Modeling Biodiesel Spray Flame Lift-Off and Emission Characteristics Using a Detailed Mechanism for Methyl Decanoate as Surrogate

Sibendu Som, Douglas E. Longman
Argonne National Laboratory

Zhaoyu Luo, Max Plomer, Tianfeng Lu
University of Connecticut

April 13th 2011

Multi-Dimensional Engine Modeling (Part 3 of 4)

SAE 2011 World Congress

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

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

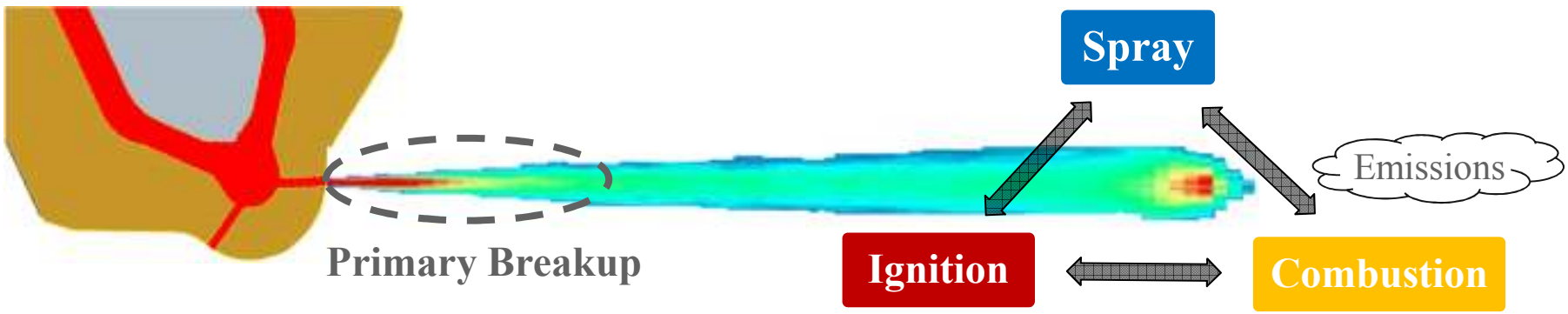
- Biodiesel is a lucrative alternate for compression ignition engines. However, differences in physical & chemical properties of biodiesel and petrodiesel are not insignificant
- Differences between biodiesel and petrodiesel using detailed computational modeling in terms of:
  - Inner nozzle flow (Som et al., SAE 2010): cavitation, turbulence, discharge coefficient
  - Non-reacting spray studies (Som et al., Fuel 2010): slower breakup with biodiesel

- Develop and validate reduced chemical kinetic models for biodiesel with a mixture of methyl decanoate + methyl decenoate + n-heptane surrogate mixture

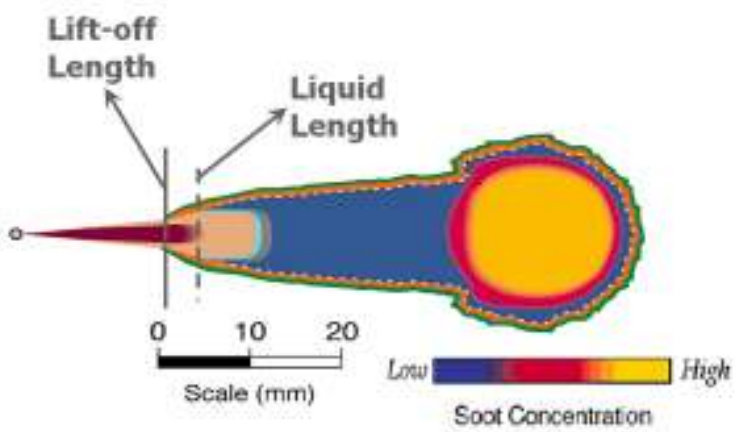
- Compare the predictive capability and scalability of different biodiesel models in literature: (a) methyl decanoate mixture as surrogate (b) methyl butanoate mixture as surrogate

Integrated Modeling Approach

Influence of Physical and Chemical properties of fuel



Conceptual Combustion Model from Sandia National Laboratory

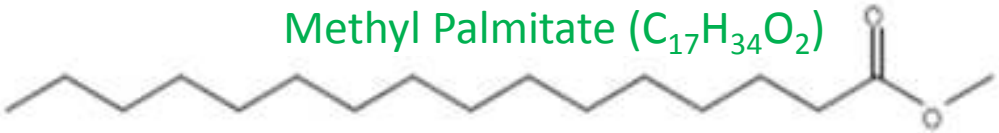


- **KH-ACT** primary breakup model: Aerodynamics, Cavitation, Turbulence
- Validation against spray data

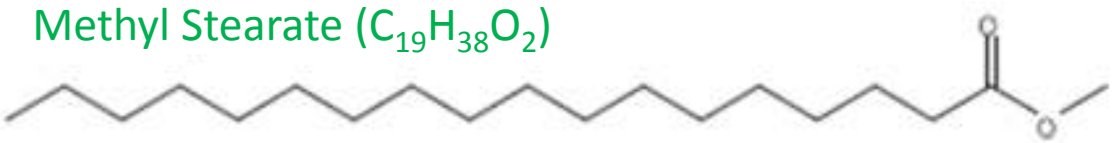
- **Detailed Chemistry**:
  Methyl Butanoate (MB)
  Methyl Decanoate (MD)
- Validation against **liquid and flame lift-off length** data
- Spray - flame interaction

