Modeling & Simulation Capabilities at Argonne for ICE Applications

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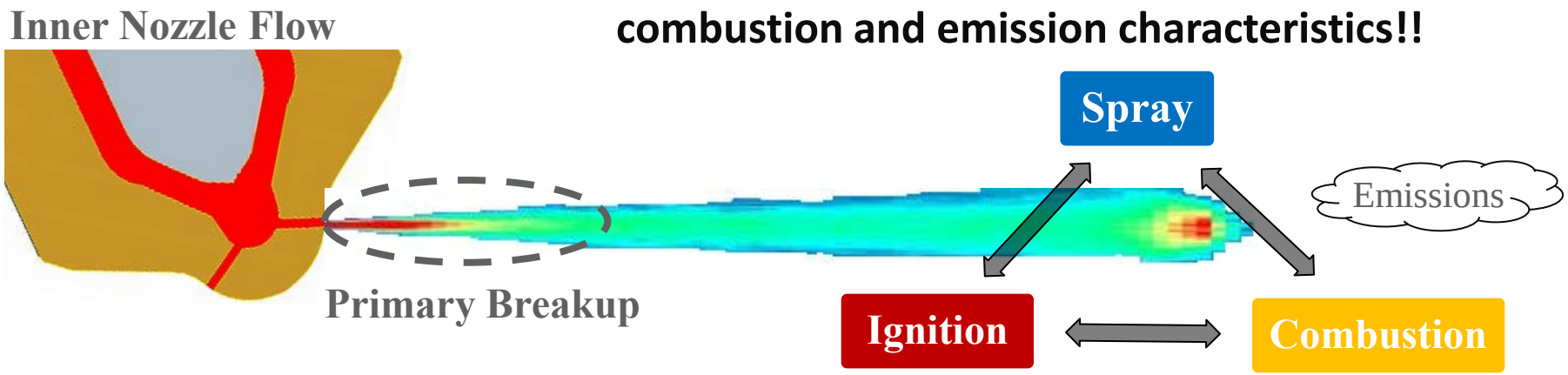
Presentation to: FORD – Diesel combustion modeling global meeting

Outline

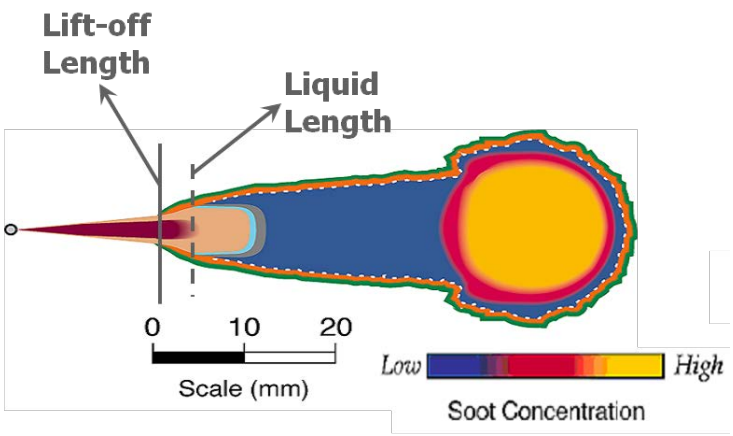
- Detailed inner-nozzle flow simulations:
  - Diesel # 2 vs. Biodiesel (SME)
  - Cylindrical, conical, hydroground nozzle geometries
- Spray modeling:
  - Development of KH-ACT spray breakup model
  - Coupling with nozzle flow simulations: Effect of nozzle orifice geometry
  - Validation against x-ray radiography data from Argonne
  - Validation against optical data from Sandia
  - Diesel vs. Biodiesel (SME)
- Combustion modeling:
  - Detailed chemistry approach integrated with spray models
  - Development of chemical kinetic models for diesel and biodiesel surrogates
  - Validation against ignition delay and flame lift-off data
- Other topics of interest to Argonne
- Opportunities of Collaboration

Integrated Modeling Approach

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



Conceptual Combustion Model from Sandia National Laboratory

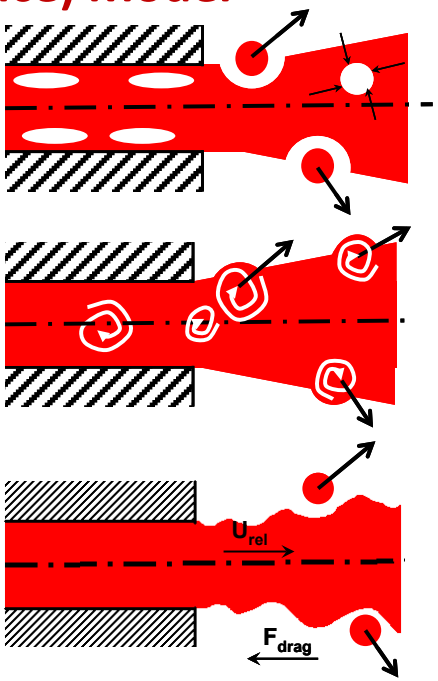


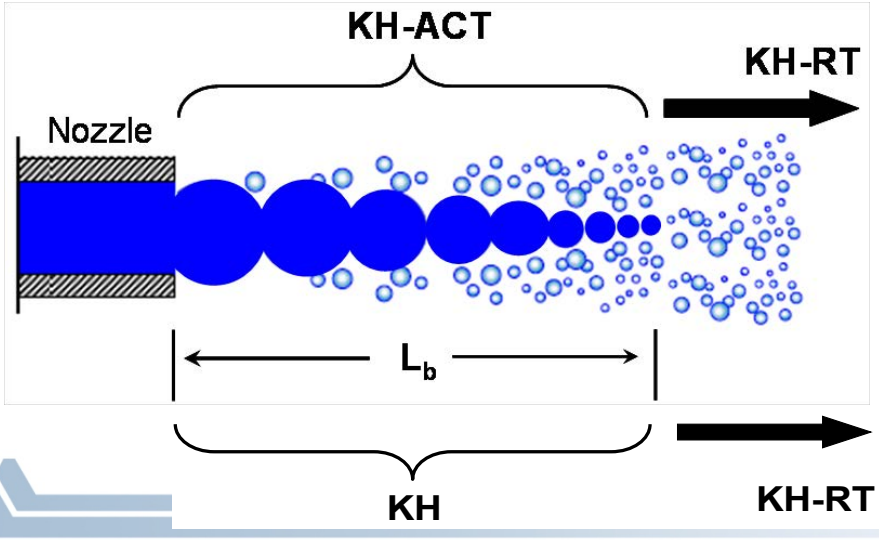
- Detailed inner-nozzle flow modeling with realistic fuel properties
- **KH-ACT** primary breakup model: Aerodynamics, Cavitation, Turbulence
- Spray Validation
  X-ray radiography data
- **Detailed Chemistry**:
  Methyl Butanoate
  Methyl Decanoate
  } **Biodiesel Surrogate**

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 Paper No.* 2009-01-0838
Som et al., *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

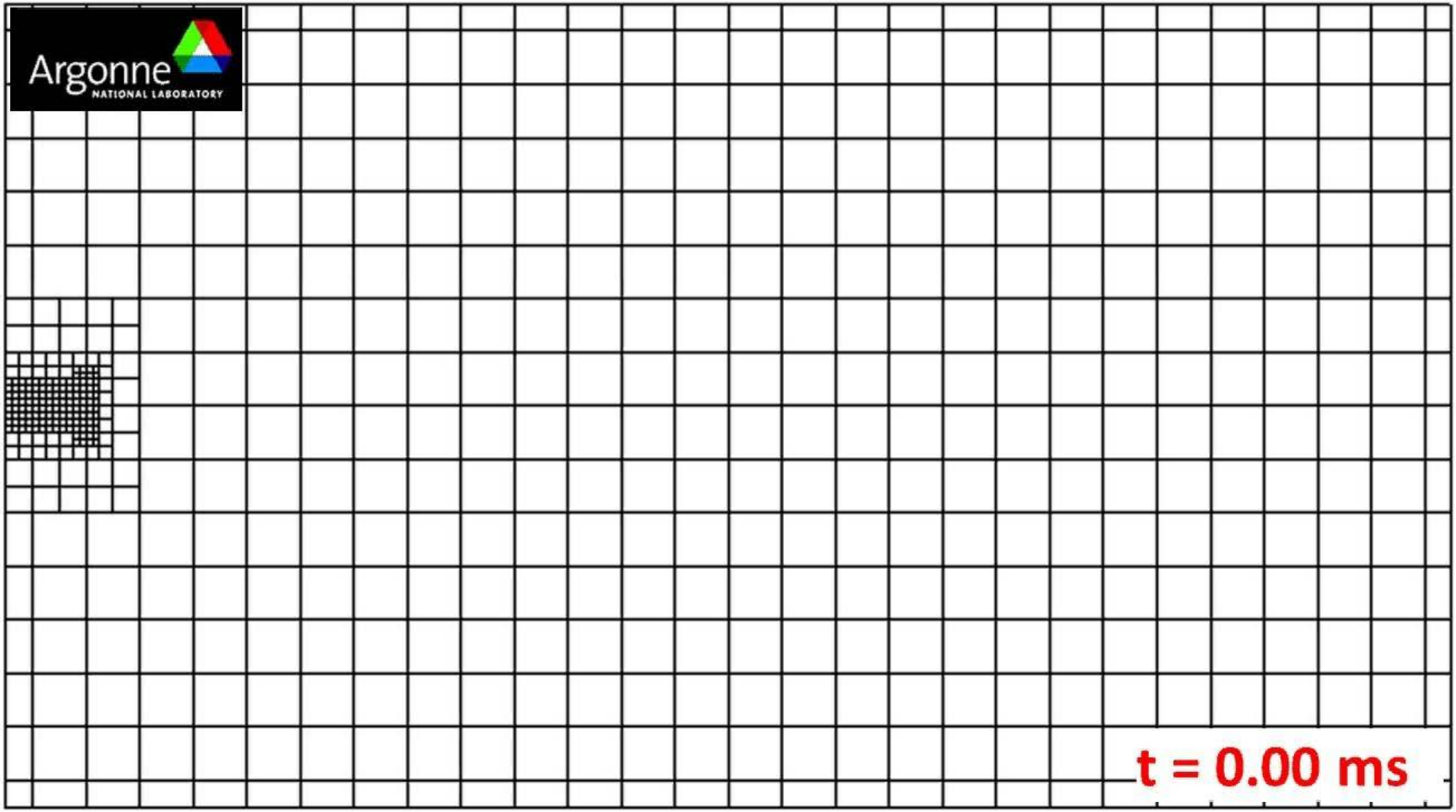
KH-ACT model implemented in CONVERGE

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

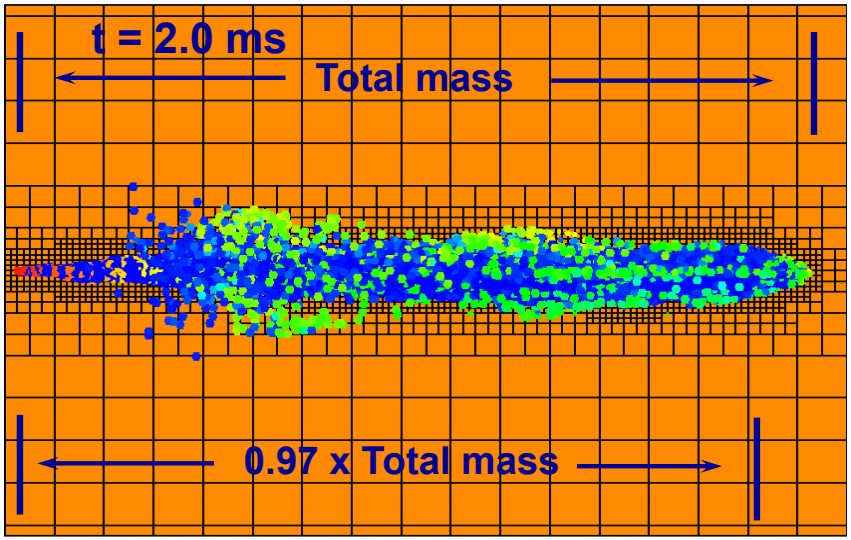
Total grid number	**30K-40K for 0.5mm – RANS simulations (Non-reacting)** **1.3 million for 0.125mm – LES case (Reacting) @ 3 ms**
Parallelizability	**Good scalability up to 48 processors**

Adaptive Mesh Generation



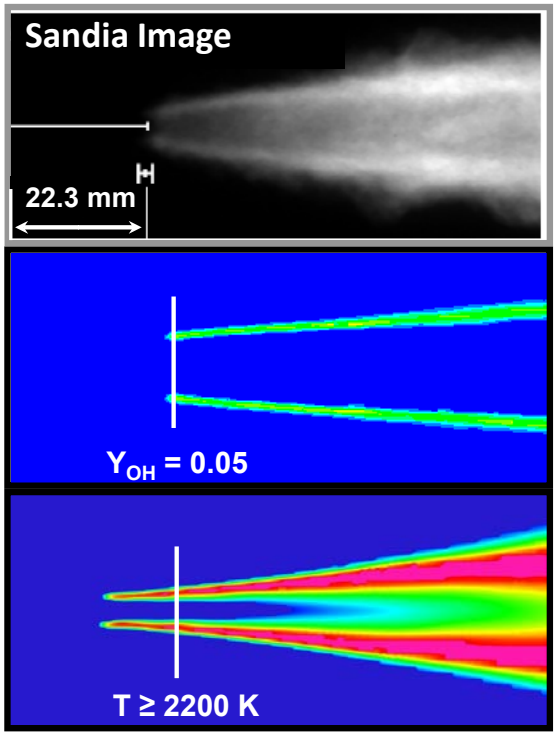
Base Grid Size = 4 mm, Minimum Grid Size = 0.5 mm

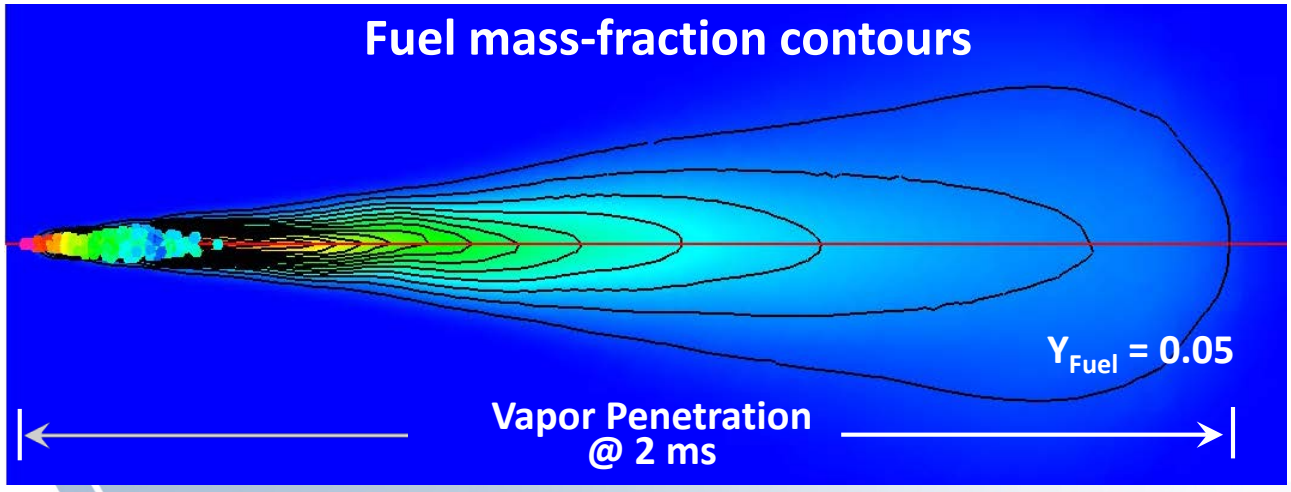
Some Definitions



Spray penetration @ 2 ms

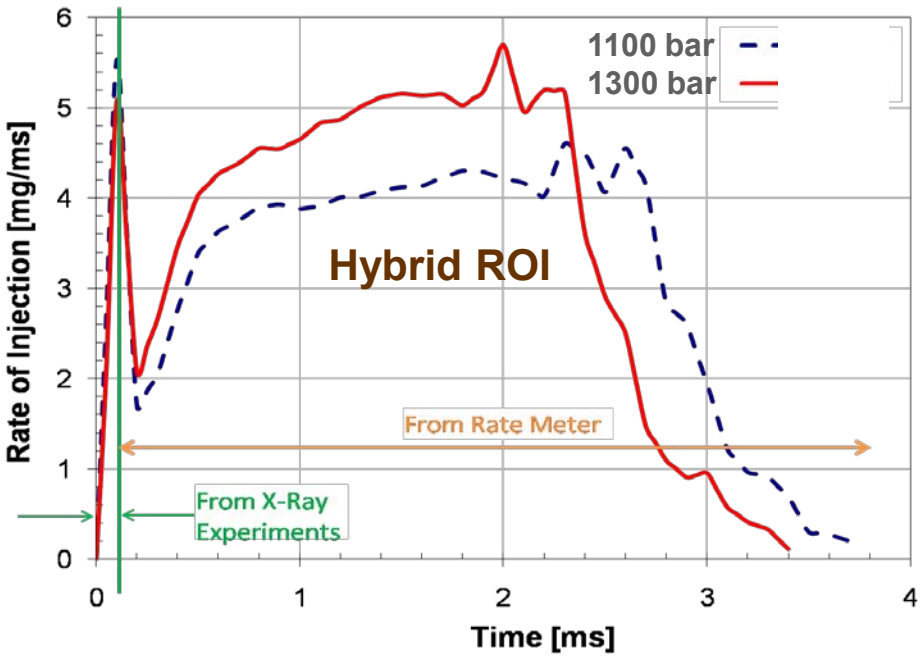
Lift-off length





Ignition delay: Ignition is said to occur when T ≥ 2000 K in a particular cell. Usually, coincides with appearance of OH.

