (MD+MD9D+NHPT) mechanism** captures flame characteristics well
- ❑ **Full-cycle engine simulations** with KH-ACT model against CAT single-cylinder engine data
  - o Engine testing currently in progress at Argonne
- ❑ Turbulence Modeling:
  - o Coupling **high-fidelity LES model** with detailed chemistry

Thank You

Contact: ssom@anl.gov dlongman@anl.gov

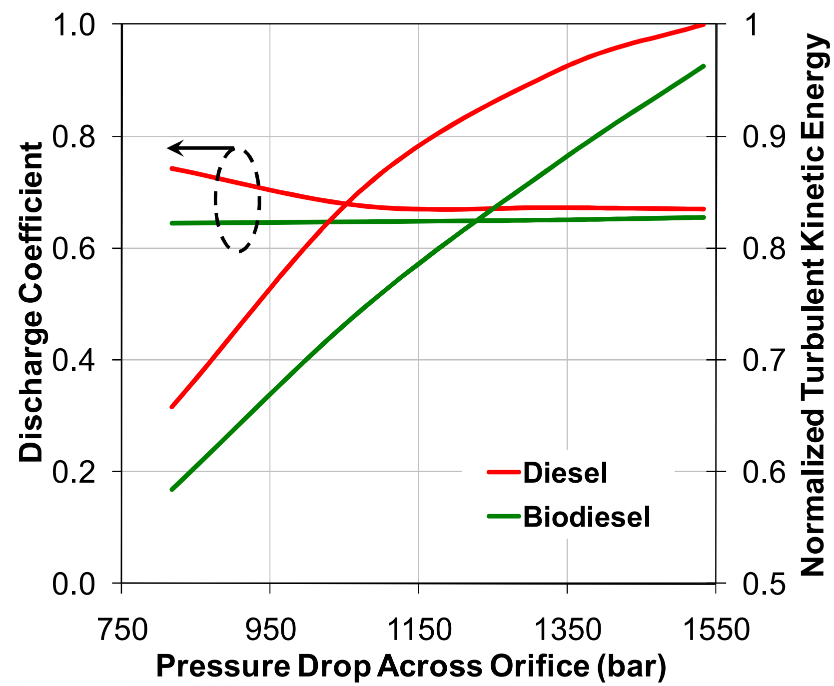
Nozzle Exit Characteristics



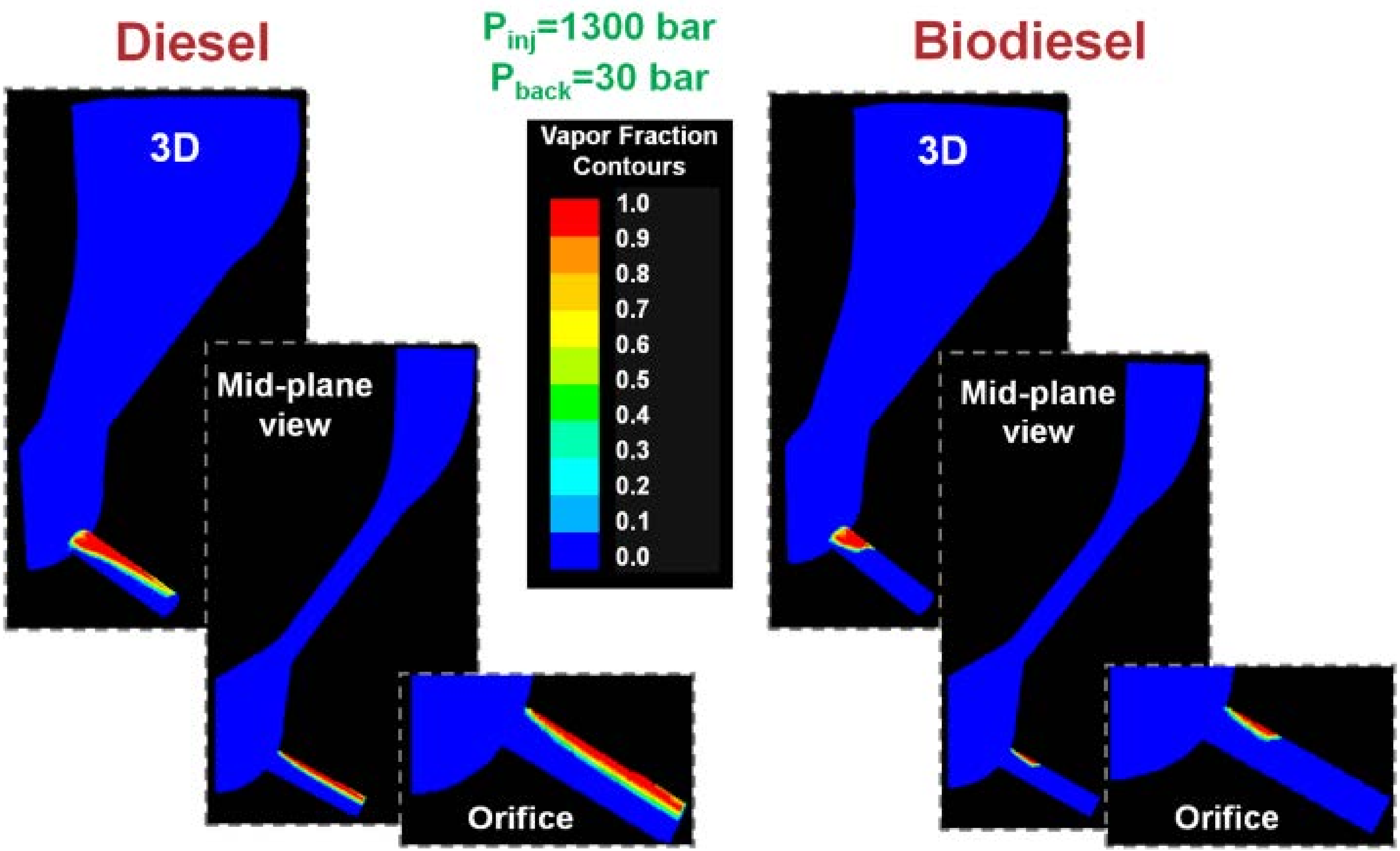