Composition of Biodiesels

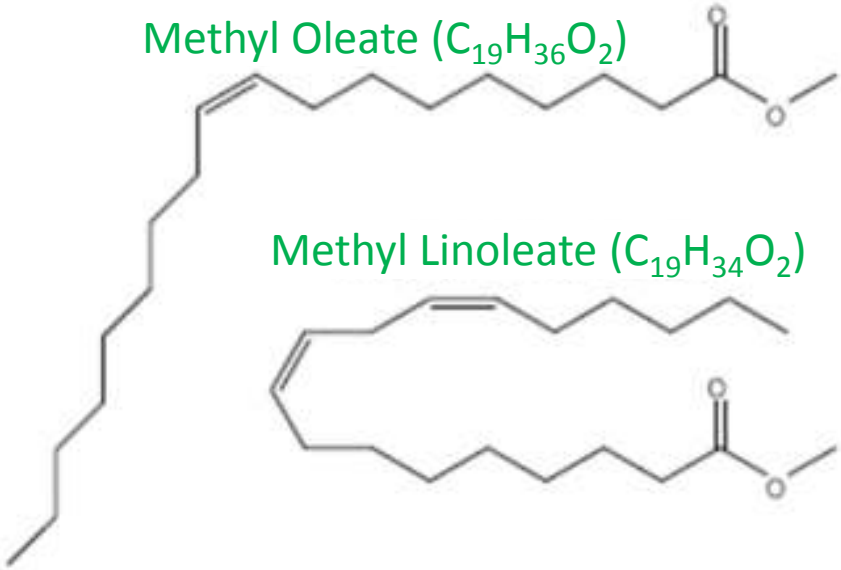
Methyl Palmitate ($C_{17}H_{34}O_2$)



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

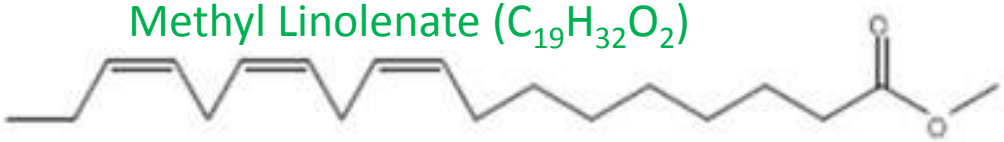


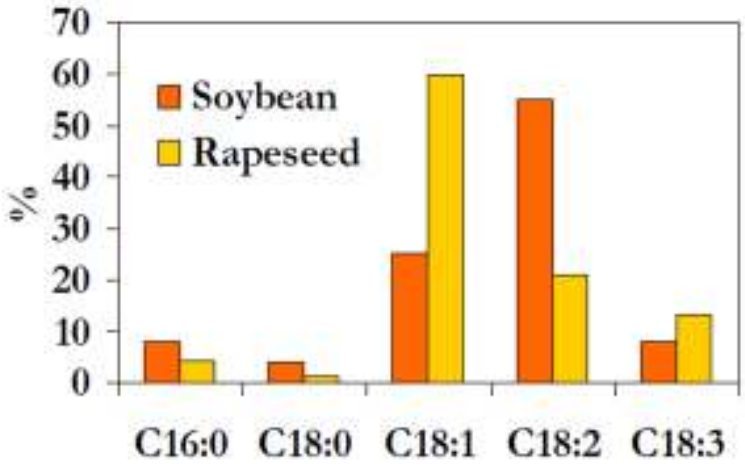
Methyl Oleate ($C_{19}H_{36}O_2$)



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

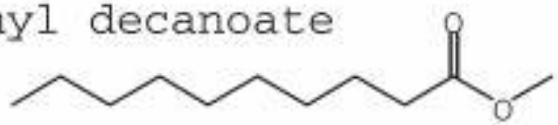
Methyl Linolenate ($C_{19}H_{32}O_2$)