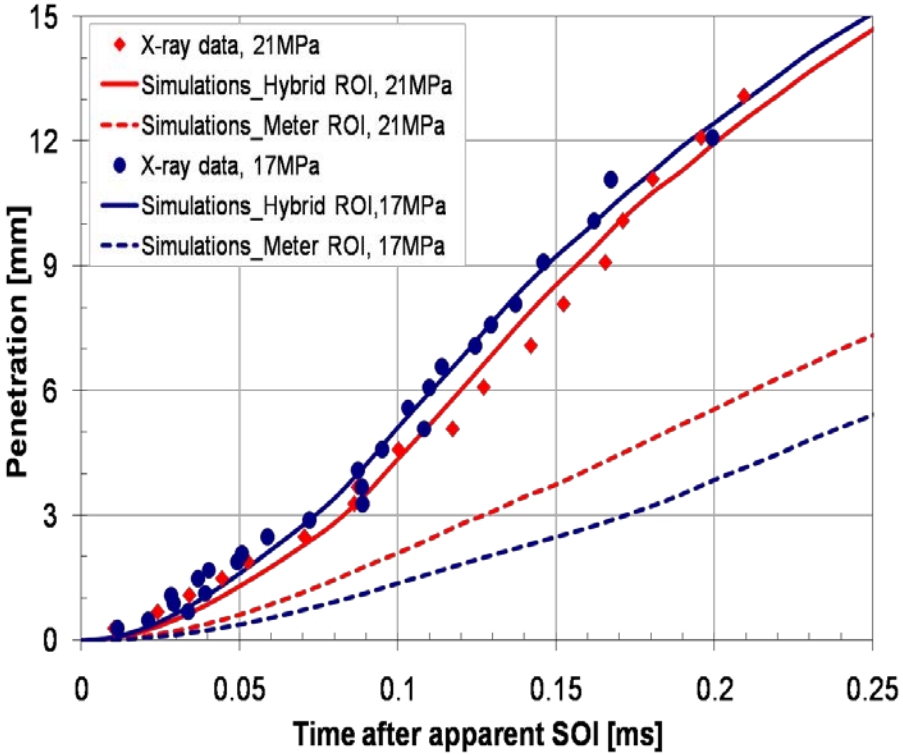
Initial Transience*



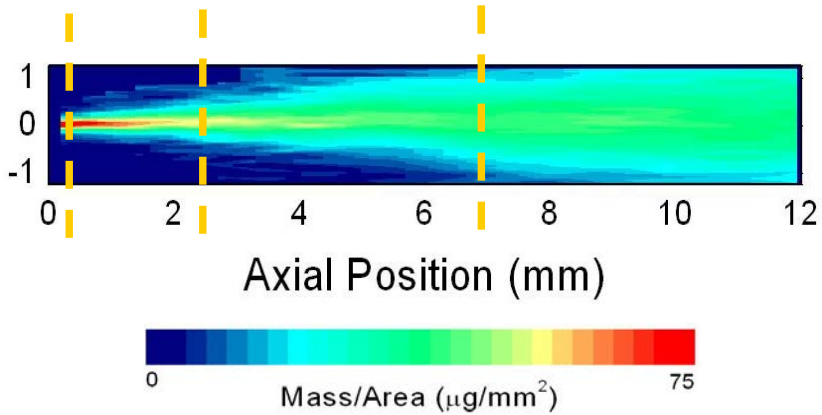
- A slow penetration region is found up to 0.1ms.
- A faster penetration region follows up to 0.2 ms, where penetration scales linearly with time.

Ramirez et al. *ILASS* 2008, *JEF* 2009

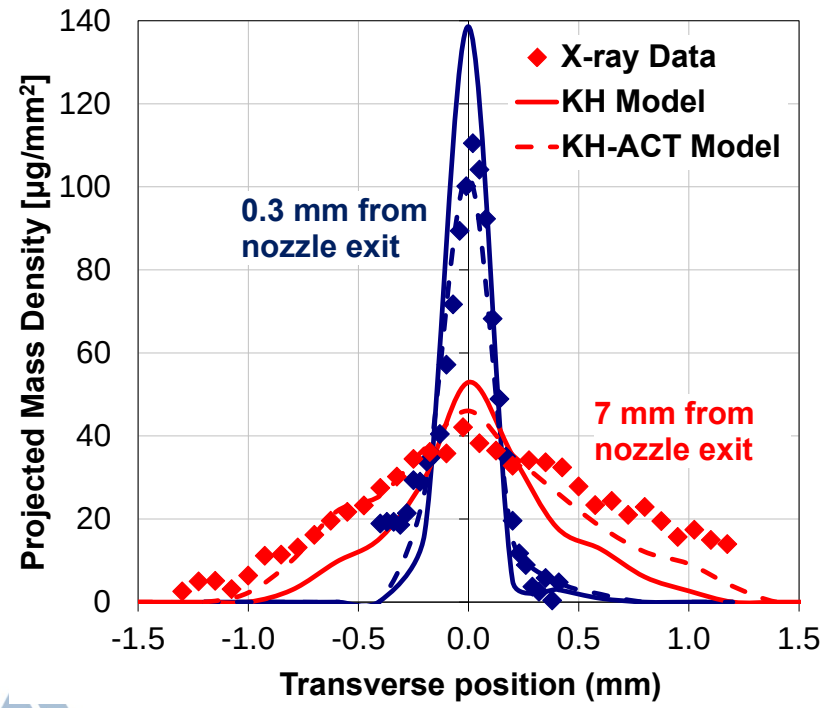
- Hybrid ROI was constructed mating information from x-ray studies and Bosch rate meter
- Only with this hybrid ROI, spray penetration trends could be accurately captured. Lower injection pressure case initially penetration further.

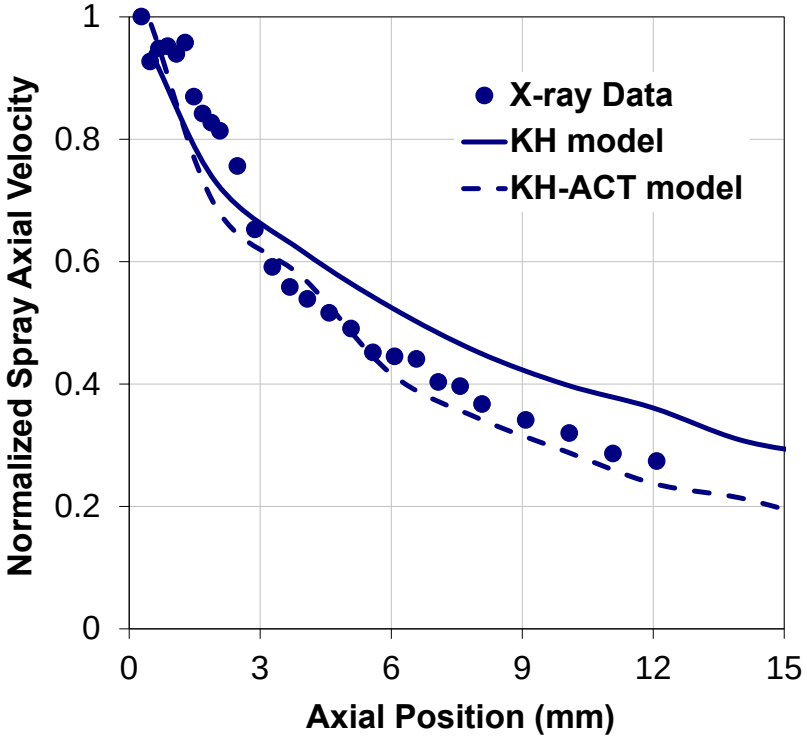


Spray Validation against X-ray Data



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



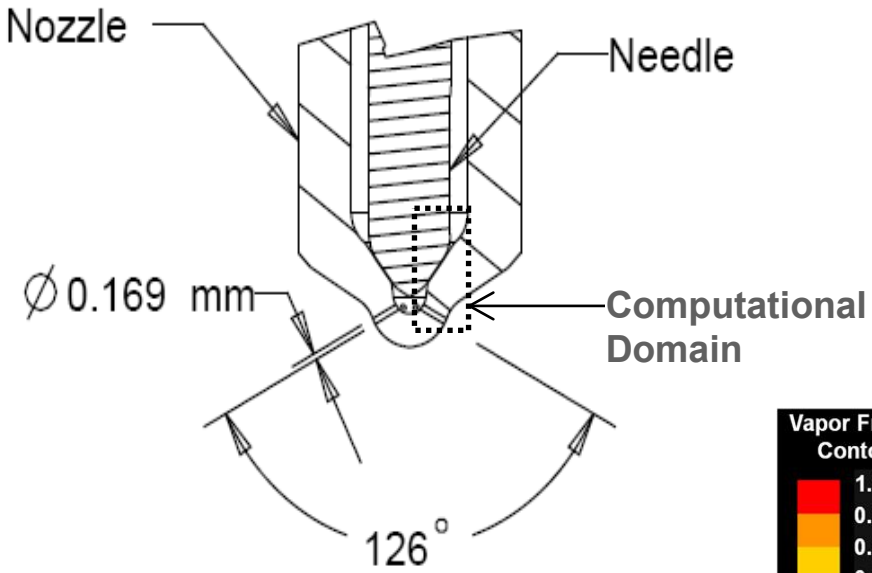


- The spray loses half of its initial velocity within the first 6 mm
- Simulation capture the Gaussian mass distributions from x-ray data well
- Spray Dispersion accurately captured by only the KH-ACT model. KH model under-predicts spray spreading

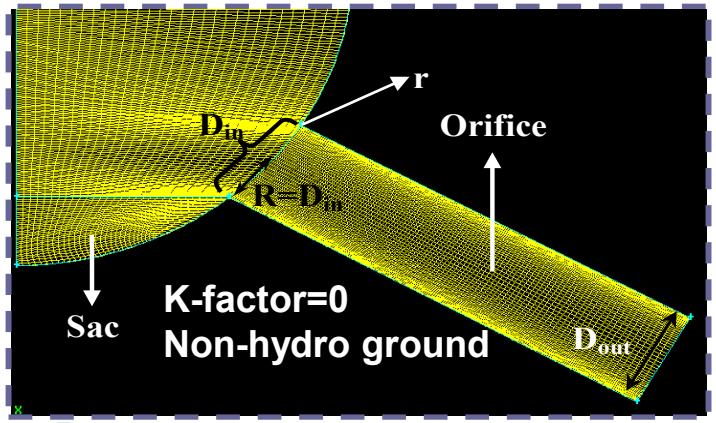
Effect of Nozzle Orifice Geometry

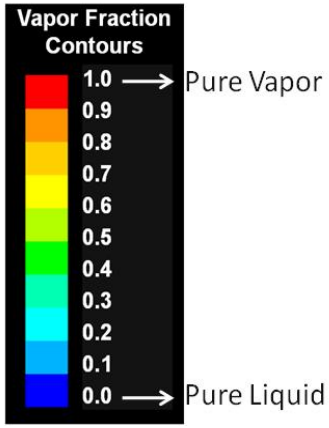
Injector Geometry and Grid Generated

6-hole production Injector

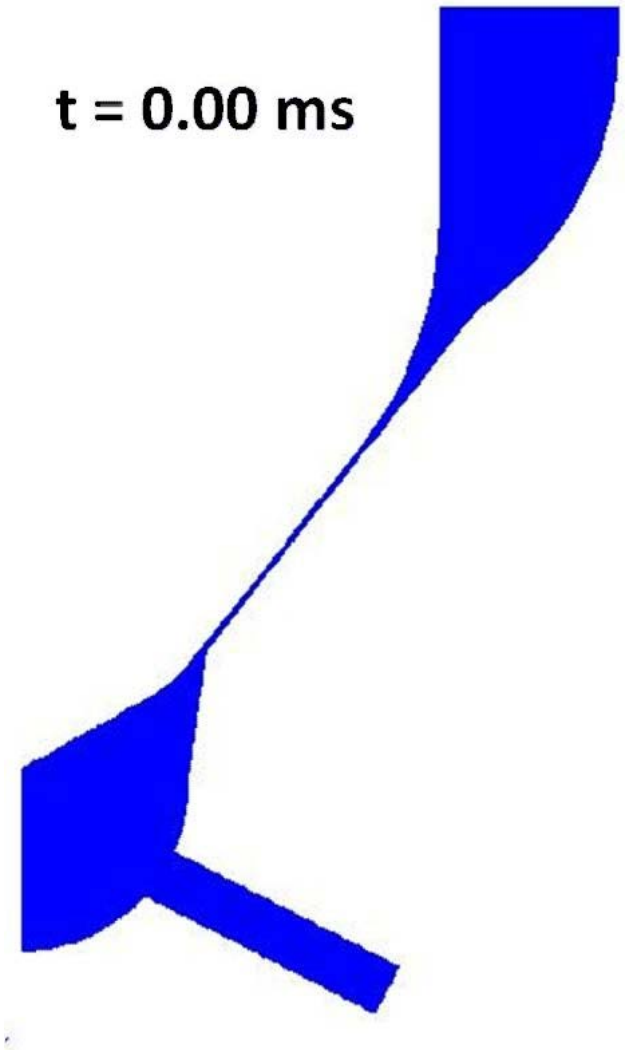


Nozzle Orifice





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

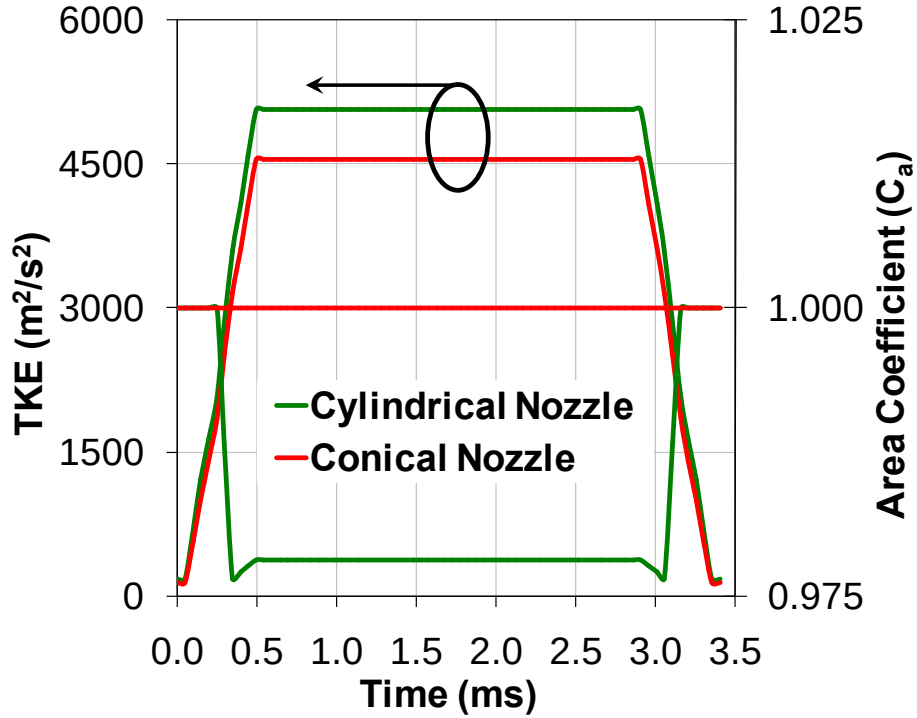


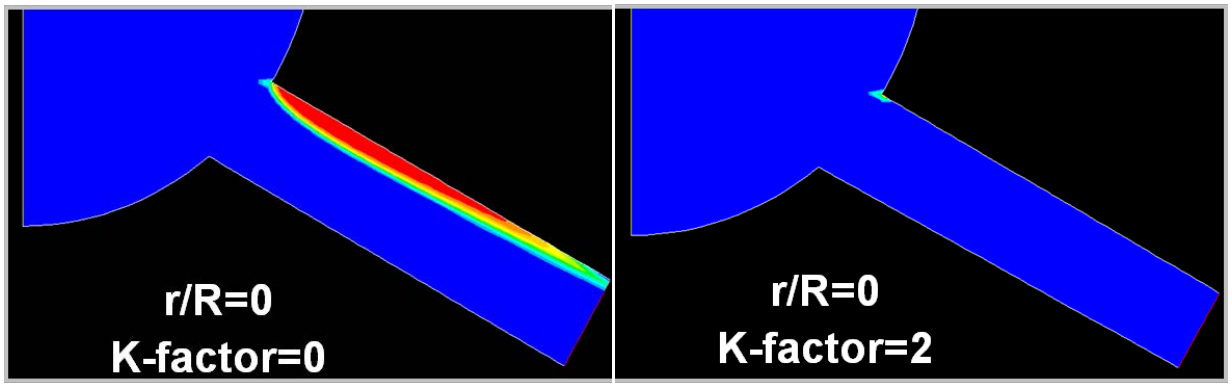
*Som et al., *FUEL* (2010)
Som et al., *JEGTP* (2010)

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

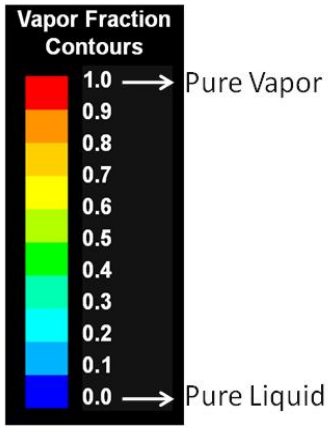
$$K_{factor} = \left(\frac{D_{in} - D_{out}}{10} \right) \mu m$$