- Lower levels of turbulence and cavitation for biodiesel
- Breakup process with biodiesel may be slower!

$$C_d = \frac{\dot{M}_{actual}}{\dot{M}_{th}} = \frac{\dot{M}_{actual}}{A_{th}\sqrt{2*\rho_f*\left(P_{inj}-P_{back}\right)}}$$

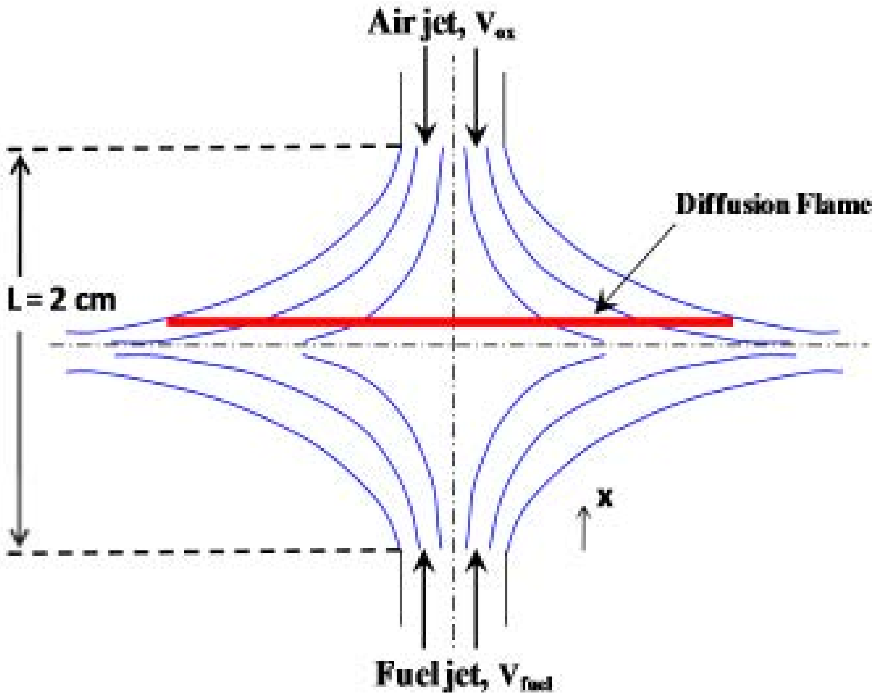
- Lower injection velocity, mass flow rate, and discharge coefficient for biodiesel
- This is due to biodiesel's significantly <u>higher molecular and turbulent viscosity</u>
- Significant differences in inner nozzle flow characteristics