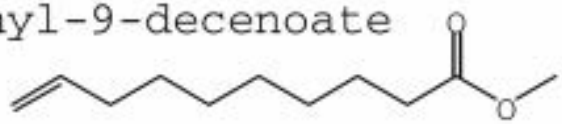


Biodiesel is a mixture of long-chain, oxygenated, unsaturated components

methyl decanoate



methyl-9-decenoate

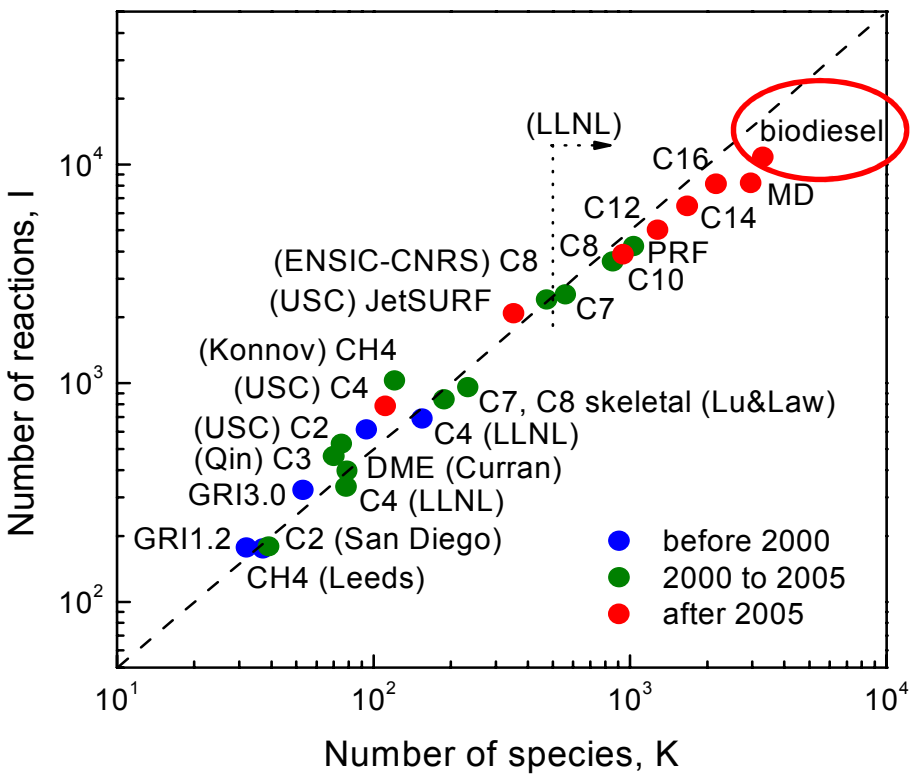


n-heptane, n-C_7H_{16}

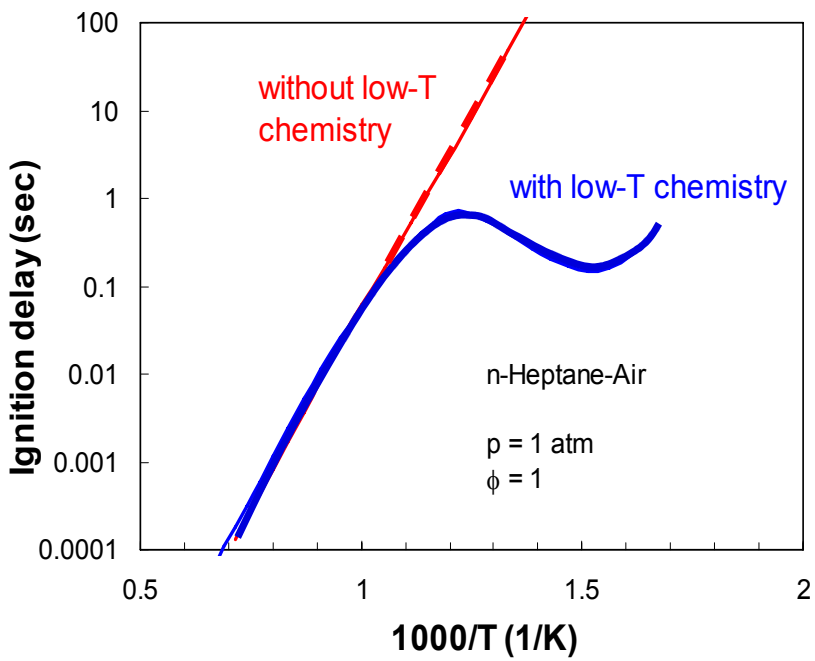
Detailed Mechanisms in Practical CFD Engine Simulations*