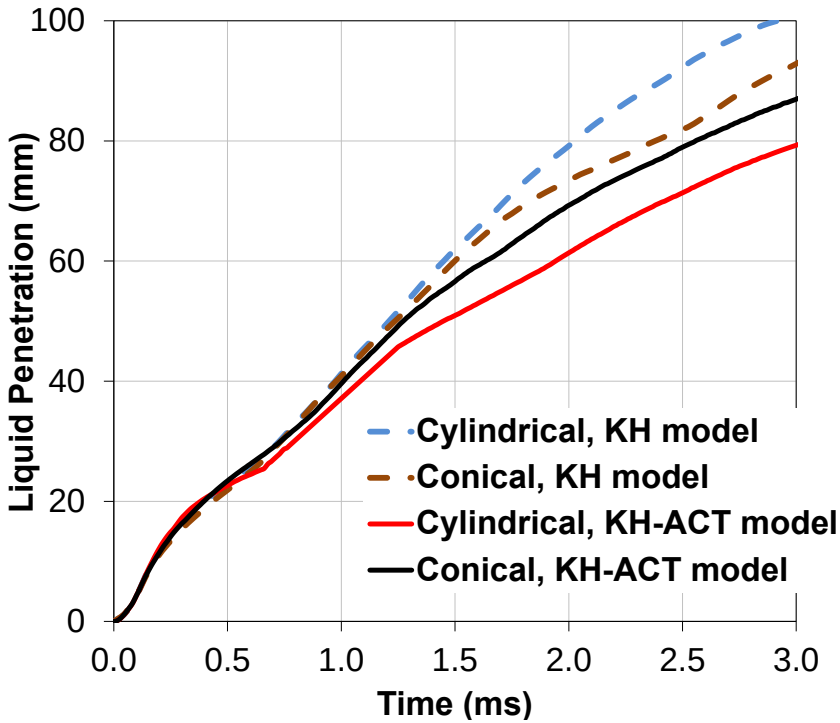


Cylindrical Nozzle

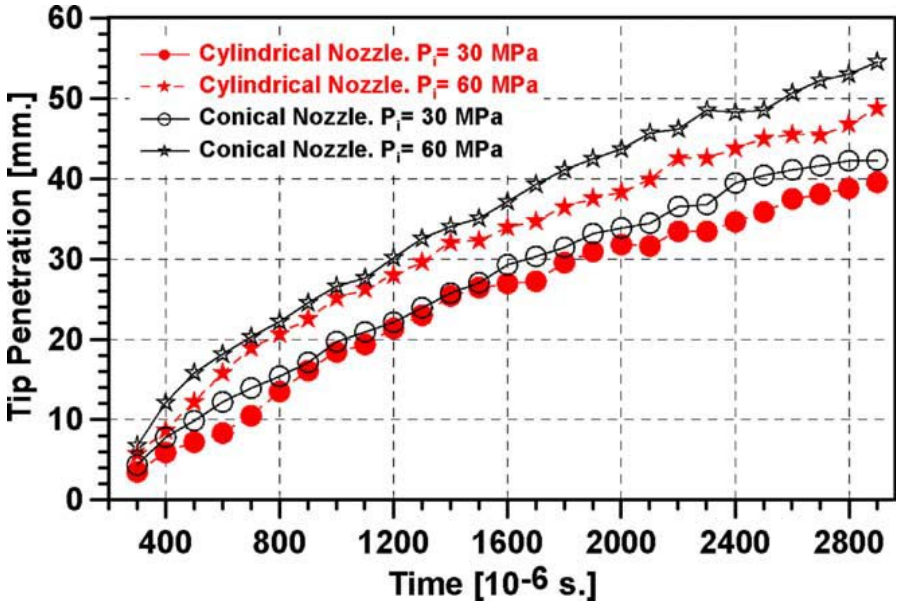
Conical Nozzle



Influence of Nozzle Geometry on Spray Penetration



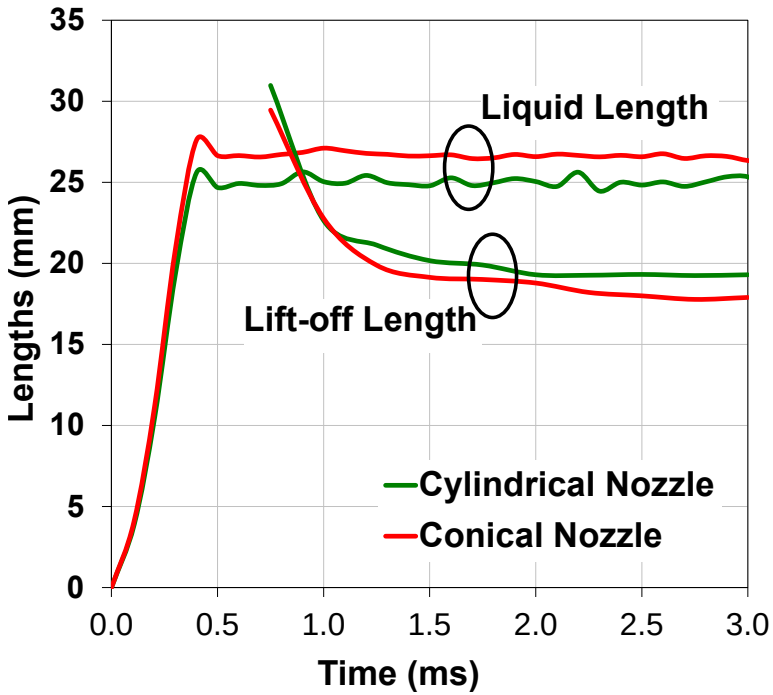
F Payri, V Bermudez, R Payri, FJ Salvador: FUEL (2004)



- 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**

Spray and Combustion Characterization

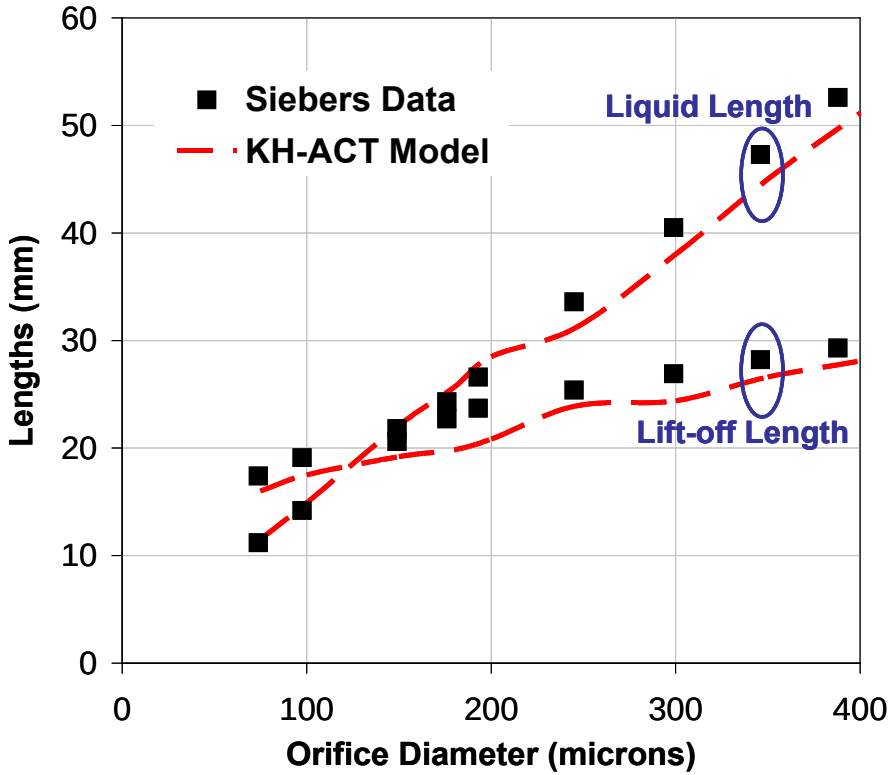


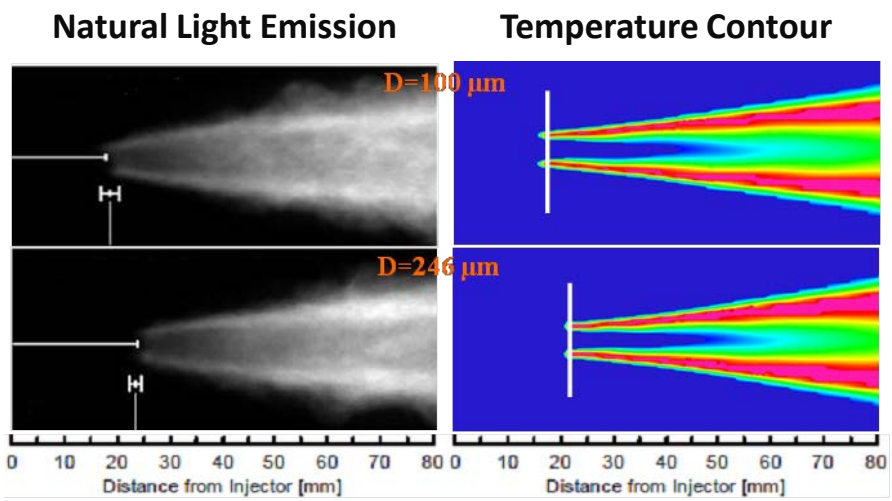
- Liquid length trends are consistent with non-evaporating spray penetration results observed earlier
- Lift-off length trends explained based on amount of fuel injected
- Liquid length always greater than lift-off length showing interaction between spray and combustion processes
- Ignition occurs earlier and closer to orifice tip for the base nozzle

Nozzle type	Ignition time (ms)	Ignition location (mm)	Liquid length (mm)	Liftoff length (mm)
Cylindrical (K=0, r/R=0)	0.42	47.2	25.1	19.3
Conical (K=2, r/R=0)	0.44	48.8	26.9	17.9

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

Effect of Orifice Diameter of Flame Lift-off





*Data from Sandia National Laboratory

$$L_f = \frac{U_0 Z_{st} D}{s_L^2(Z_{st})}$$

- The non-premixed gas jet theory fails to explain this dependence on orifice diameter since it predicts flame lift-off to be independent of the orifice diameter.
- This trend can be explained by the fact that the fuel injection rate and hence the total mass injected increases with increase in orifice diameter. Hence, to form a conducive fuel-air mixture for ignition, the amount of air to be entrained also increases thus increasing the flame lift-off length.

Flame Index for Diesel Engine Applications

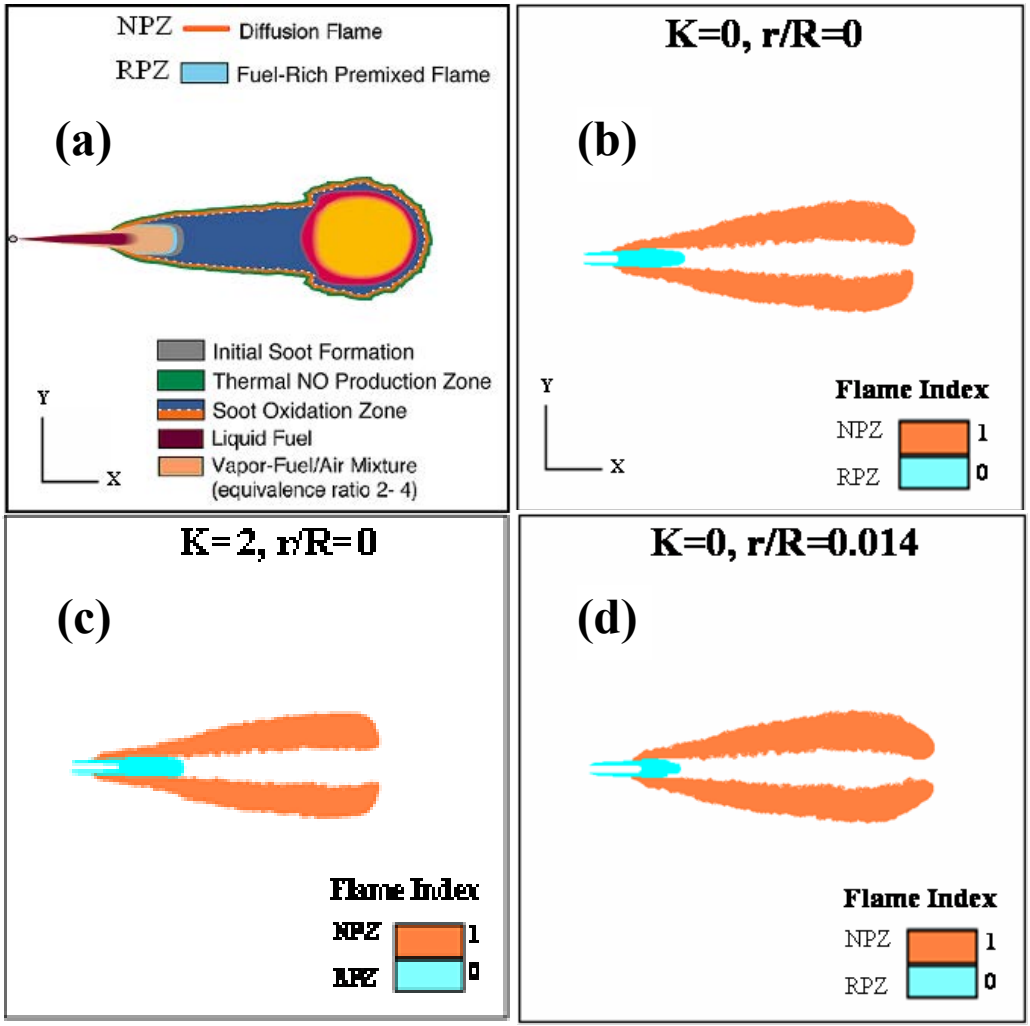
$$G_{CO.O_2} = \nabla Y_{CO} . \nabla Y_{O_2}$$

$$\xi_p = \frac{1}{2}\left(1 + \frac{G_{CO.O_2}}{\left|G_{CO.O_2}\right|}\right)$$

$\xi_p = 0 \Rightarrow$ Rich Premixed Reaction Zone

$\xi_p = 1 \Rightarrow$ Non-Premixed Reaction Zone

- Developed based on CO rather than fuel species gradient
- Typical double flame structure
- RPZ and NPZ influences NOx and soot production
- Conical nozzle: RPZ enhanced
  Hydroground nozzle: NPZ enhanced

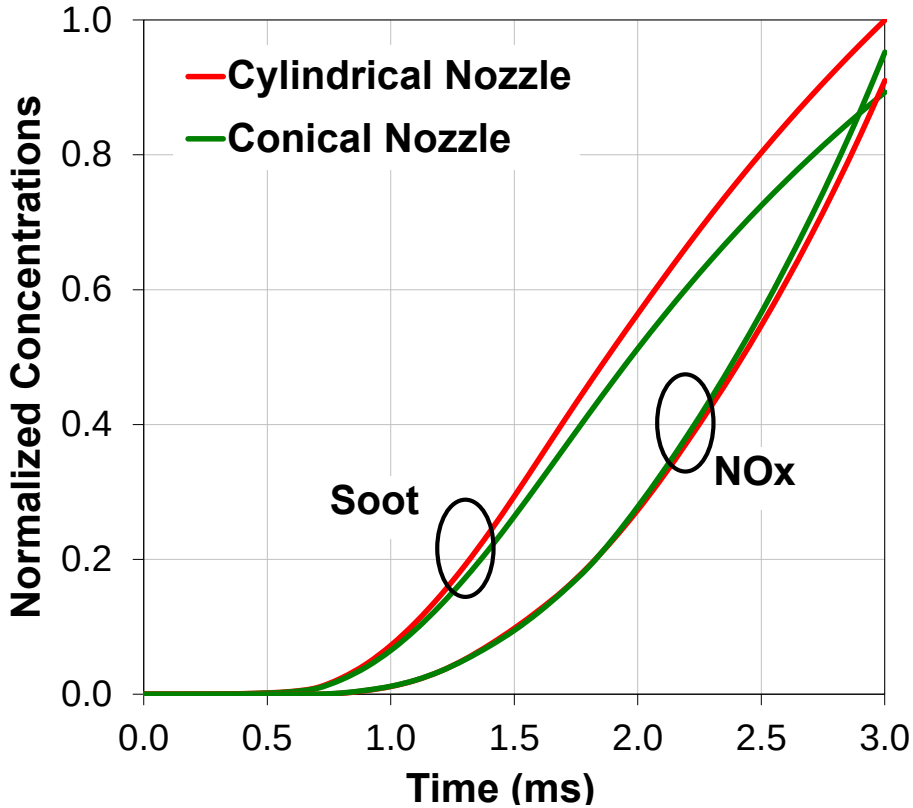


K=0, r/R=0: Cylindrical Nozzle

K=2,r/R=0: Conical Nozzle

* Som et al., *Combustion and Flame* 2010

Emission Characterization



$$\dot{m}_a \propto \sqrt{\rho_a \rho_f}\, dU_f\, x \tan\left(\theta/2\right)$$

$$\dot{m}_a \propto dU_f$$

$$\Phi\left(\overline{L_f}\right) = \frac{30}{\left\{\sqrt{1+16\left(L_f/x^+\right)^2}-1\right\}}$$

* JD Naber, DL Siebers. SAE No. 960034

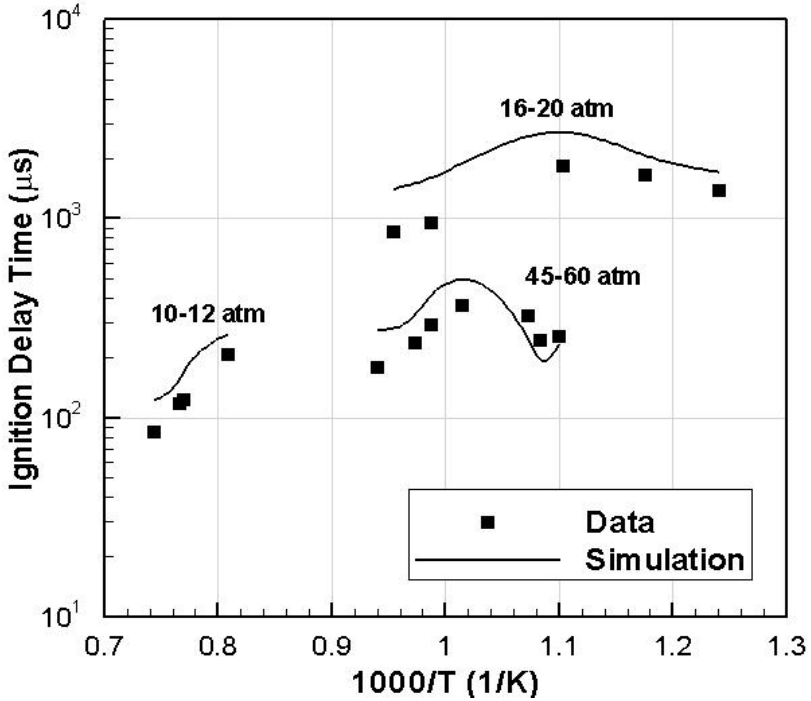
↑ Liftoff length => ↓ fuel richness => ↓ soot production

- Normalization performed based on maximum soot/NOx production
- Classical tradeoff between NOx and soot observed
- The NOx and soot production could be explained based on RPZ and NPZ characteristics and liftoff length trends