Vapor Distribution

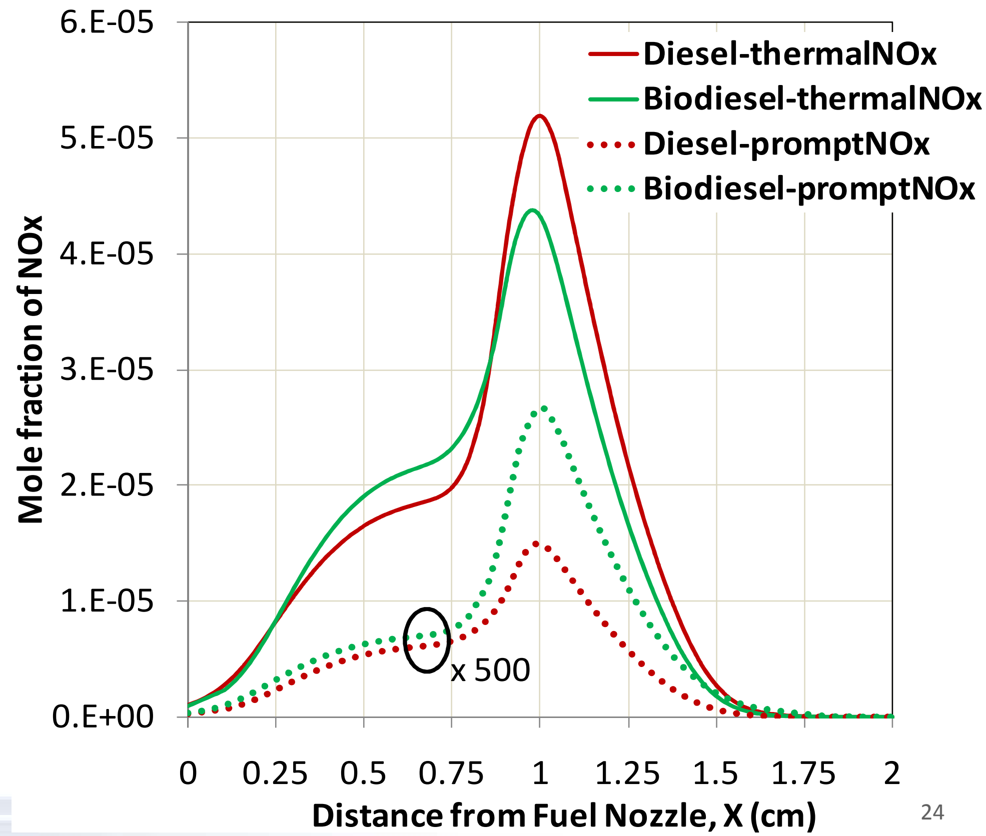


Emission Characteristics in 1-D Configuration

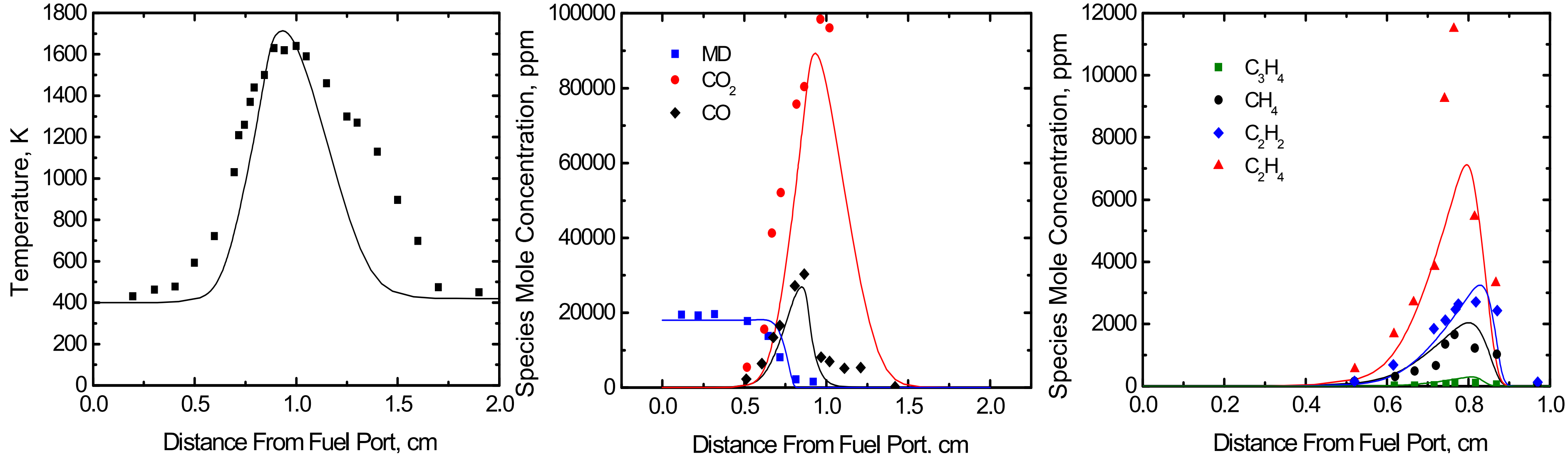


- Counter-flow configuration to study the NOx chemistry further
- GRI-3.0 NOx chemistry consisting of prompt, thermal, N_2O
- Simulations performed in CHEMKIN 4

- Prompt NOx higher for biodiesel compared to diesel
- Thermal NOx higher for diesel
  - Radical pool not captured properly by the mechanisms