- 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

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

Lu-123*
123 species, 394 reactions

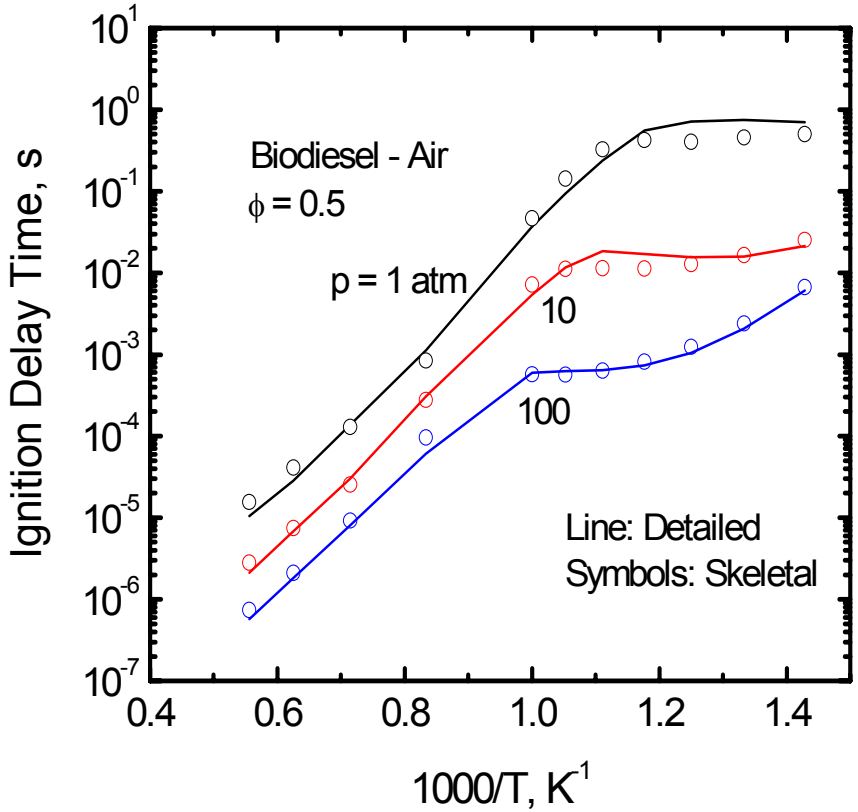
Lu-89
89 species, 367 reactions

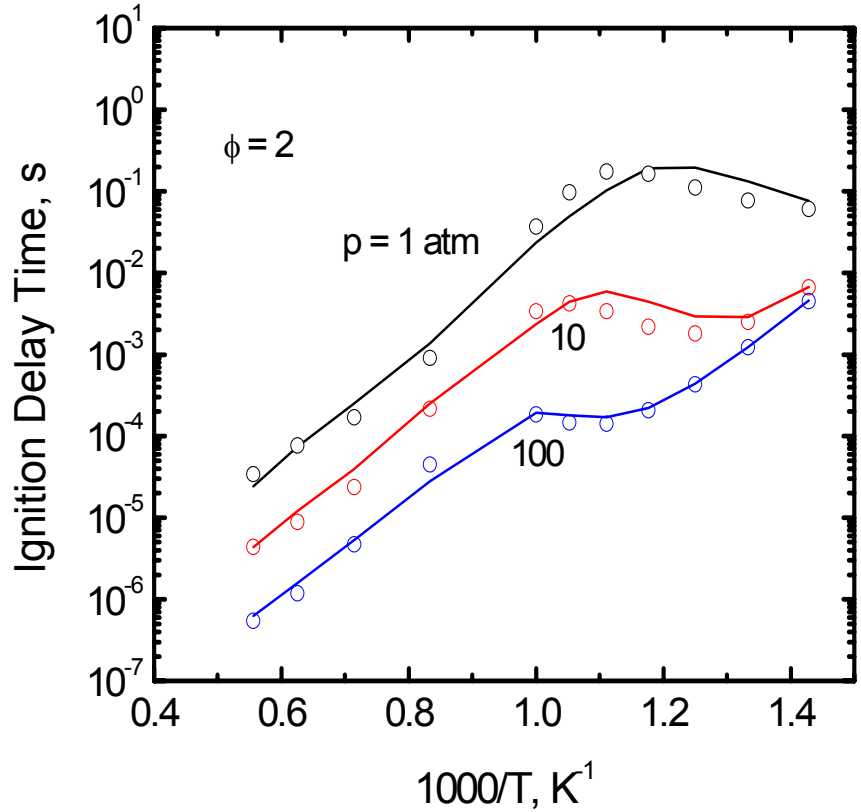
Range of operation:

- ✓ 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 Detailed Mechanism



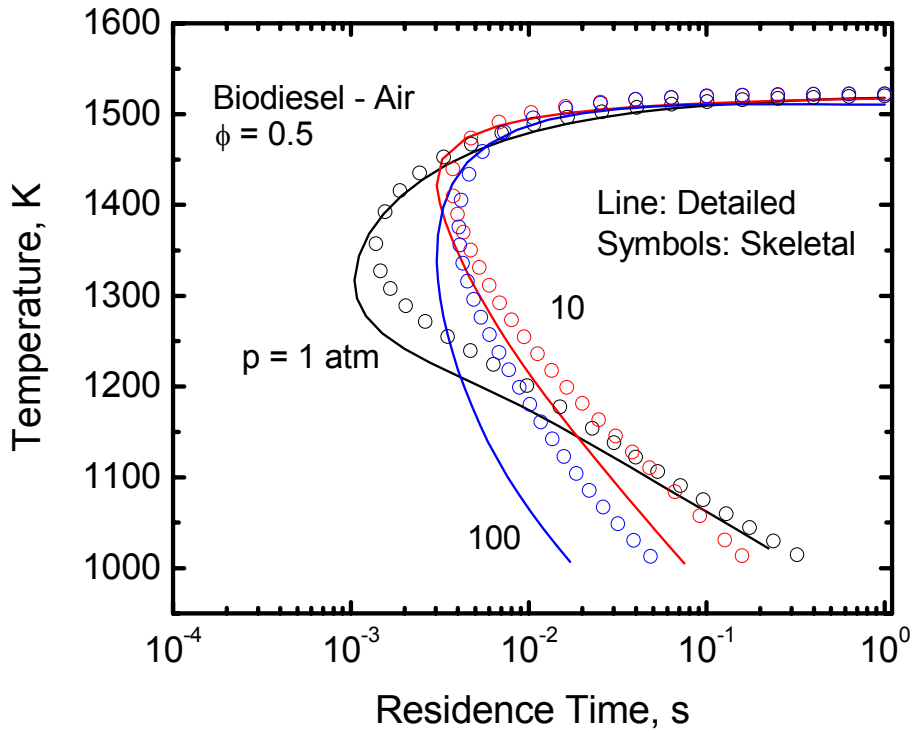


Detailed mechanism: 3329 species;10,806 reactions

- Reduced mechanism is able to predict ignition delay characteristics accurately!
- NTC region is also being well captured by both 89 and 123 species mechanisms