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

Detailed Chemistry from Combustion Modeling Perspective

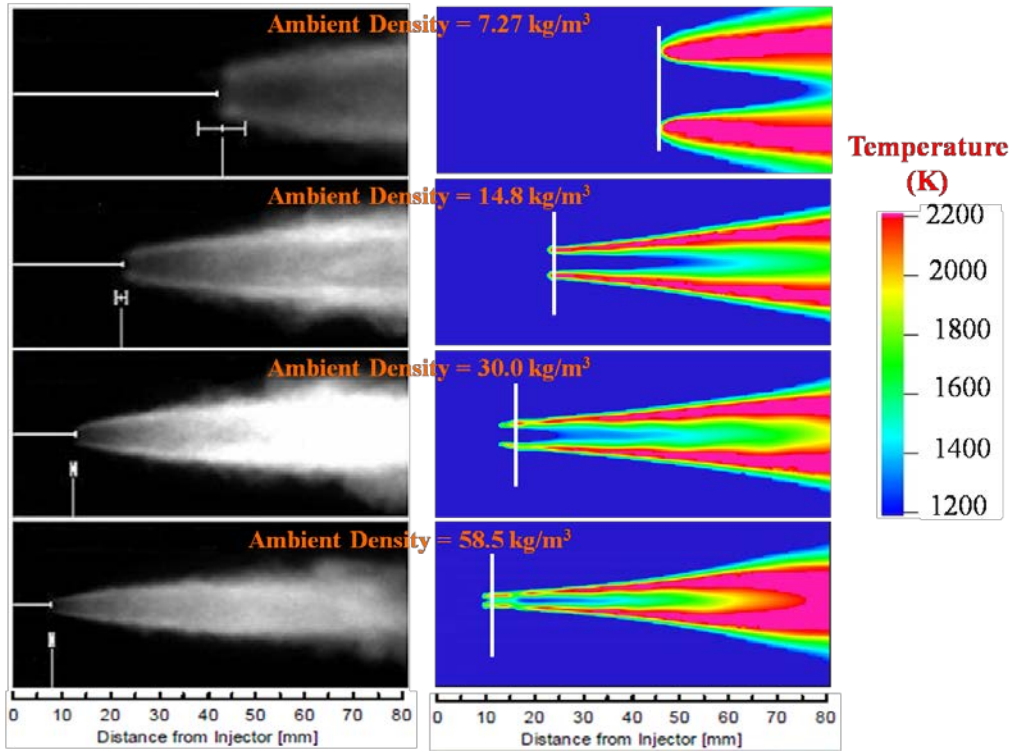
Capture Ignition delay accurately



- Shock-tube data from Hanson's group
- Detailed Chemistry (n-heptane): 42 species, 168 reactions
- Accurately captures NTC characteristics

Model Flame lift-off characteristics

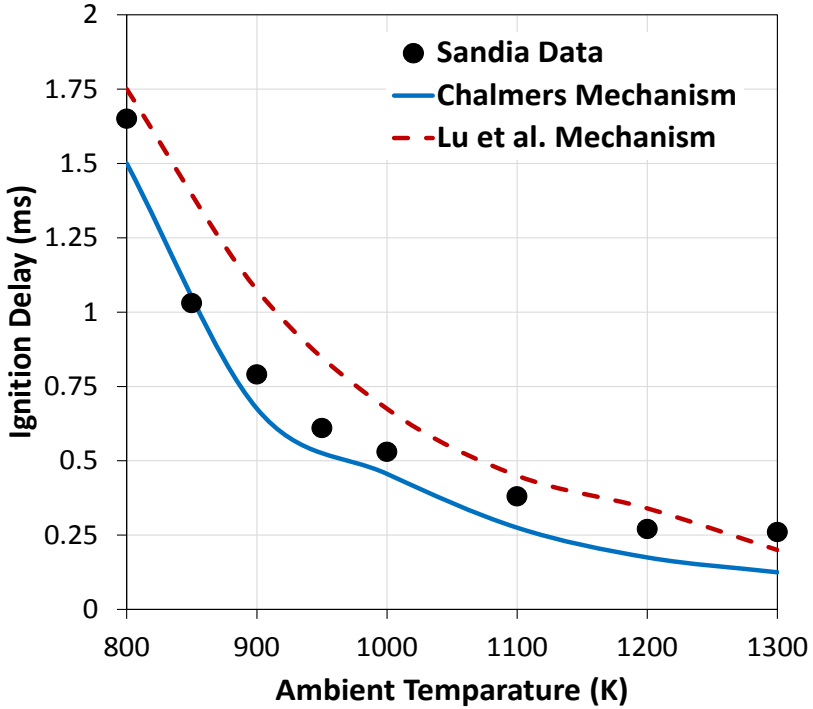
Data Simulations

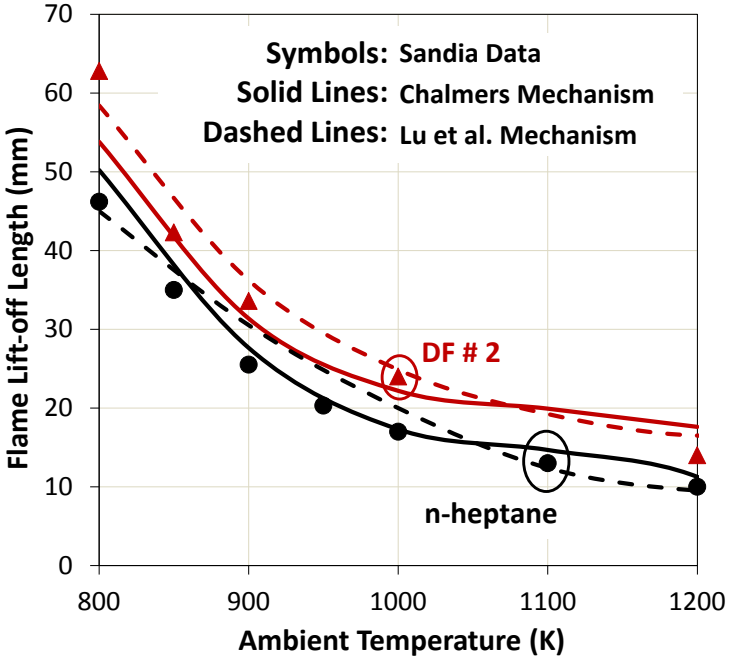


- Data from Sandia National Laboratory
- Lift-off trends well predicted
- About 15% under-prediction at low ambient densities

Reliable Chemical Kinetic Models CAN Improve Combustion Predictions!

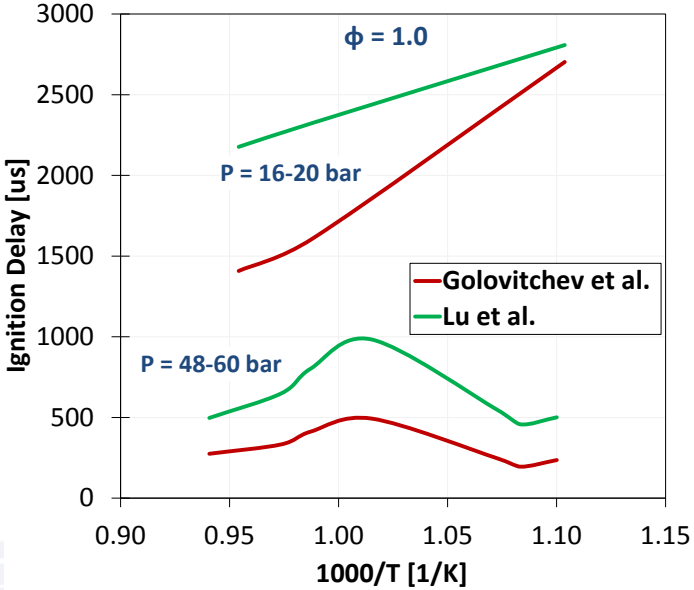
Diesel Surrogate Modeling





1) 42 species, 283 reactions (**Golovitchev et al.**): SAE Paper 2000-01-1891.
2) 68 species, 168 reactions (**Lu et al.**): Combustion and Flame 2009.

Lu et al. mechanism does a marginally better job in predicting diesel # 2 characteristics

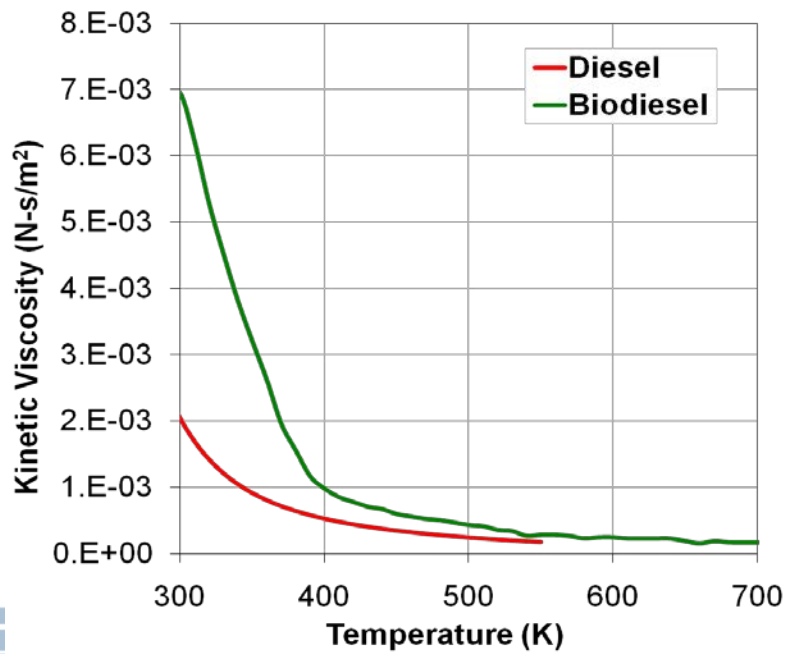


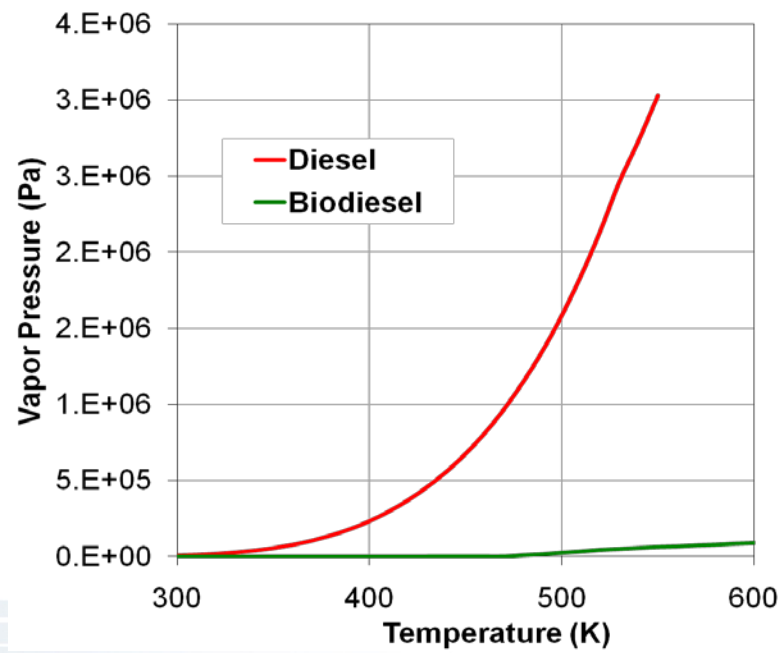
Diesel vs. Biodiesel

Differences in Fuel Properties*

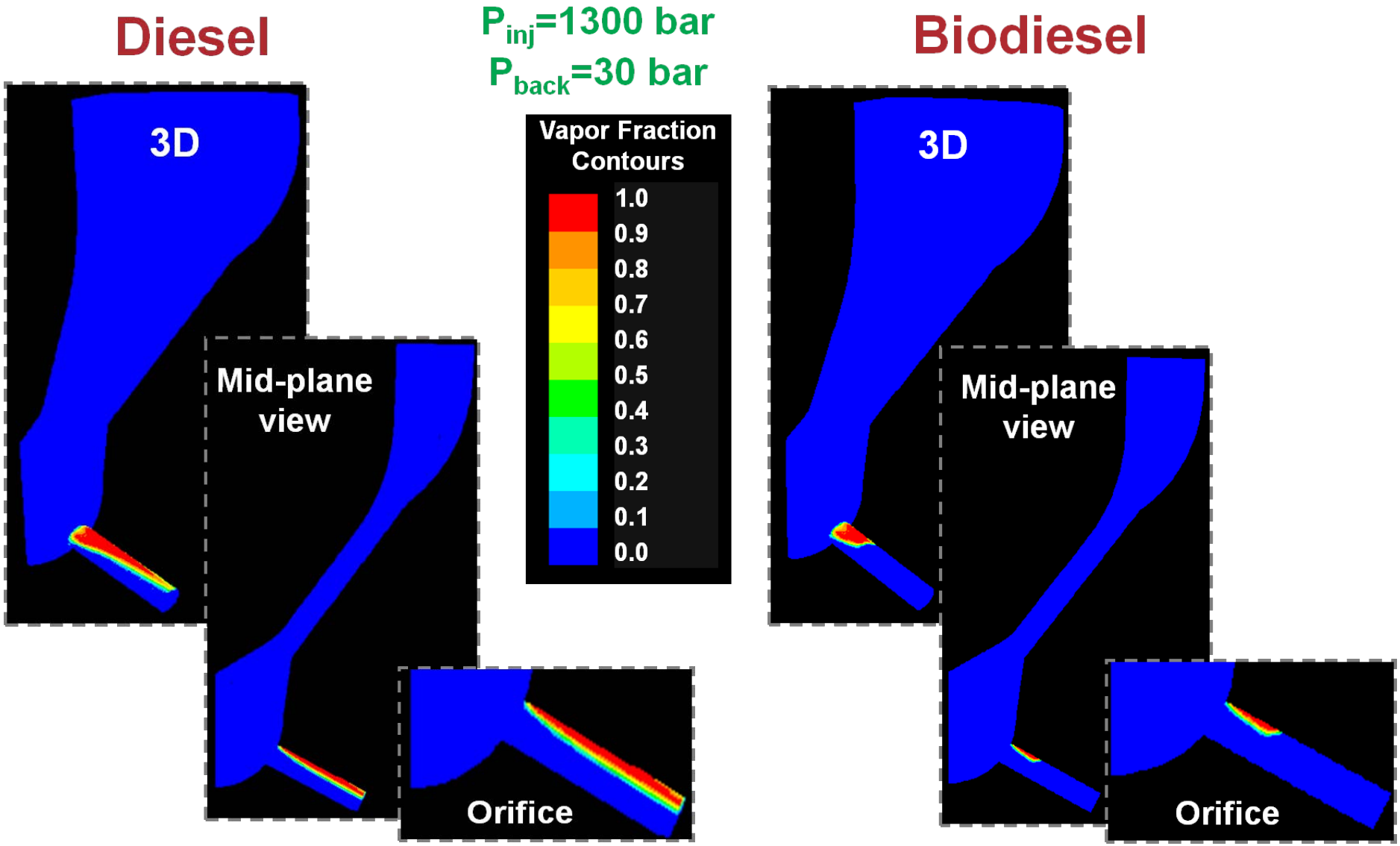
Fuel Property	Diesel	Biodiesel (SME)
Carbon Content [wt %]	87	76.74
Hydrogen Content [wt %]	13	12.01
Oxygen Content [wt %]	0	11.25
Density @ 15°C (kg/m3)	**820**	**877.2**
Surface Tension @ 25°C (N/m)	**0.020**	**0.0296**
Heat of Combustion (MJ/Kg)	**42.0**	**37.4**
Heat of Vaporization (KJ/Kg)	**361.0**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

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



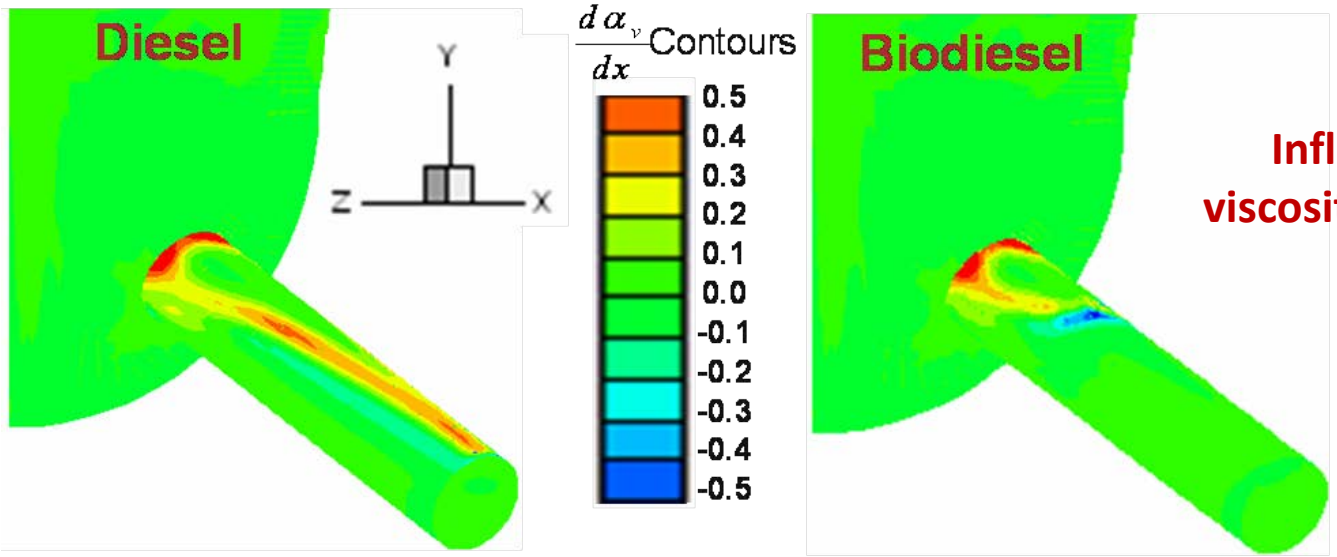


Vapor Distribution

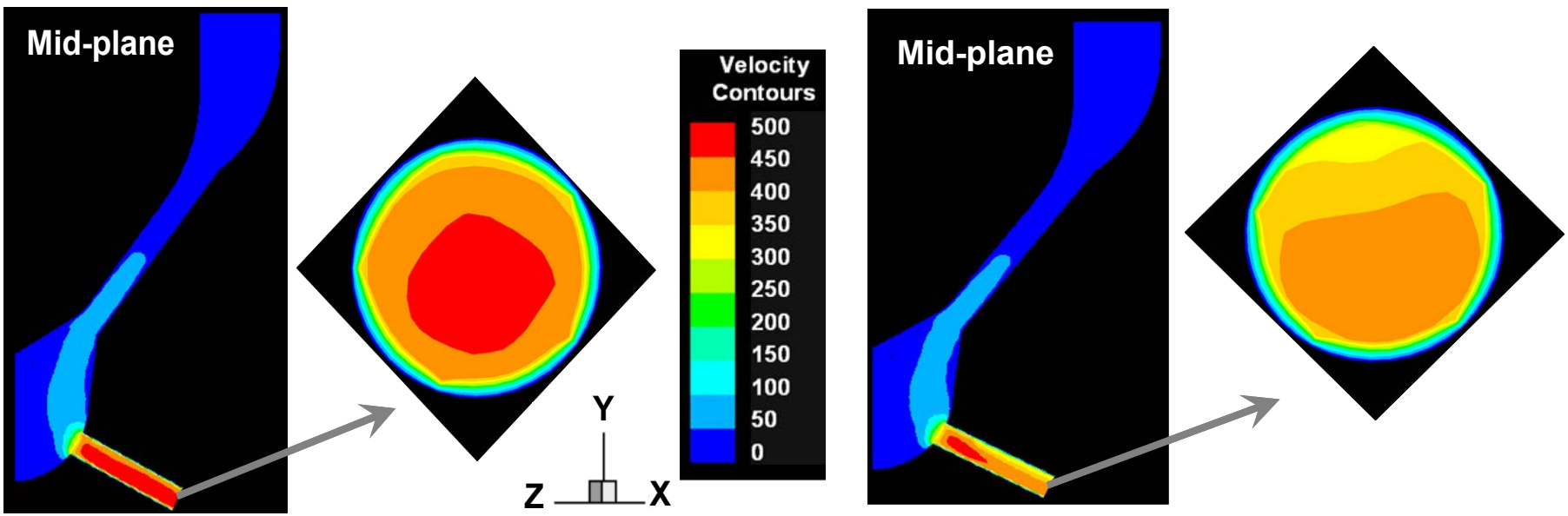


*Som et al., *FUEL* (2010)