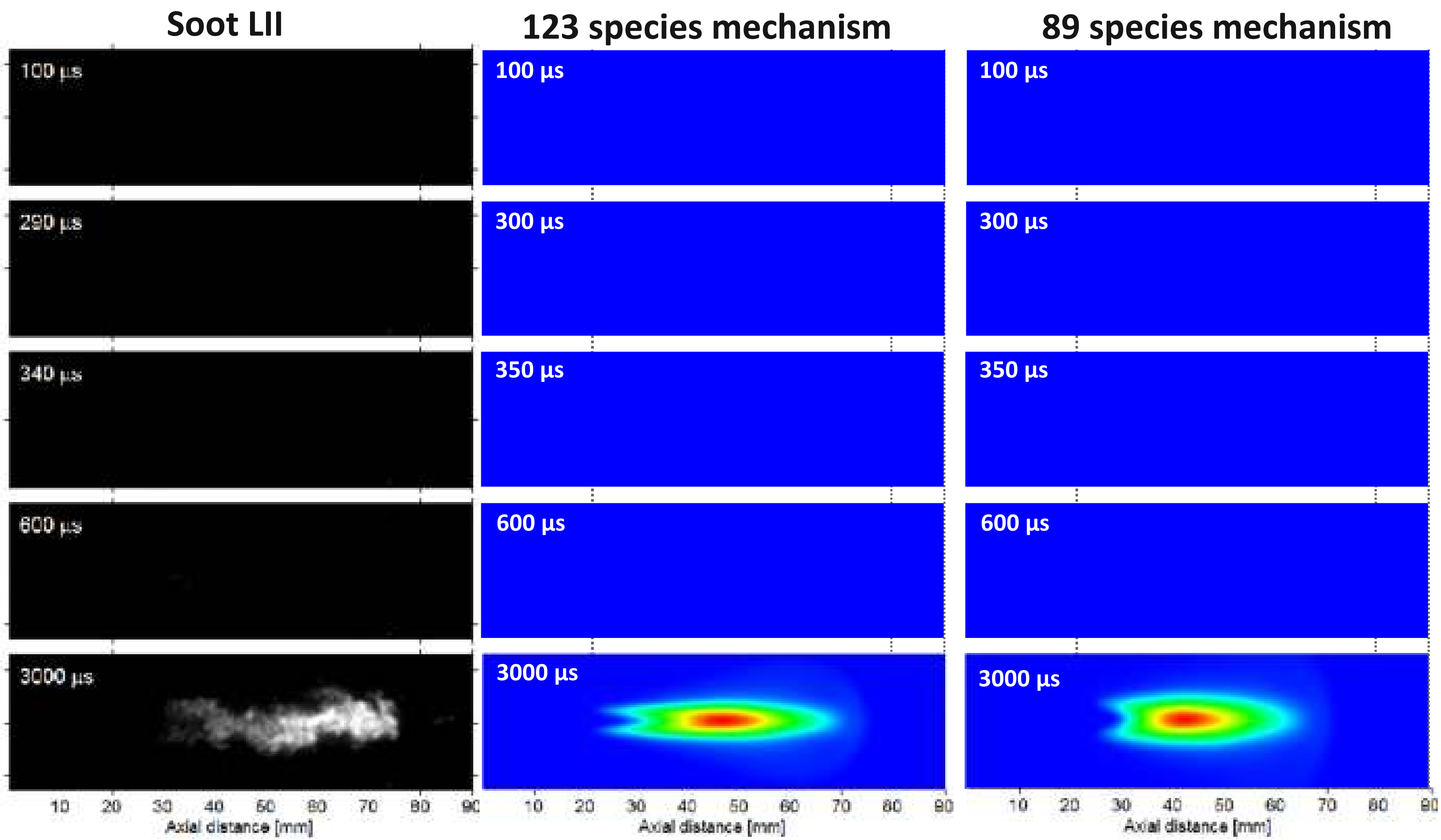
Biodiesel Kinetic Model* for High-T Applications



- Detailed Mechanism (Methyl Decanoate + Methyl Decenoate + N-heptane) from LLNL 2010: 3329 species, 10806 reactions
- Directed Relation Graph (DRG) reduction: 472 species, 2237 reactions
- Isomer lumping and DRG reduction: 242 species, 1819 reactions
- Sensitivity analysis aided DRG: 118 species, 83 reactions final mechanism
- Range of operation:
  - Pressure: 1-100 atm
  - Equivalence ratio: 0.5-2.0
  - Initial temperature > 1000 K