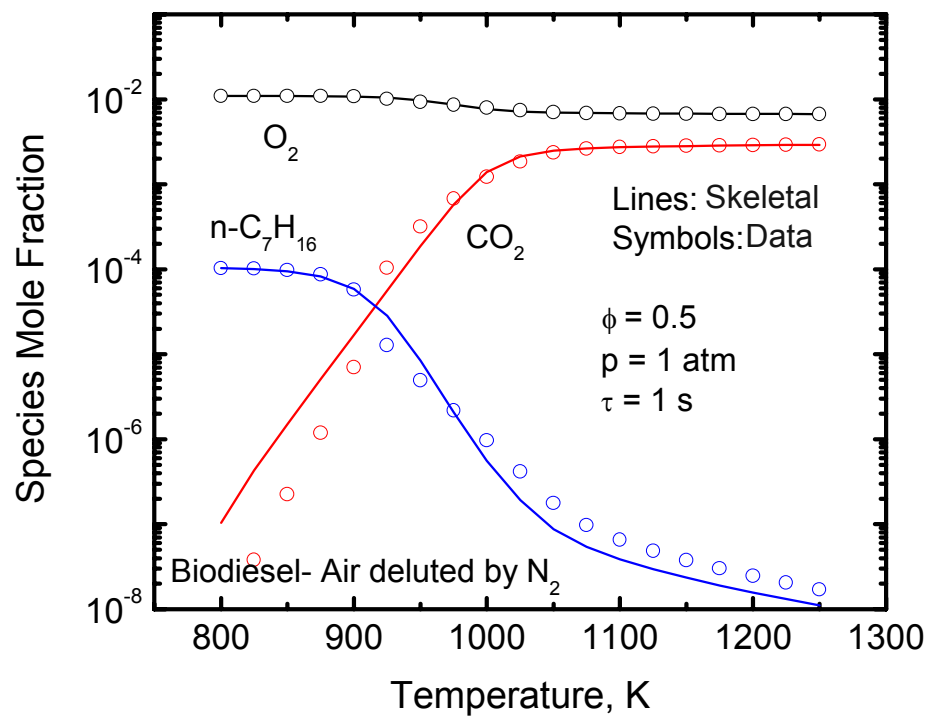
Validation Continued

Extinction profiles in perfectly stirred reactors (PSR)



Species concentrations in jet stirred reactors (JSR)

Data: Dagaut et al. PCI 2007



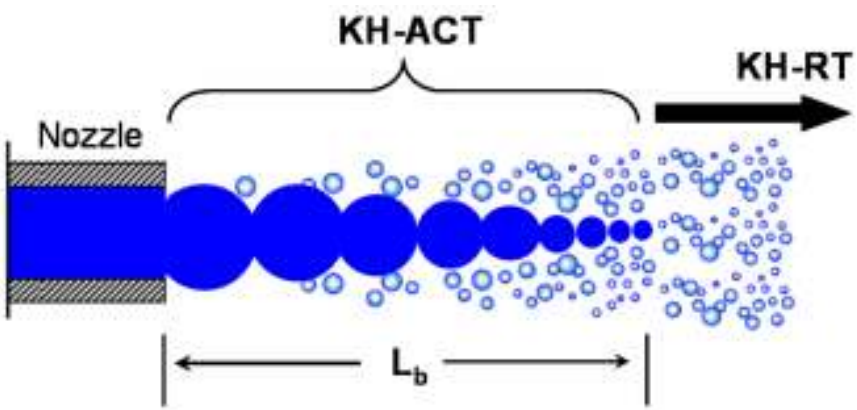
Both 89 species and 123 species mechanism yielded similar results!

123 species biodiesel surrogate mechanism is perhaps the biggest mechanism run for 3D CFD predictions under engine like conditions!

Modeling Set-up in CONVERGE*

- Liquid Injection using Blob model
- KH-ACT, KH-RT breakup models
- Collision and coalescence model
- **Multi-component** Evaporation model
- Dynamic drag model on droplet
- Turbulent dispersion model
- RNG K-ε turbulence model
- Detailed Chemistry Approach
- NOx and soot oxidation models
- Adaptive Mesh Resolution (**AMR**)

*** CONVERGE Manual**
*** Senecal et al., SAE 2007-01-0159**
*** S. Som, PhD thesis, UIC 2009**
*** S. Som et al., ASME-ICE 2011**
*** S. Som et al., Combustion and Flame 2010**



	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

Biodiesel: Case set-up

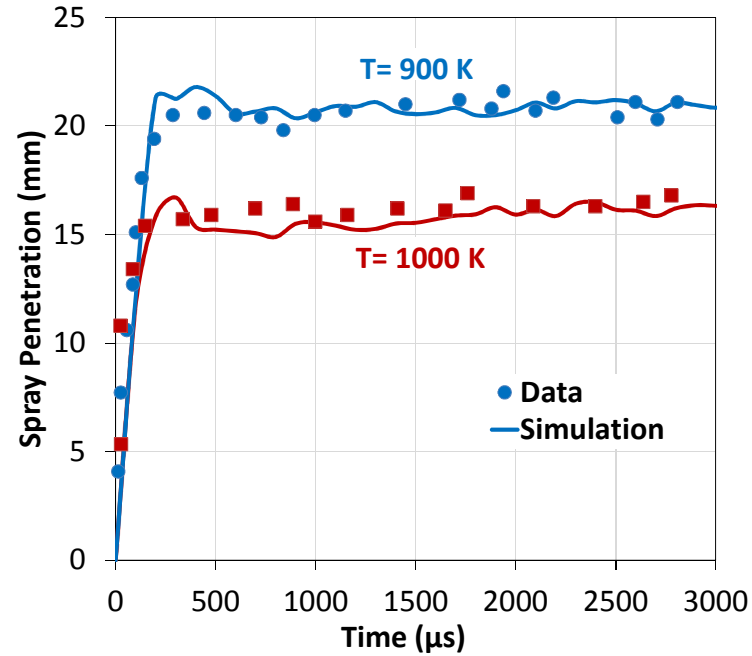
Injection & Ambient conditions for Biodiesel studies at Sandia*