Vapor Volume Fraction & Velocity Distribution

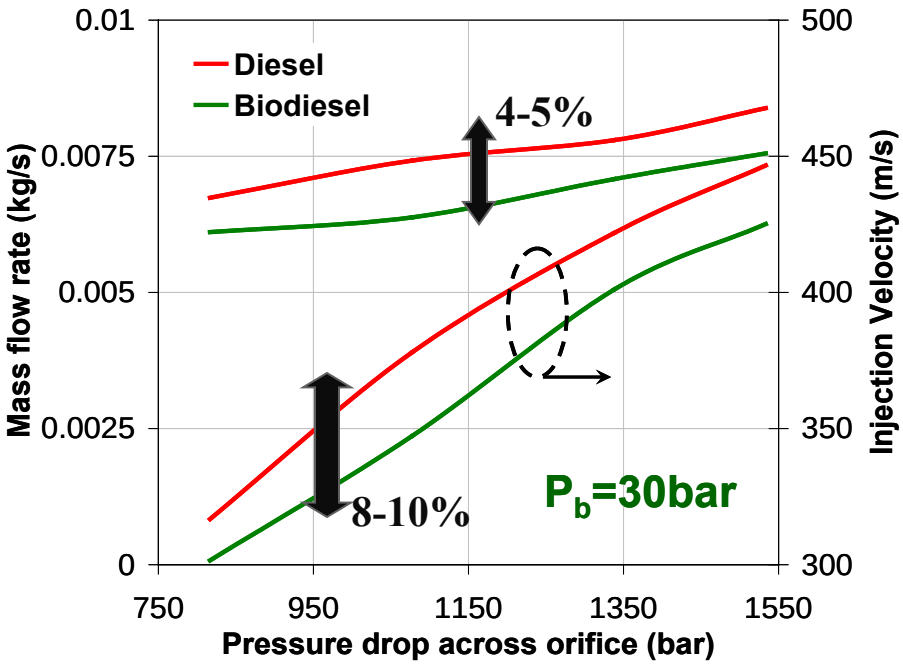


Influenced by density, viscosity, and vapor pressure



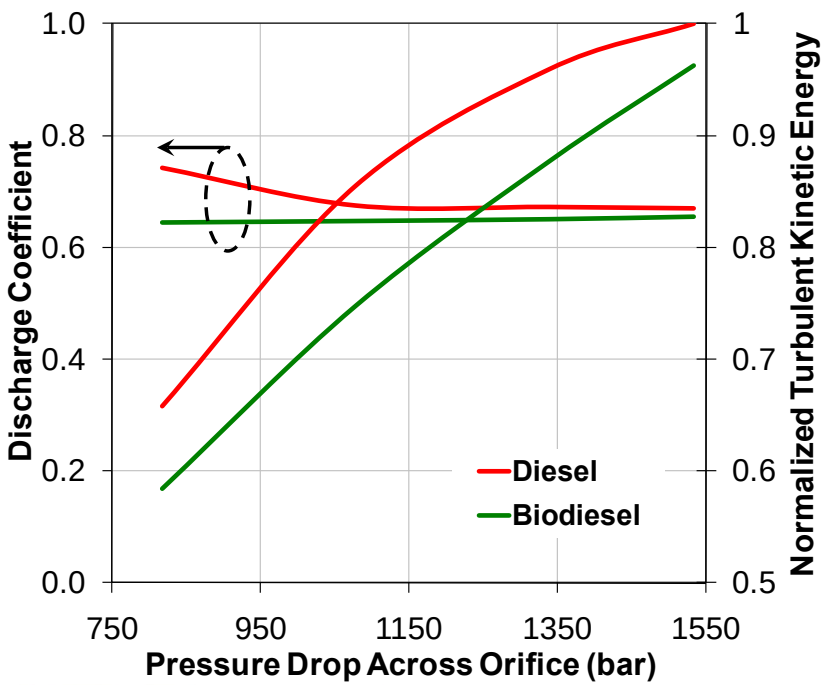
*Som et al., *FUEL* (2010)

Nozzle Exit Characteristics



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

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

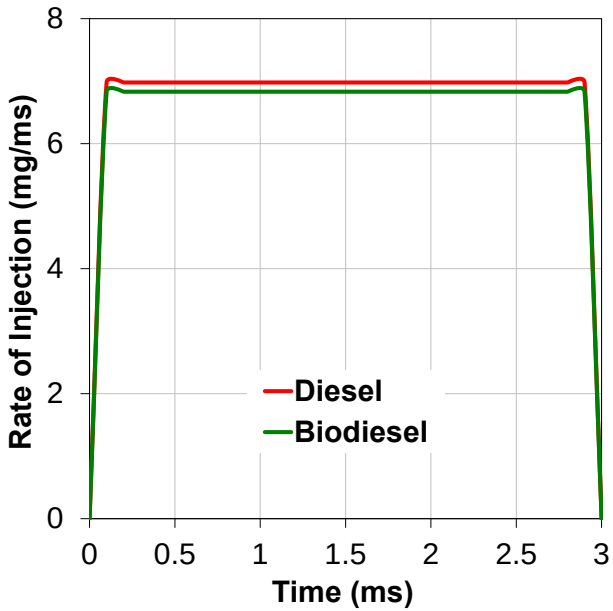


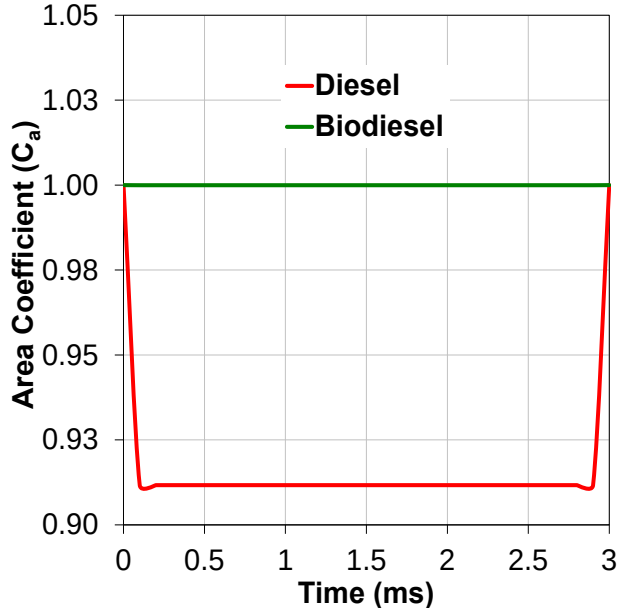
- Lower injection velocity, mass flow rate, and discharge coefficient for biodiesel
- This is due to biodiesel's significantly <u>higher molecular and turbulent viscosity</u>
- Significant differences in inner nozzle flow characteristics

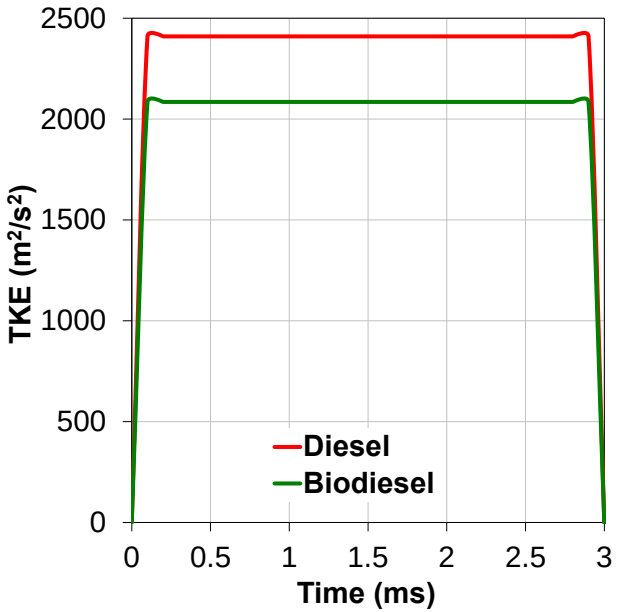
*Som et al., *FUEL* (2010)

Quasi Dynamic Coupling Strategy*

Boundary condition for KH-ACT model



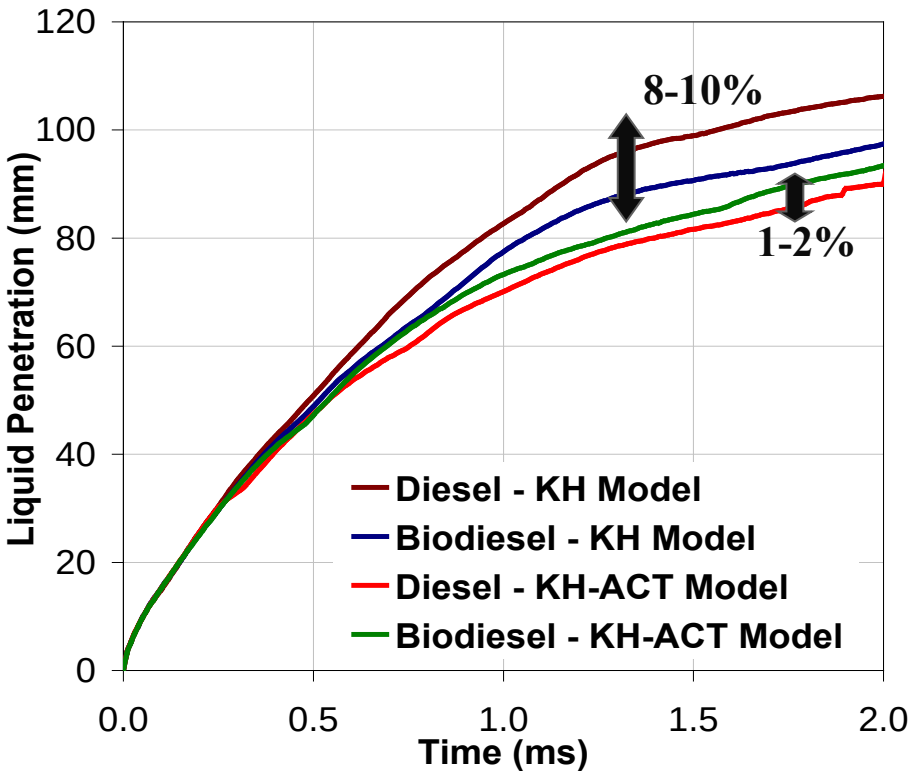




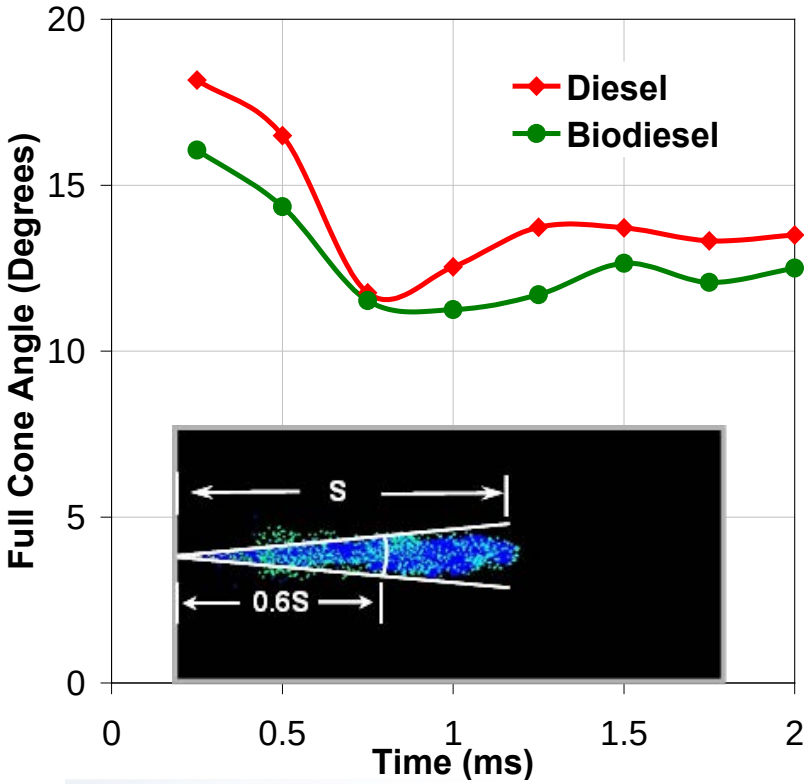
Property	Diesel	Biodiesel
Injection Pressure (bar)	1100 | 1300	1100 | 1300
Total Mass Injected (mg)	17.54 | 20.94	17.18 | 20.50
Discharge Coefficient (C_d)	0.64 | 0.64	0.61 | 0.62
Area Coefficient (C_a)	0.92 | 0.92	1 | 1
TKE (m^2/s^2)	1409 | 2410	1356 | 2135
Injection Duration (ms)	3	3
Ambient Density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

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

Spray Penetration & Cone-angle



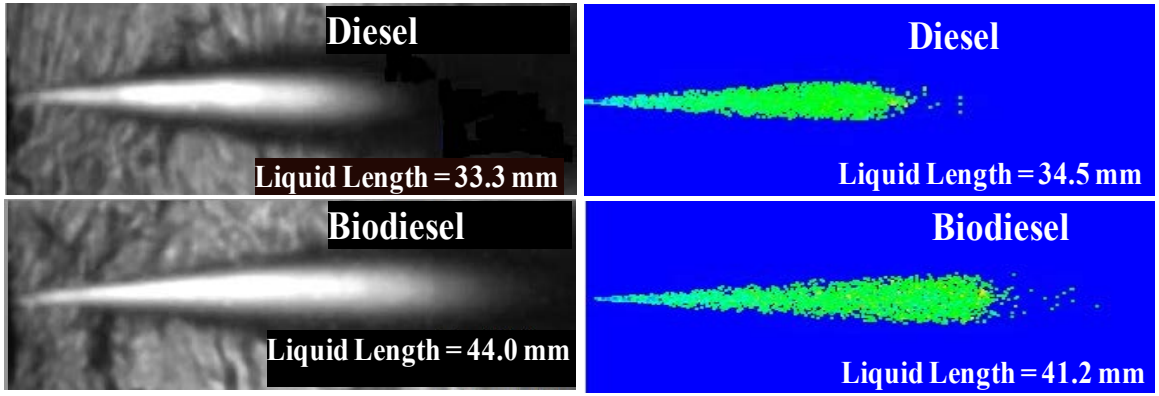
- Experimental trend: Biodiesel penetrates more than diesel
- KH-ACT model accurately captures the experimental trend i.e., biodiesel penetrates marginally more than Diesel



- 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

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

Evaporating Sprays: Liquid

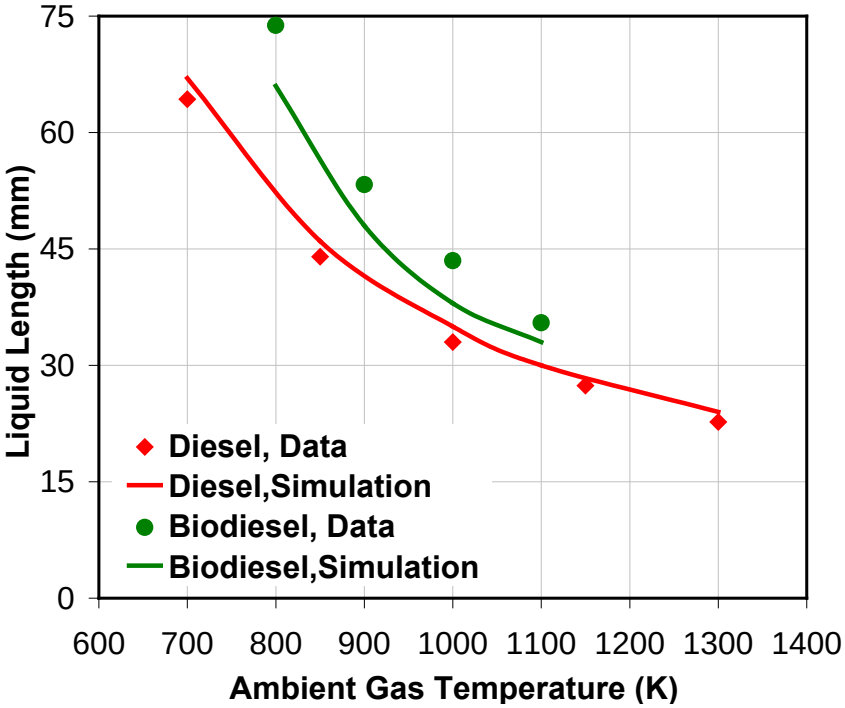


Data from:

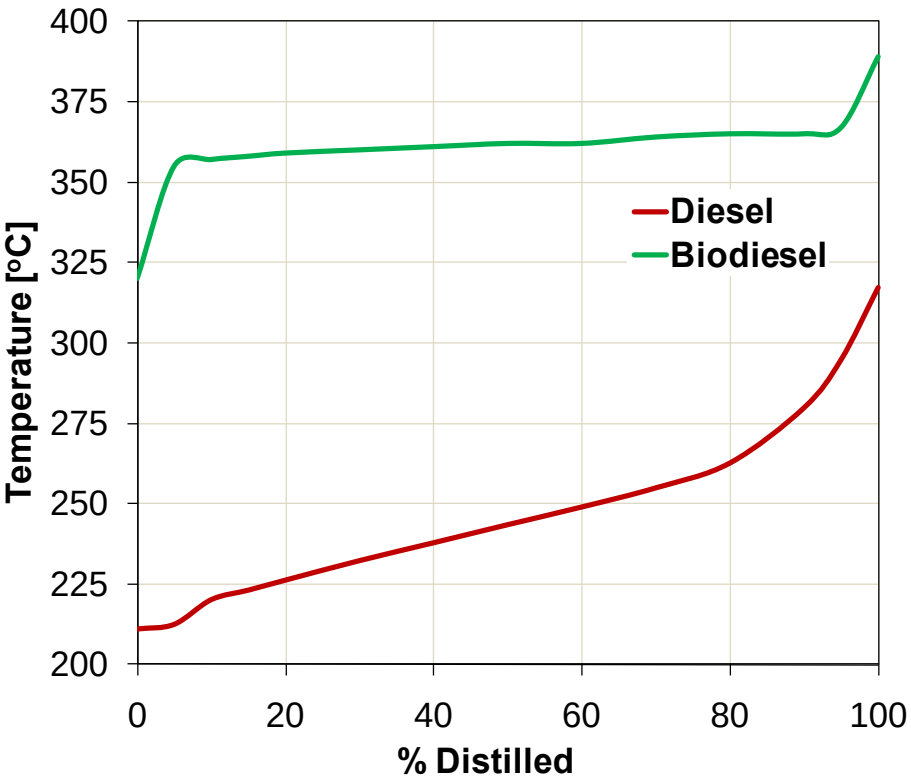
1) DL Siebers: SAE 980809

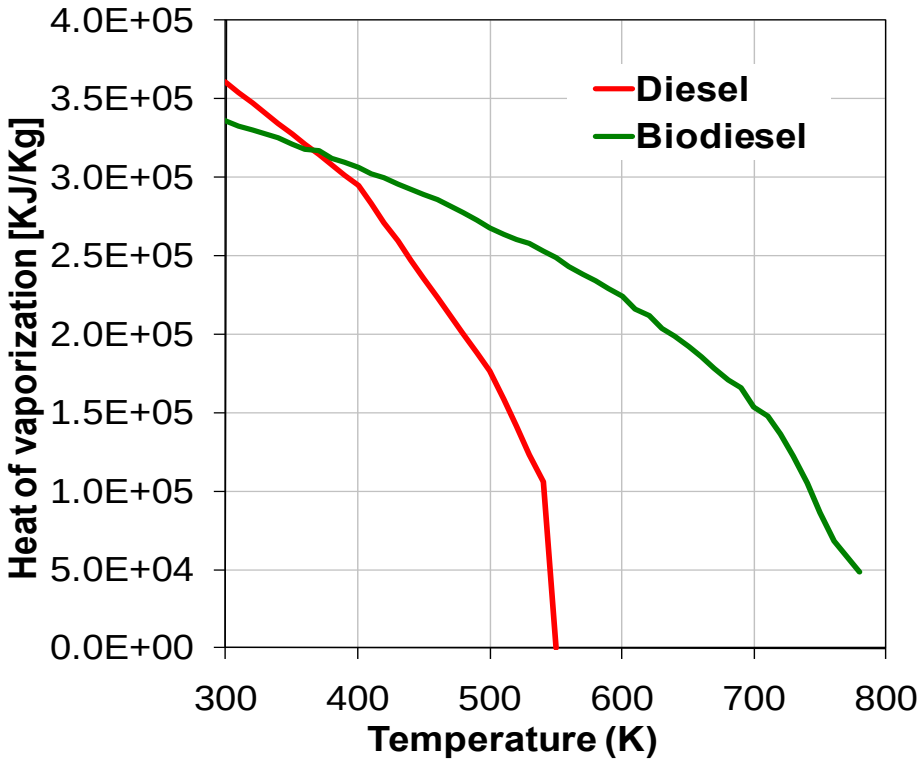
2) BS Higgins, CJ Mueller, DL Siebers: SAE 1999-01-0519

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?





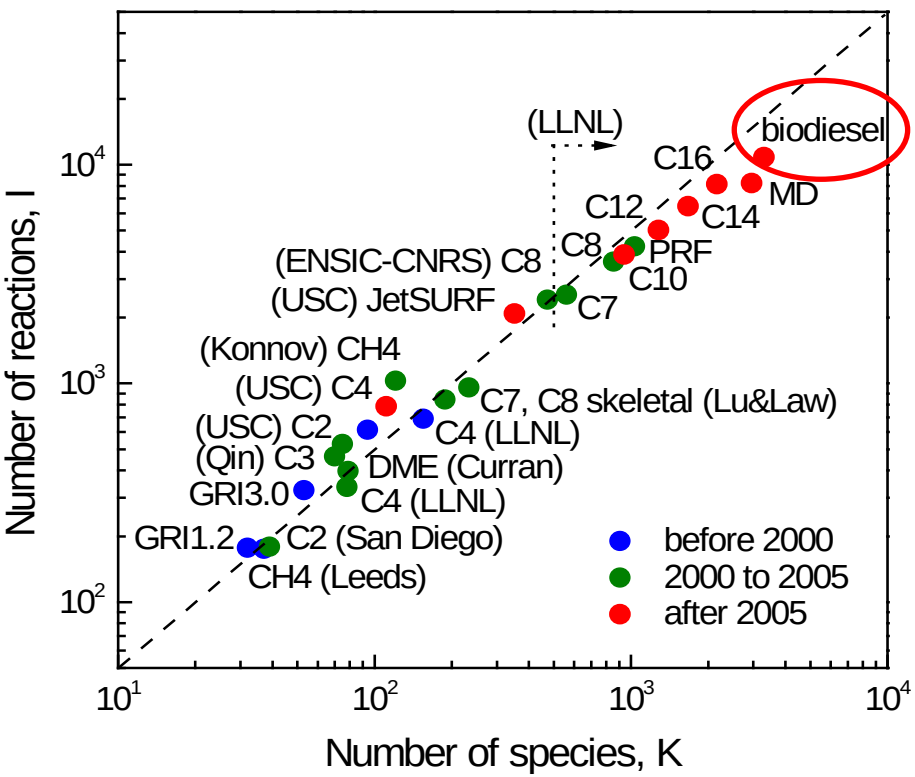
Slower breakup for biodiesel* is due to lesser amount of inner nozzle turbulence and cavitation. This results is increased spray penetration and reduction in spray cone-angle!

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

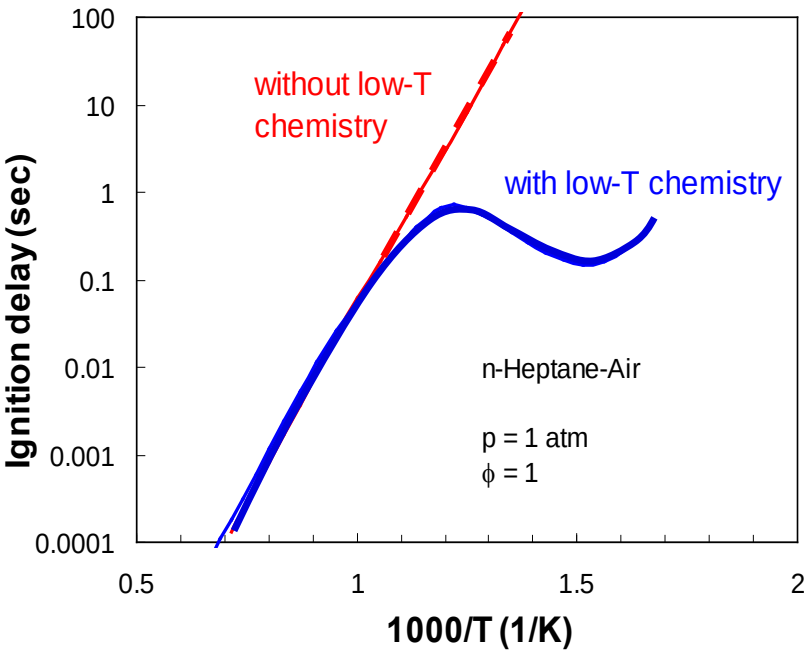
Detailed Mechanisms in Practical CFD Engine Simulations*

- Large mechanism size

3329 species;10,806 reactions



- Detailed chemistry is important



Mechanism reduction needed for CFD simulations with large mechanisms

*** Z Luo, M Plomer, T Lu, M Maciaszek, S Som, DE Longman. Energy and Fuels (24) 2010**

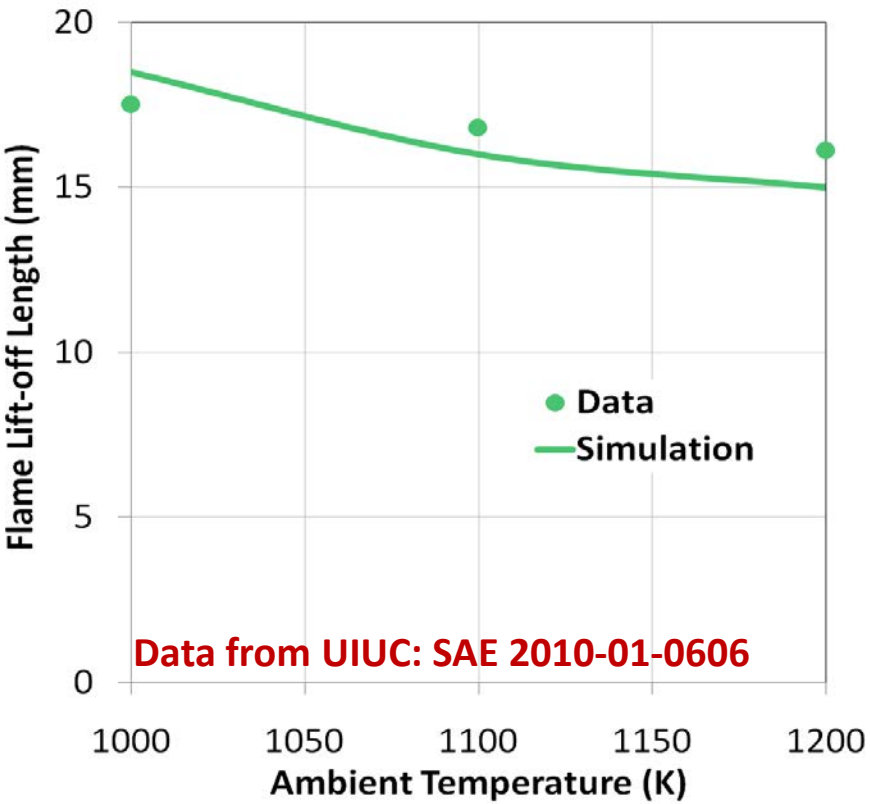
Biodiesel Surrogates for Engine Modeling

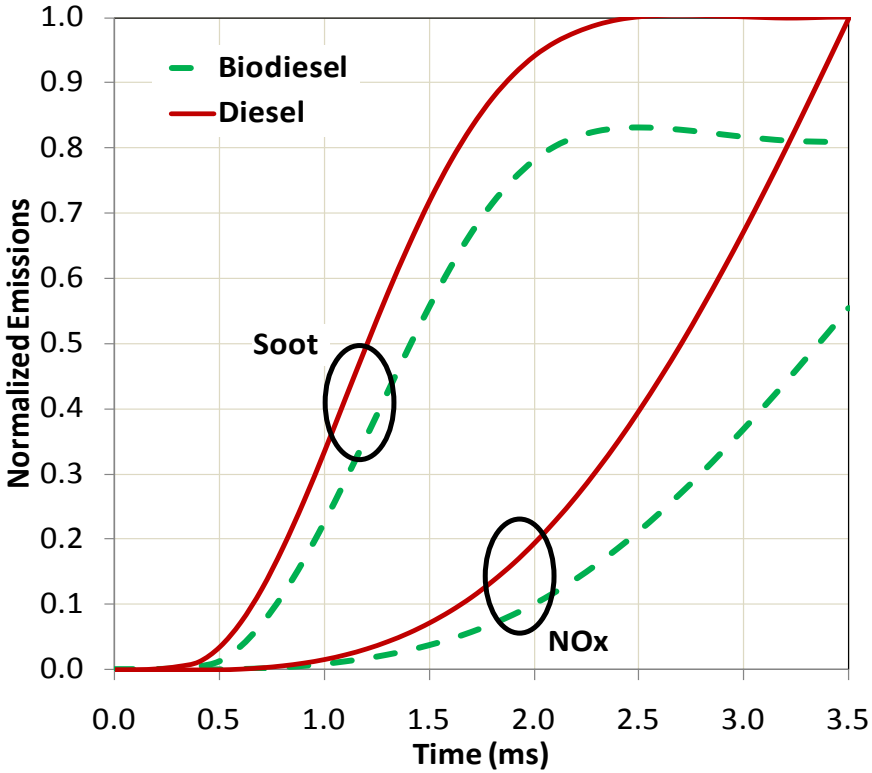
- Methyl butanoate: 41 species, 150 reactions (Brakora et al; 2008)
  - Include low temperature chemistry
  - Cannot well represent the real biodiesel chemical kinetics
- Methyl decanoate (MD):648 species and 2998 reactions (Sarathy et al; 2011)
  - Include low temperature chemistry
  - Too large to be applied in practical engine simulations
- MD, Methyl-9-decenoate and n-heptane:118 species and 837 reactions(Luo et al;2010)
  - Suitable for high temperature flame simulations
  - Did not include low temperature chemistry

Desired reduced biodiesel mechanism:

- Small in mechanism size (about 100-125 species)
- Represent the real biodiesel properties well
- Including low and high temperature chemistry
- No tuning of rate parameters to match specific data-sets

Combustion Modeling with Detailed Chemistry*



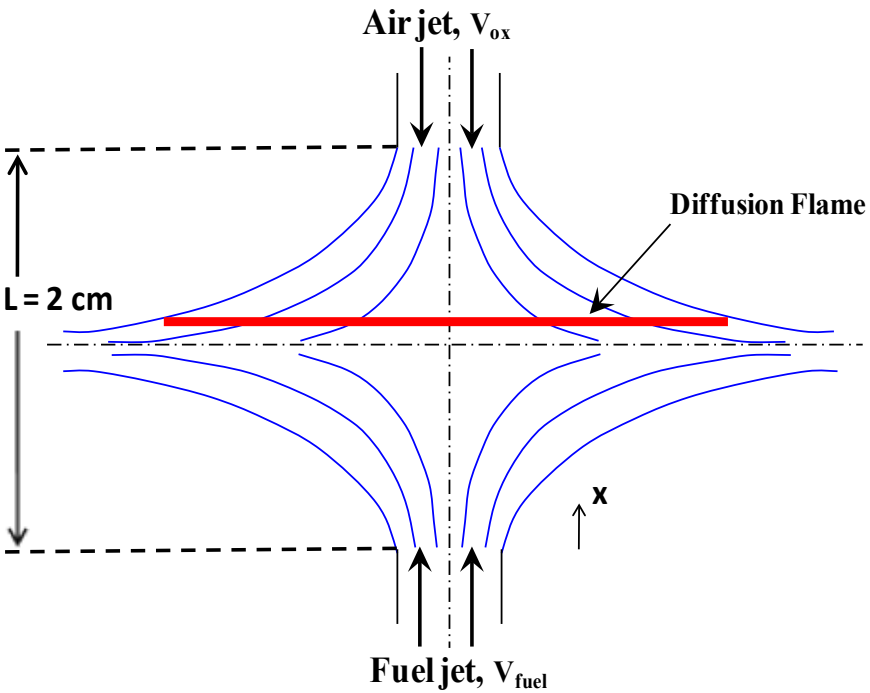


- Diesel surrogate (n-heptane): 42 species, 168 reaction mechanism from Chalmers University
- Biodiesel surrogate (methyl butanoate): 41 species, 150 reaction mechanism {Brakora et al. SAE 2008-01-1378}

- Lower soot emission trends with biodiesel well captured
- Biodiesel surrogate not able to capture the accurate NOx trends!