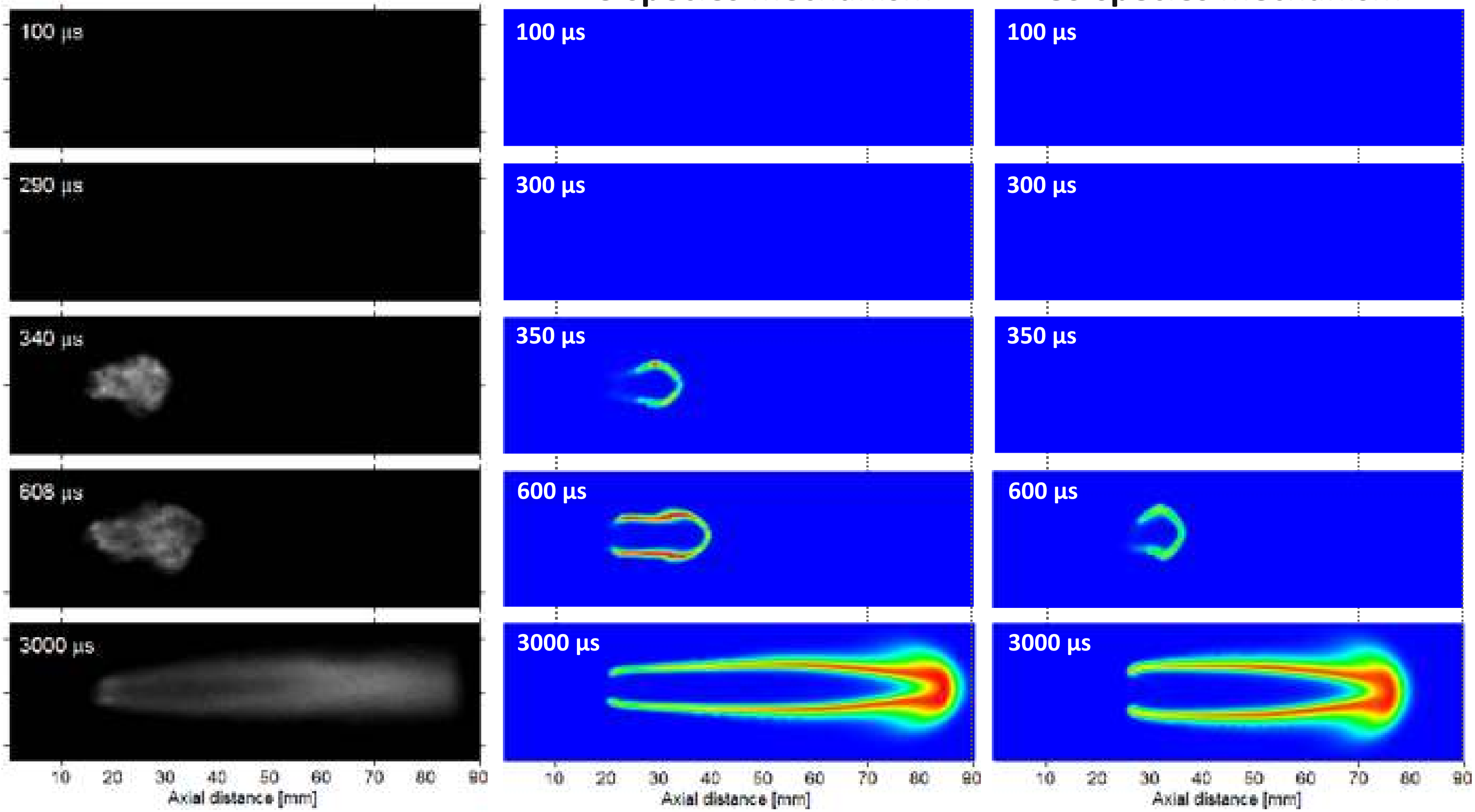
* **Z. Luo, M. Plomer, T. Lu, S. Som, D.E. Longman, *Energy & Fuels* (2010)**