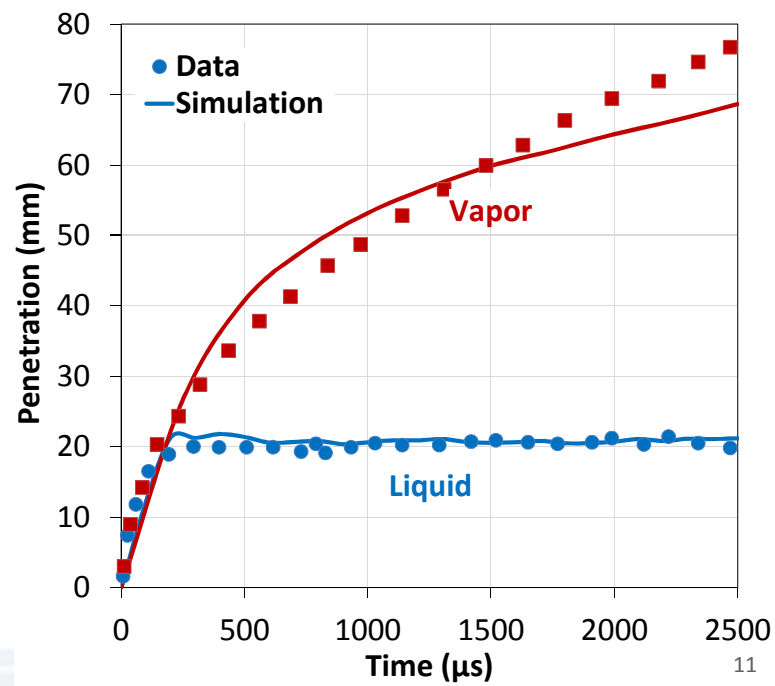
Parameter	Quantity
Injection System	Bosch Common Rail
Nozzle Description	Single-hole, mini-sac
Duration of Injection [ms]	
Orifice Diameter [µm]	90
Injection Pressure [Bar]	1400
Fill Gas Composition (mole fraction)	N_2=0.7515, O_2=0.15, CO_2=0.0622, H_2O=0.0363
Chamber Density [kg/m³]	22.8
Chamber Temperature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

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

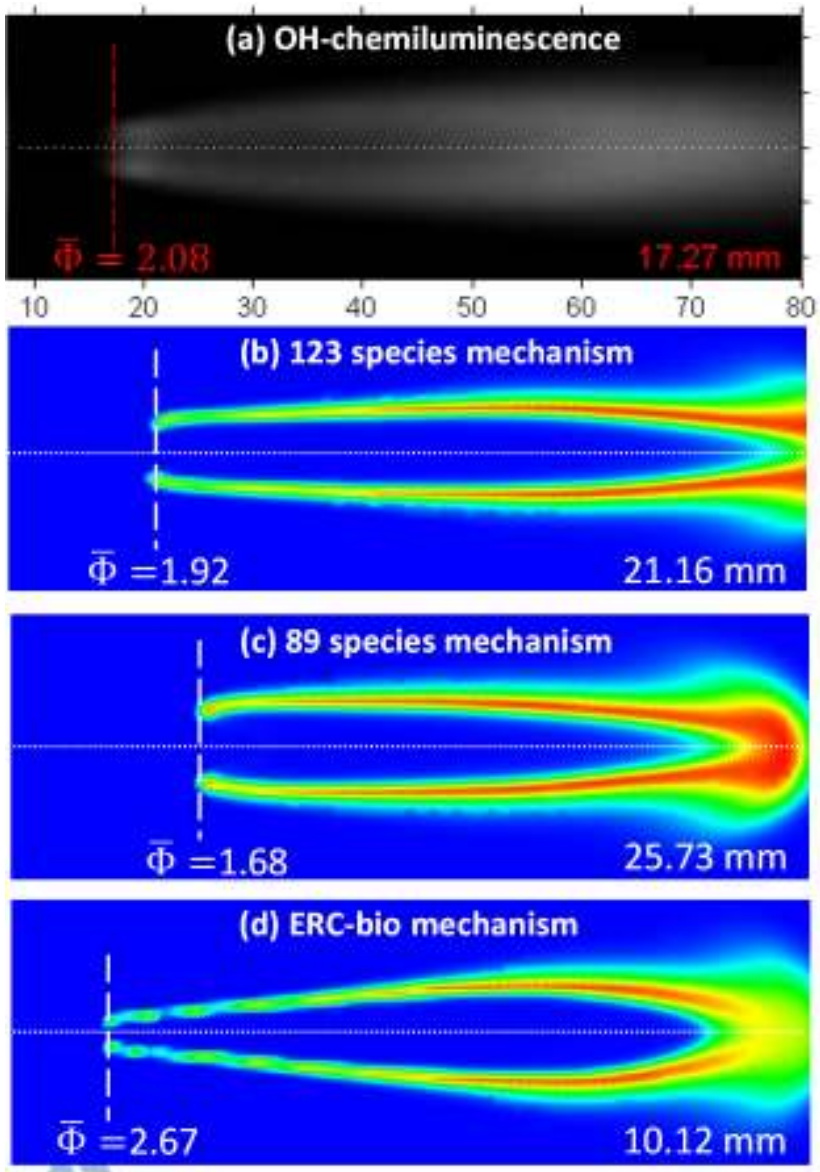
JG Nerva, CL Genzale, JMG Oliver, LM Pickett. Fundamental Spray and Combustion Measurements of Biodiesel under Diesel steady conditions. *Under preparation*