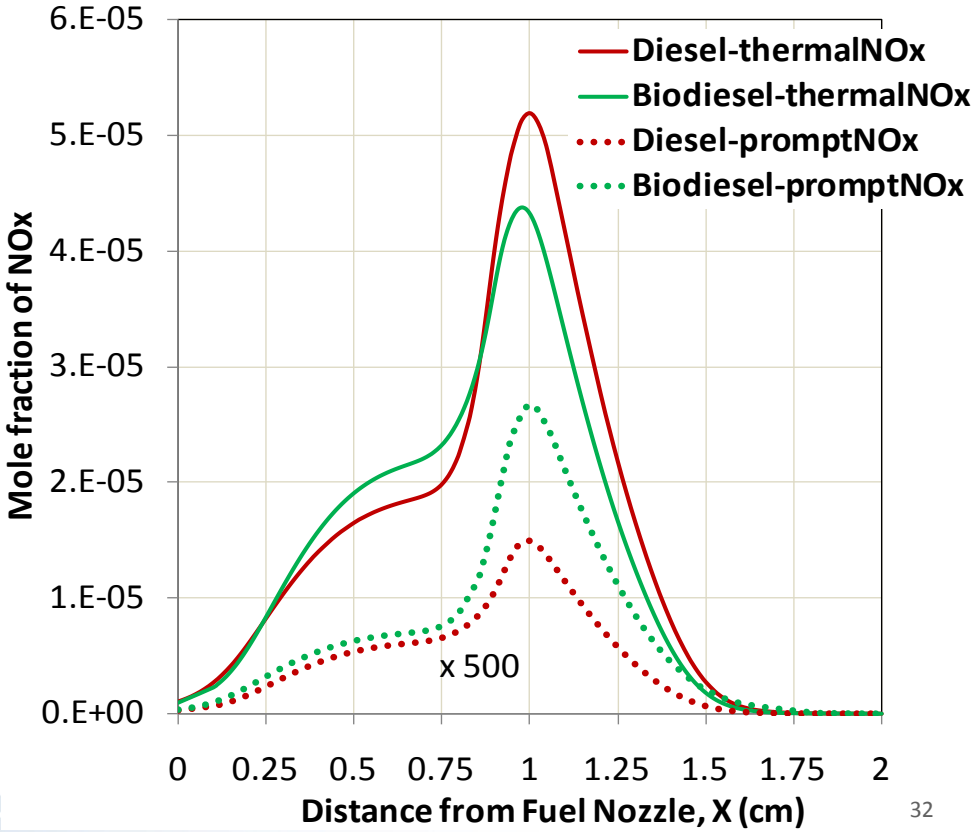
***S Som, DE Longman. Energy and Fuels (25) 2011**

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



Mechanism Reduction Methodology

Detailed Mechanism (from LLNL)
3329 species, 10806 reactions

DRG

Skeletal Mechanism
664 species, 2672 reactions

Isomer lumping

Skeletal Mechanism
641 species, 2670 reactions

DRGASA & Error Cancelation

123 species, 394 reactions

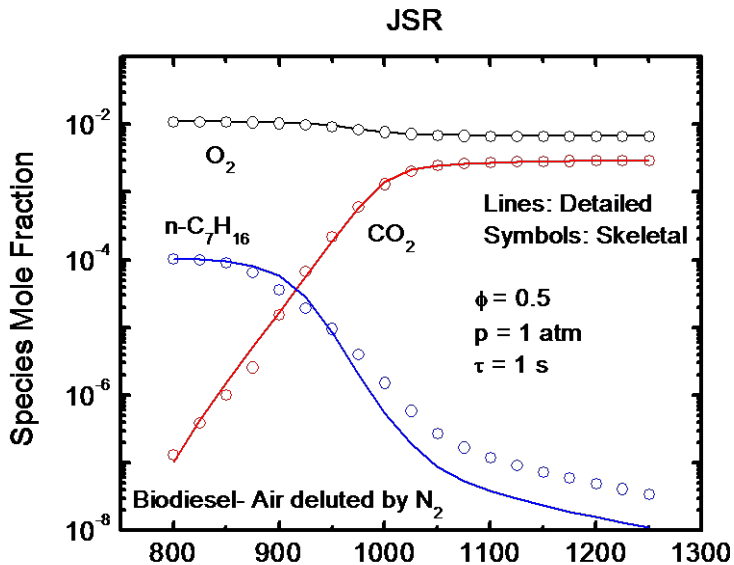
89 species, 367 reactions

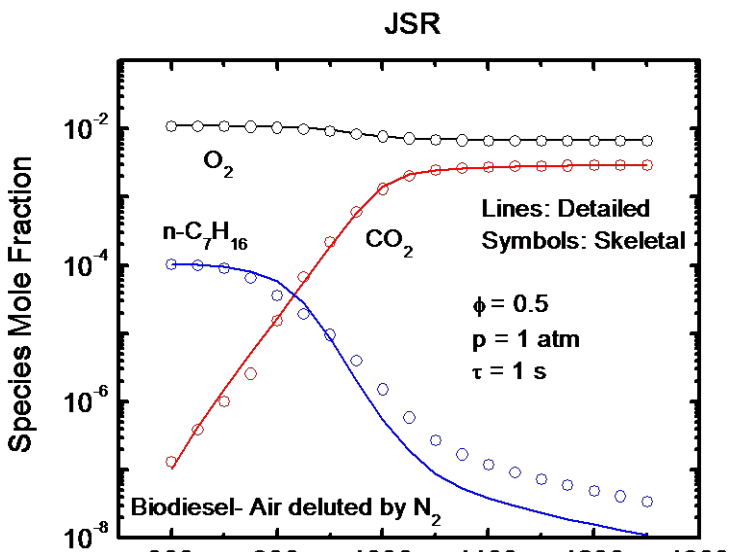
Range of operation:

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

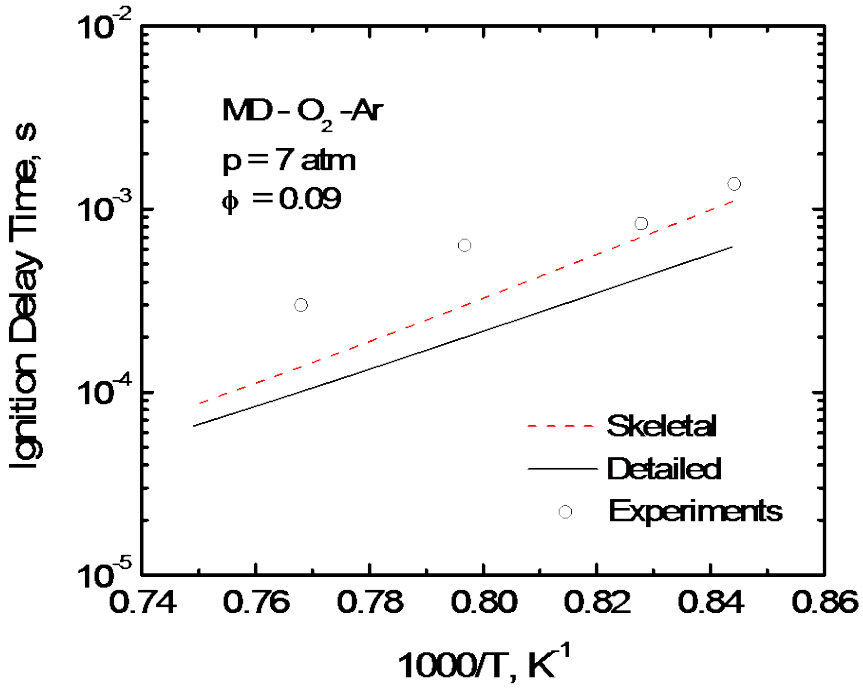
*** Z. Luo, M. Plomer, T. Lu, S. Som, D.E. Longman, 2G02. *US National Combustion Institute meeting, March 2011***

Validation against Idealized Combustion Systems





Data: Dagaut et al. PCI 2007



Data: Dievart et al. 7th US Combustion Institute meeting, 2011

*** Z. Luo, M. Plomer, T. Lu, S. Som, D.E. Longman. Submitted to Combustion Theory and Modeling**

Biodiesel: Case set-up

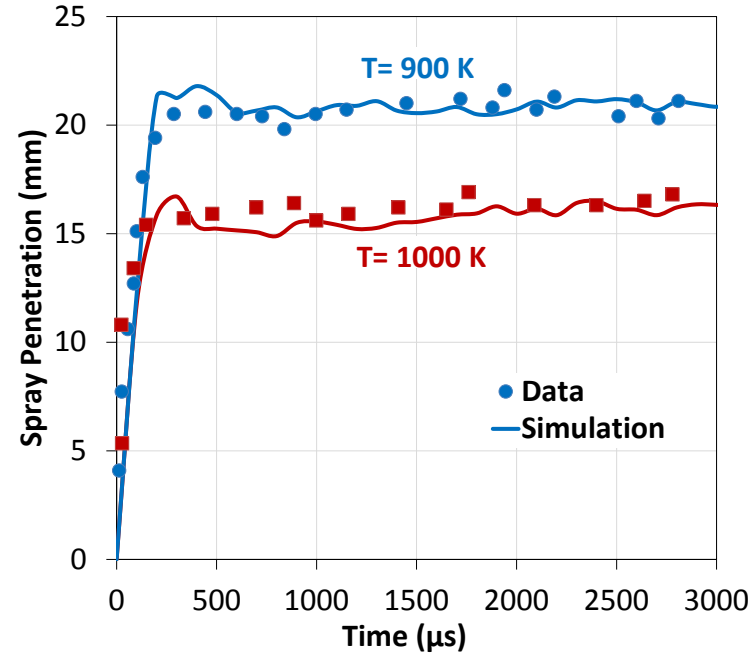
Injection & Ambient conditions for Biodiesel studies at Sandia*

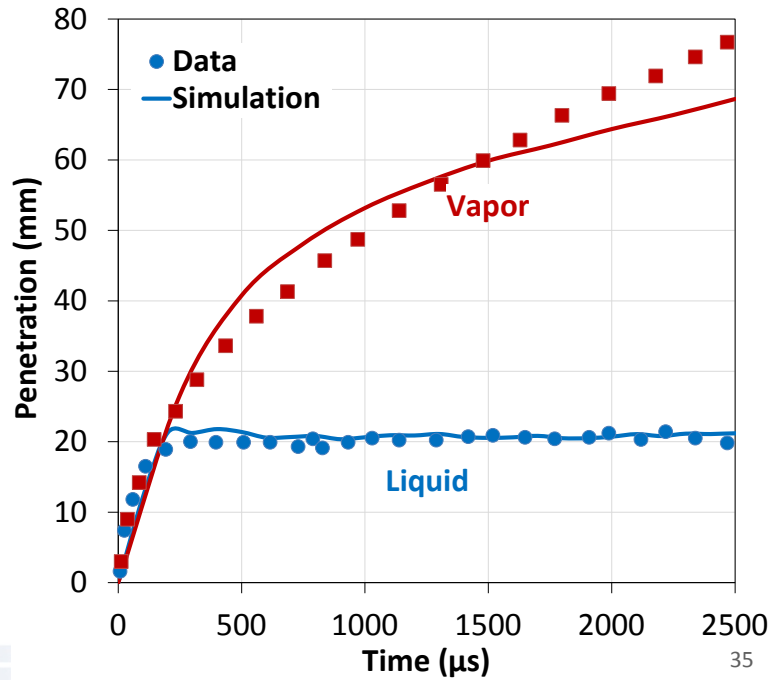
Parameter	Quantity
Injection System	Bosch Common Rail
Nozzle Description	Single-hole, mini-sac
Duration of Injection [ms]	7.5
Orifice Diameter [µm]	90
Injection Pressure [Bar]	1400
Fill Gas Composition (mole-fraction)	N_2=0.7515, O_2=0.15, CO_2=0.0622, H_2O=0.0363
Chamber Density [kg/m^3]	22.8
Chamber 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*

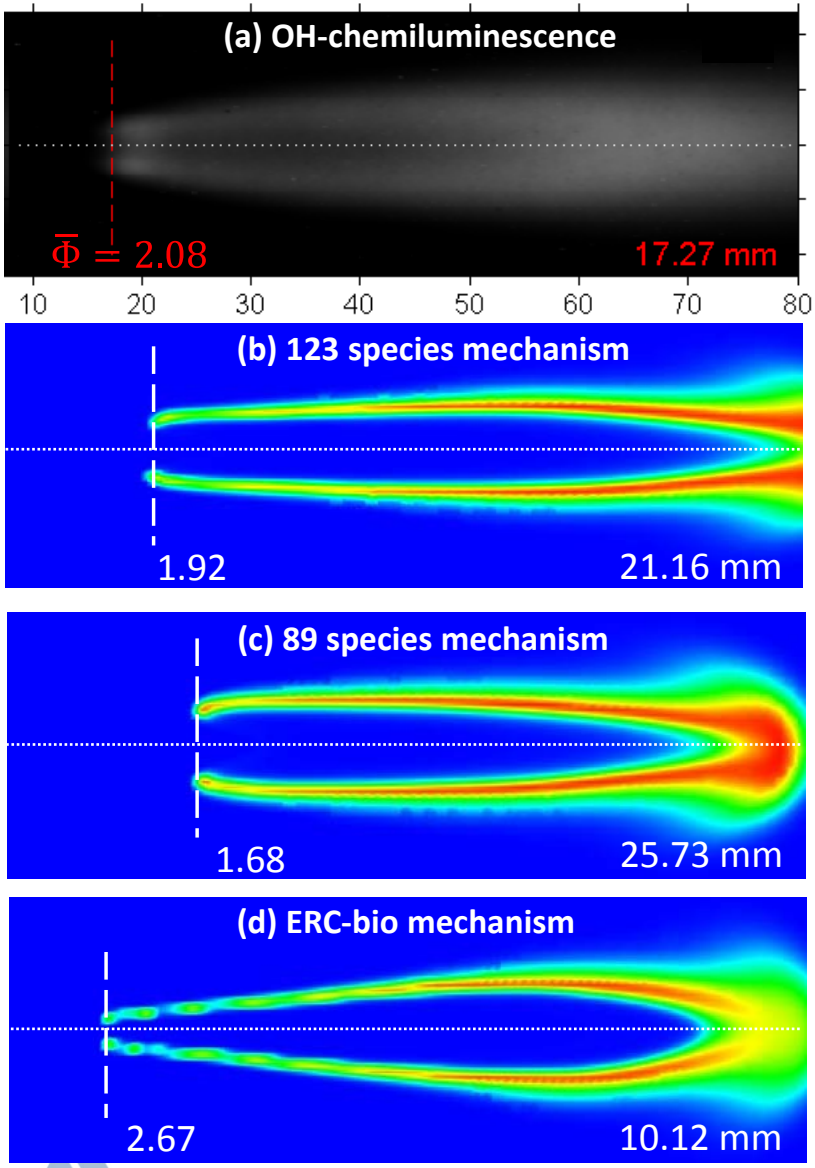
Non-reacting spray characteristics well predicted by the simulations!





Som et al. ASME ICE2011-60051

Validation of Different Reaction Mechanisms

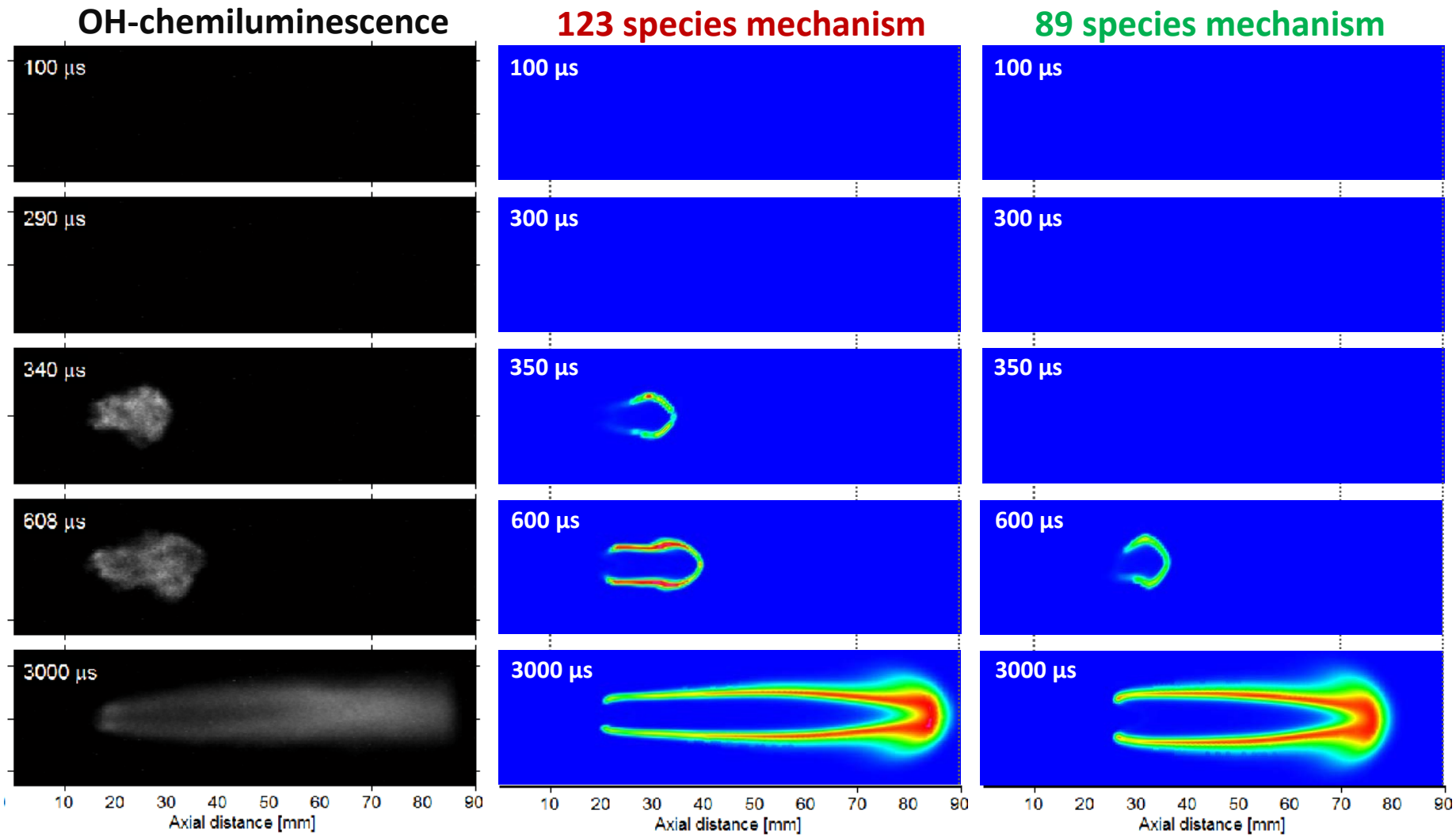


- 123 species, 394 reactions. Paper # IC18. US National Combustion Meeting, March 2011
- 89 species, 364 reactions. SAE World Congress 2011
- ERC-bio mechanism: 41 species, 150 reactions. SAE Paper No. 2008-01-1378

	Ignition Delay (μs)
Sandia Data	396
123 species	510
89 species	580
ERC-Bio mechanism	220

✓ 123 species mechanism does the best job in predicting ignition delay and flame lift-off. Over-prediction of about 25% only.