Soot Validation with MD+MD9D+NHPT Mechanism



Further Validation of Biodiesel Kinetic Models

OH-chemiluminescence | 123 species mechanism | 89 species mechanism



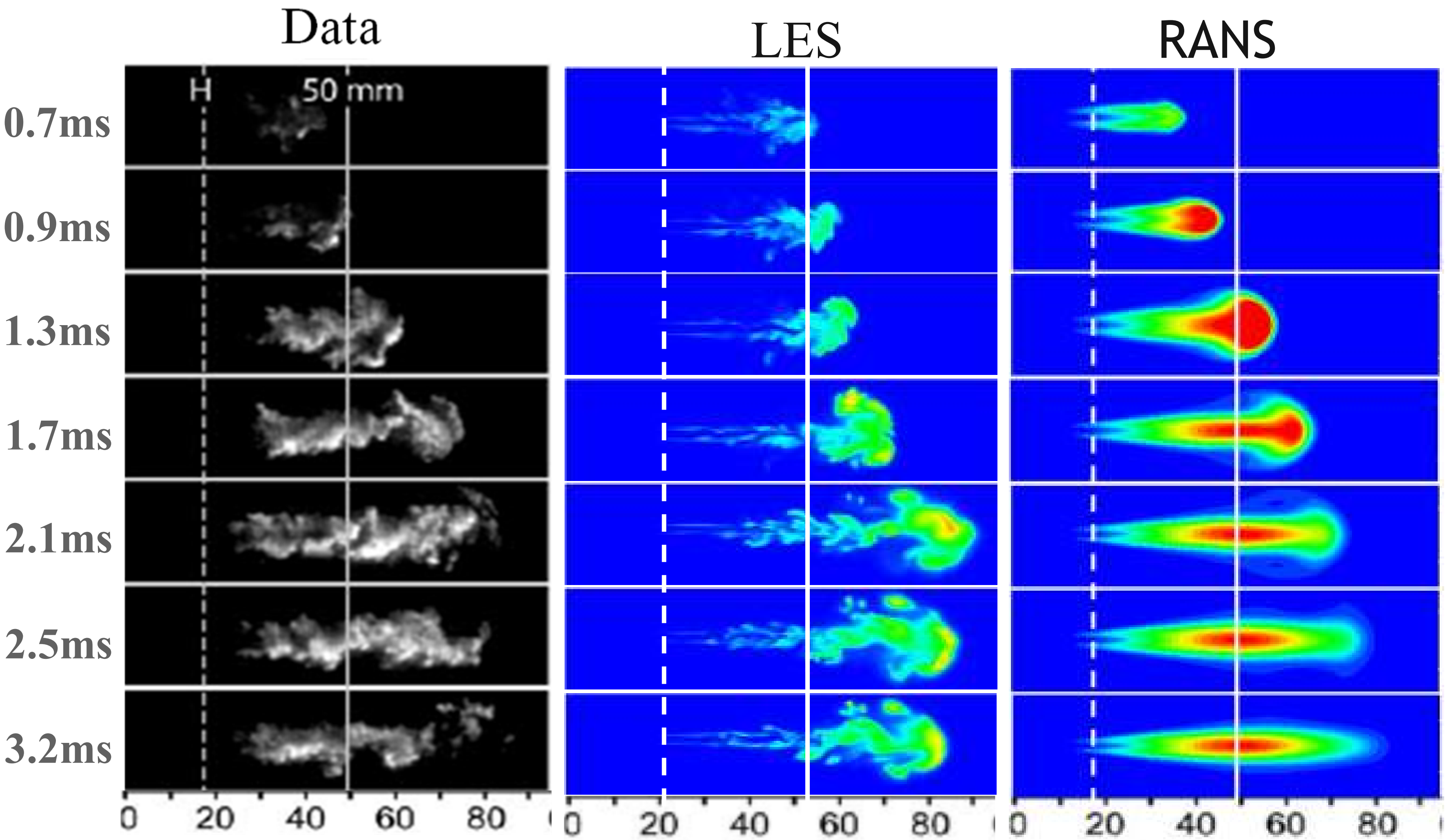
~ 160 hours on 8 processors | **~ 85 hours on 8 processors**

LES Modeling with Detailed Chemistry

Smagorinsky based LES Model:

- 0.125 mm minimum grid size
- 2 millions grid points for resolving a 108 mm (each side) cube
- 8-10 days on 24 processors

Soot Prediction with RANS & LES Models



LM Pickett & DE Siebers, Combustion and Flame 2004

2 million cells

0.3 million cells

C_2H_2 used as a soot precursor!