Non-reacting spray characteristics well predicted by the simulations!





Validation of Different Reaction Mechanisms

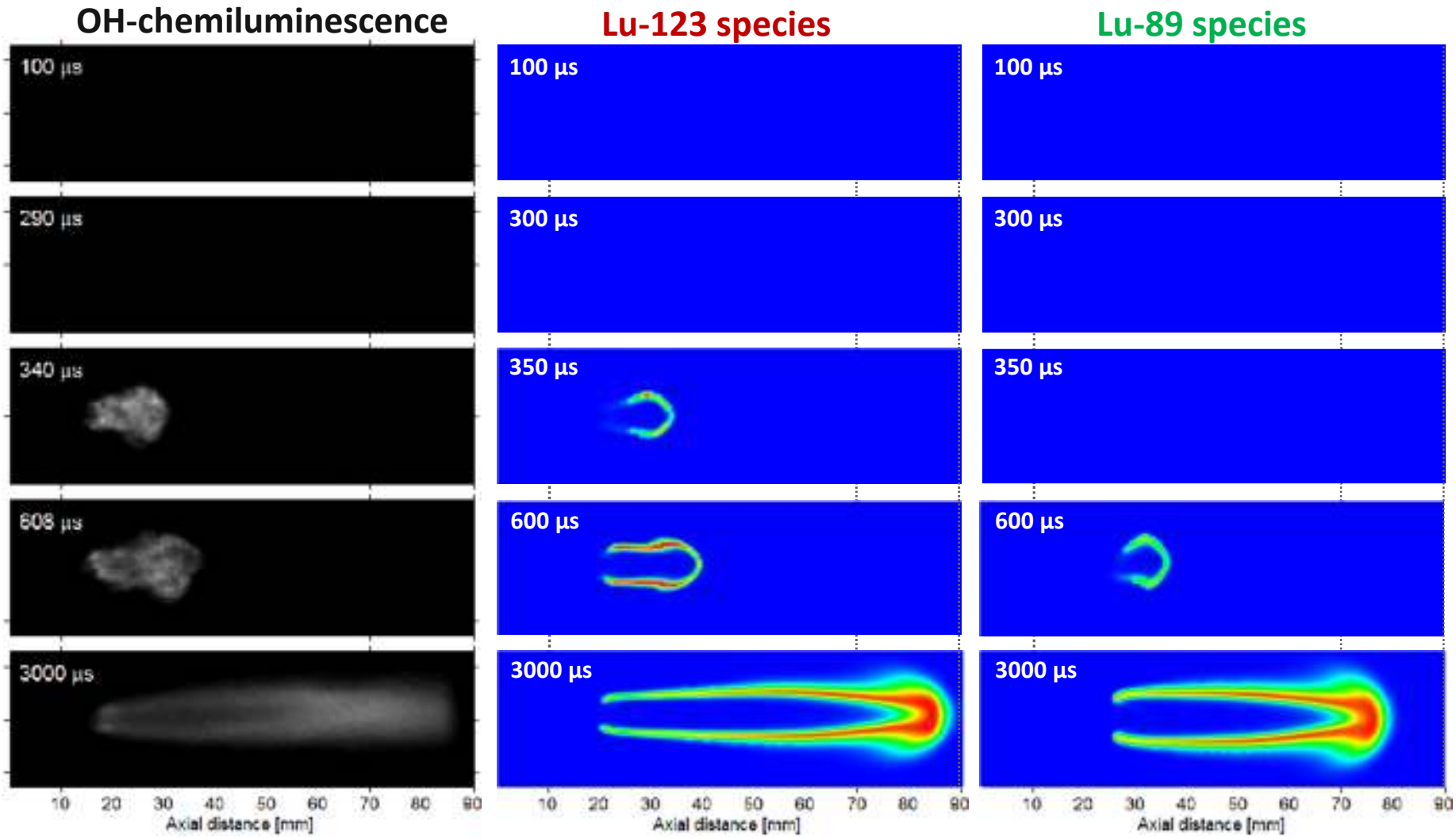


- Lu – 123: 123 species, 394 reactions. Paper # IC18. US National Combustion Meeting, March 2011
- Lu – 89 : 89 species, 364 reactions
- ERC-bio mechanism: 41 species, 150 reactions. SAE Paper No. 2008-01-1378