Further Validation of Biodiesel Kinetic Models

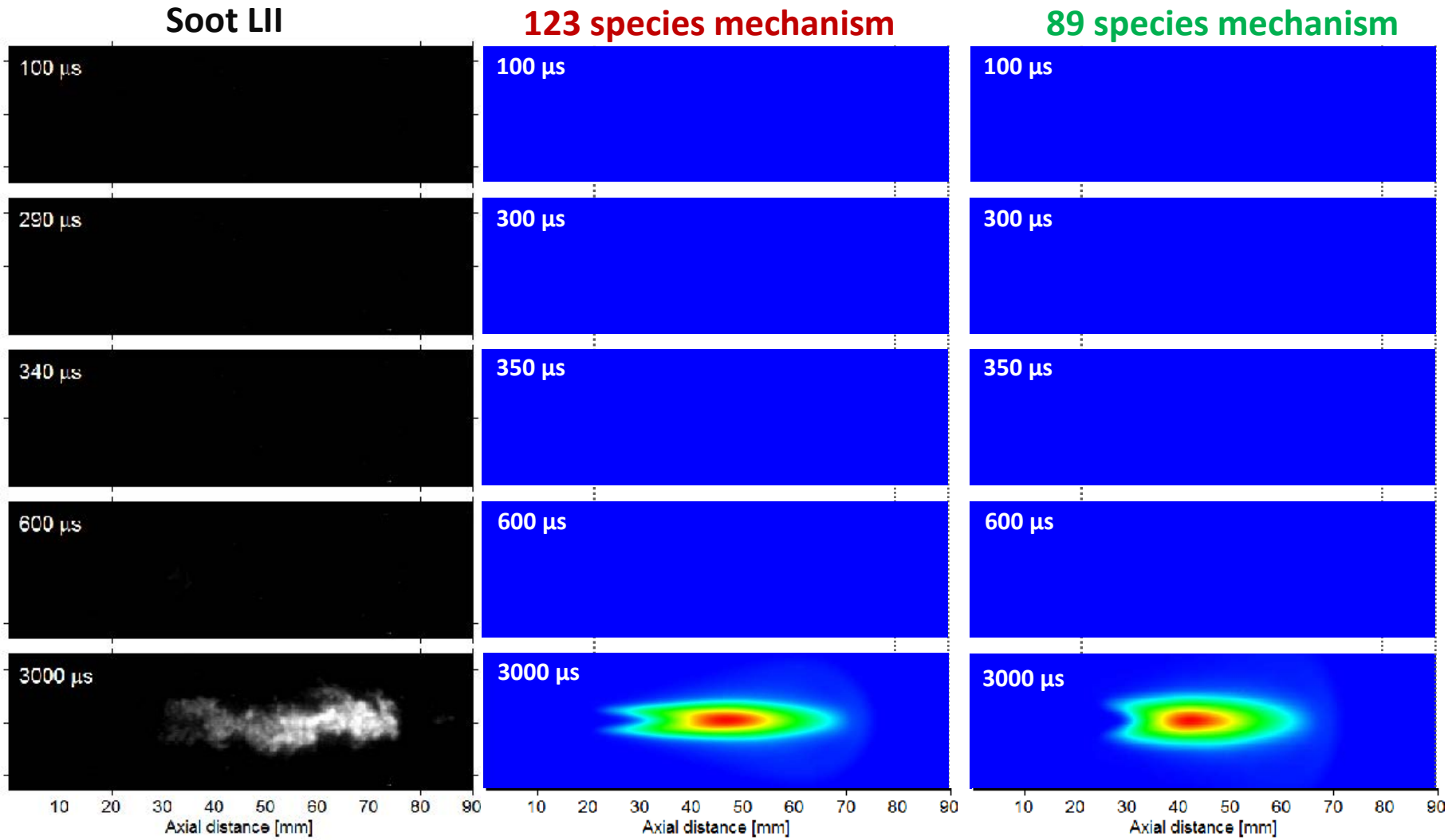


~ 160 hours on 8 processors

~ 85 hours on 8 processors

Som et al. ASME ICE2011-60051

Soot Validation with MD+MD9D+NHPT Mechanism

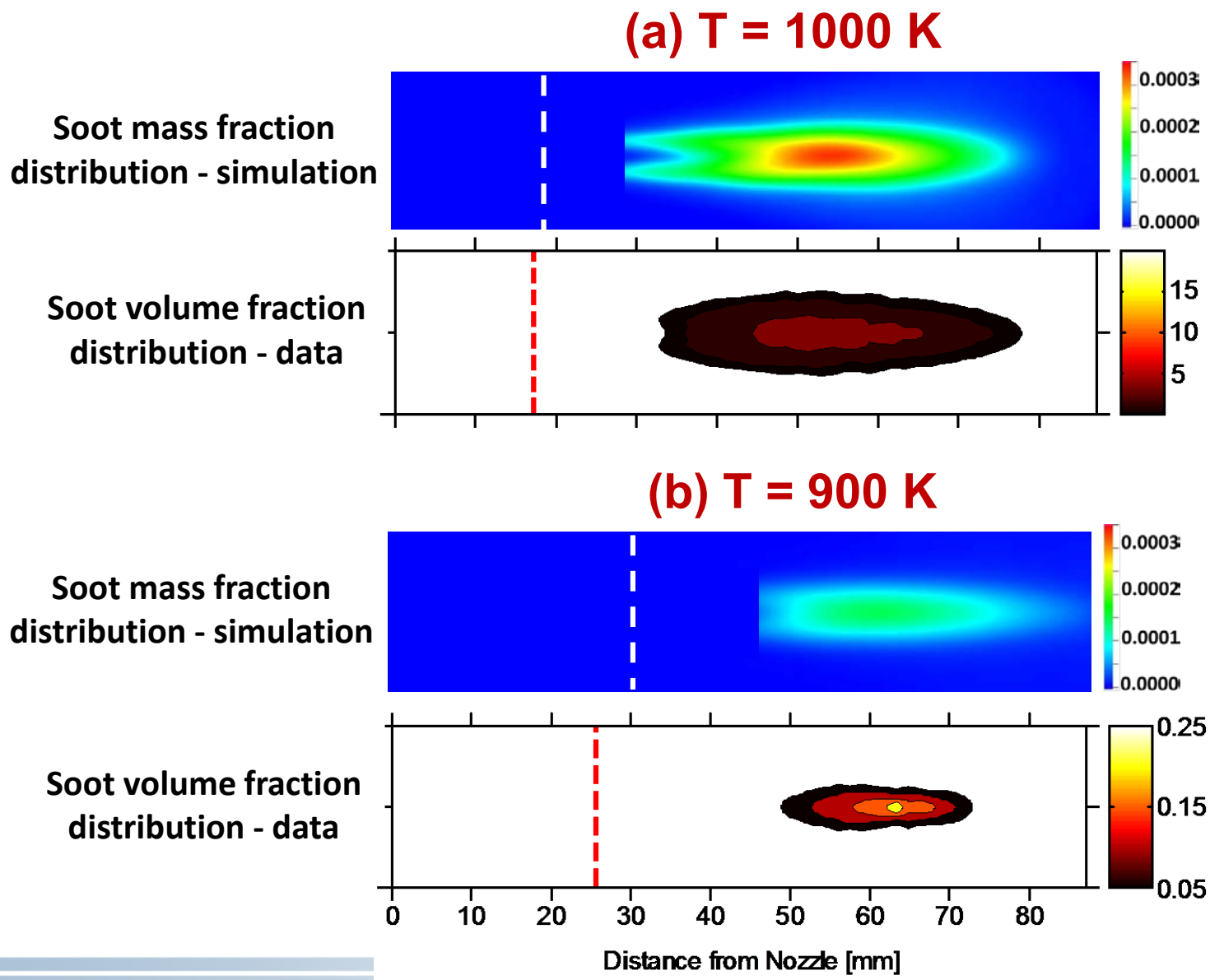


Som et al. SAE World Congress 2011

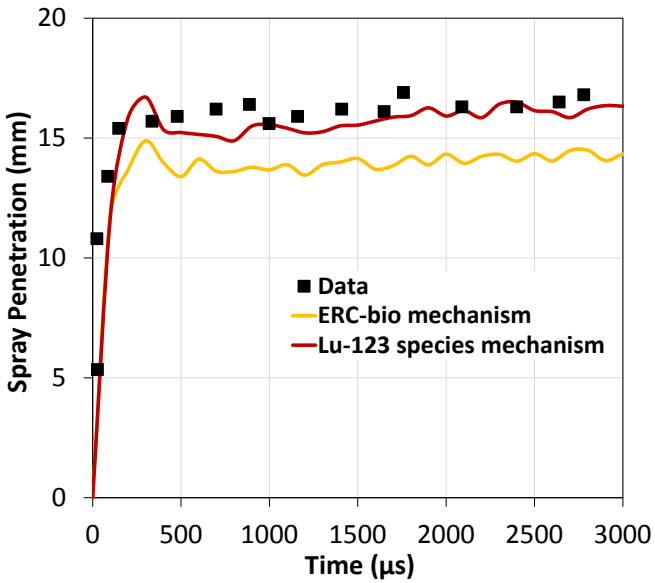
C_2H_2 used as a soot precursor!

Prediction of Soot Distribution

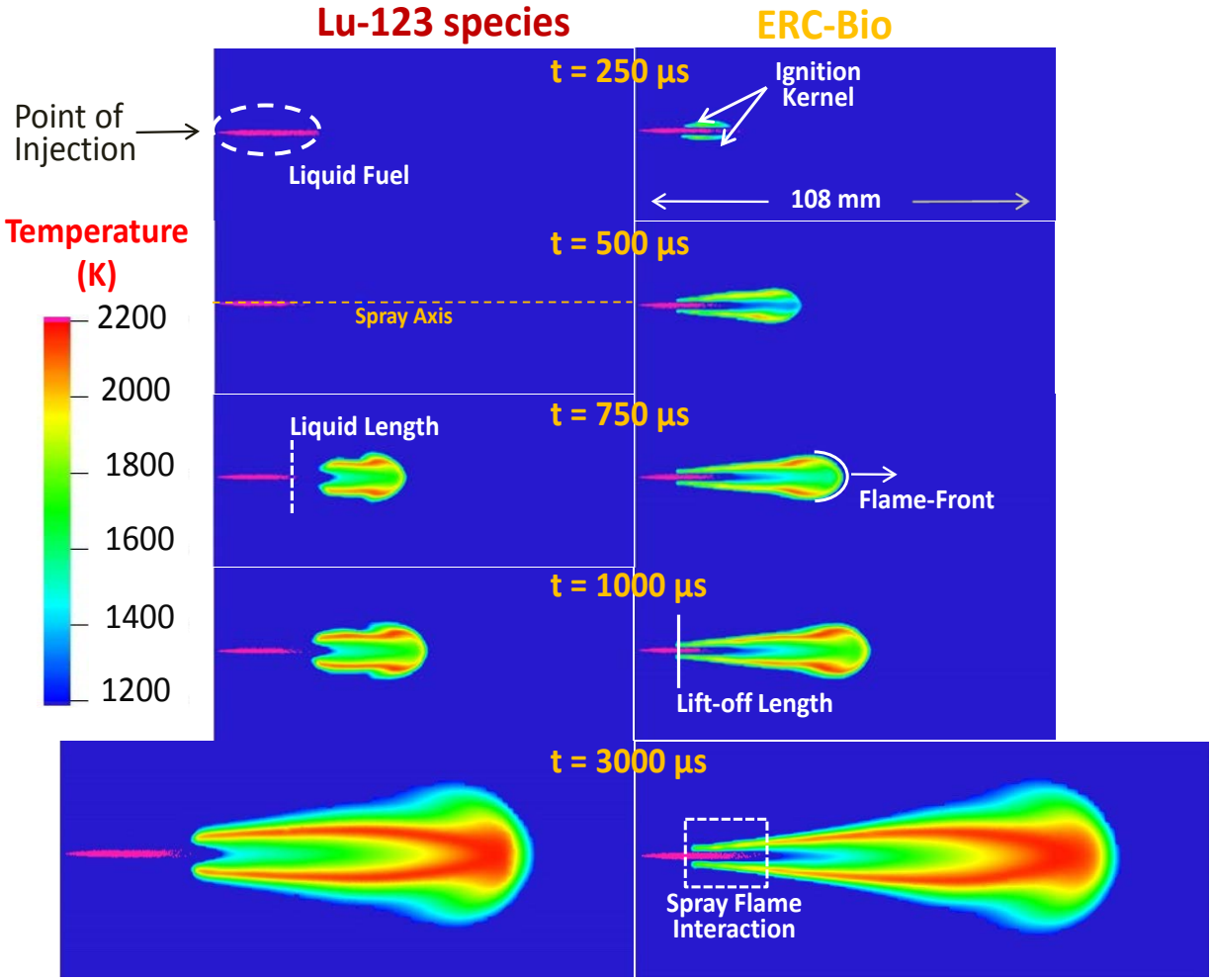
89 species mechanism



Flame Structure with Different Mechanisms



* Som et al. SAE World Congress 2011



Due to <u>enhanced spray-flame interaction</u>, liquid length is lower with the ERC-MB mechanism!

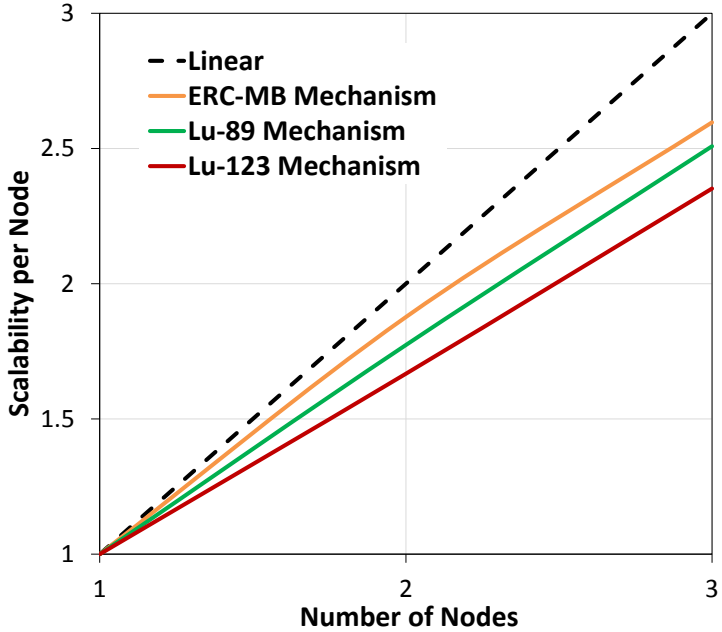
Computational Cost & Scalability

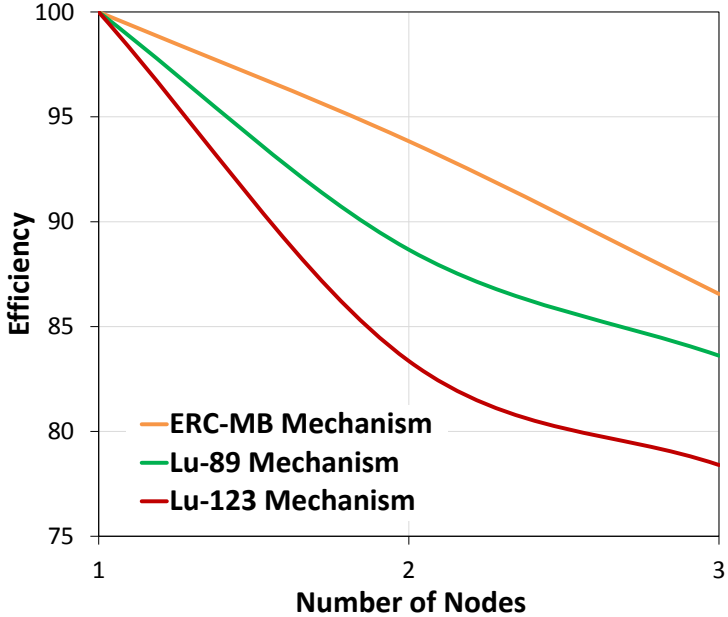
	Computational Time (for one node)
Lu-123 species	74 hours
Lu-89 species	38 hours
ERC-MB	13 hours

Scalability per node = T_1/T_n
Efficiency per node = $T_1 x100/nT_n$
n = Number of compute nodes
Each node has 8 processors

Fusion Cluster @ Argonne:

- ✓ 320 compute nodes
- ✓ Each with a 2.6 GHz Pentium Xeon Memory
- ✓ Total of 2560 processors
- ✓ 36-96 GB of RAM per node
- ✓ Infini-Band QDR Network





Other Topics of Interest to Argonne

- Inner nozzle flow modeling with biodiesel from different feedstocks, alcohols: SAE World Congress 2011
- High-fidelity large eddy simulation: ASME-ICE 2011
- Engine Combustion Network (ECN) – 1: Standardization of definitions of spray and combustion parameters for modelers and experimentalists
- Detailed full-cycle engine modeling
  - Possible dual fuel studies
- Implementation of dynamic coupling, cavitation model, and KH-ACT models as standard options for CONVERGE
- High-performance computing: Getting our feet wet!

Opportunities for Collaboration

- **KH-ACT primary breakup model:**
  - ✓ Facilitates coupling between nozzle flow and spray
  - ✓ More realistic near nozzle flow modeling
  - ✓ Dynamic coupling will also be implemented in FY12
- **Reduced reaction mechanisms:**
  - ✓ Any fuel molecule of interest
  - ✓ We will provide a well validated (0D, 1D, 3D) reaction mechanism
  - ✓ Typical size: 75-100 species, 400-500 reactions
- **LES Modeling:**
  - ✓ Scientific LES, rather than depending on heavy sub-grid scale modeling
  - ✓ Both qualitative and quantitative improvements with using LES
- **High-performance Computing:**
  - ✓ Availability of big clusters already running CONVERGE
  - ✓ Any problem too big for Ford can be run: Non-proprietary, collaborative
  - ✓ Possibility of procuring computational resources for proprietary work

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 at **University of Connecticut**

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Thank You

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