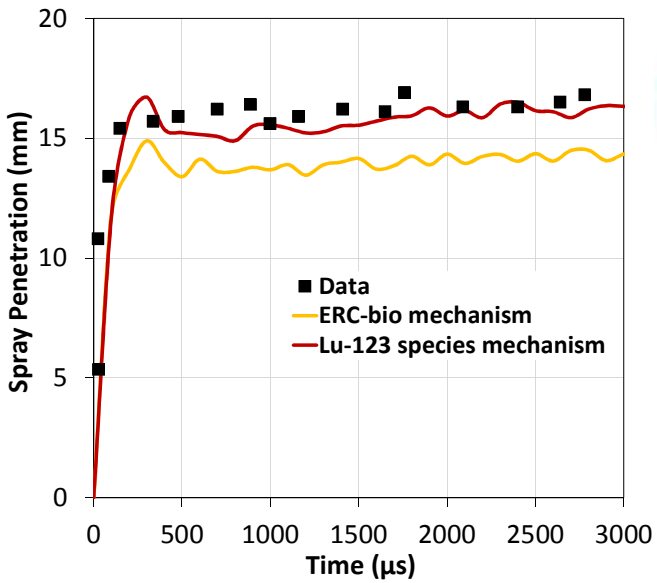
	Ignition Delay (μs)
Sandia Data	396
Lu - 123 species	510
Lu - 89 species	580
ERC-Bio mechanism	220

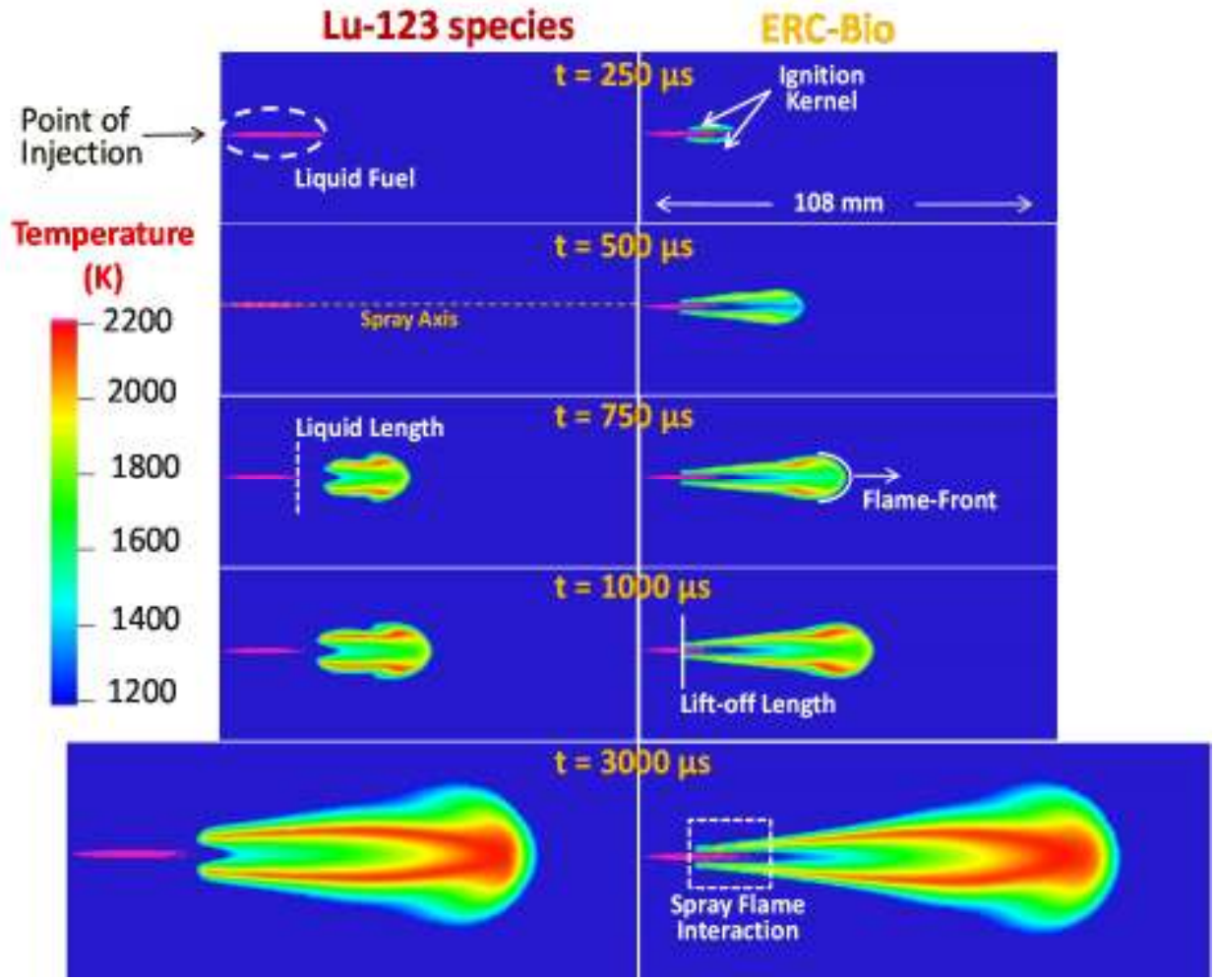
✓ Lu-123 species mechanism does the best job in predicting ignition delay and flame lift-off. Over-prediction of about 25% only.

Further Validation of Biodiesel Kinetic Models



Flame Structure with Different Mechanisms





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

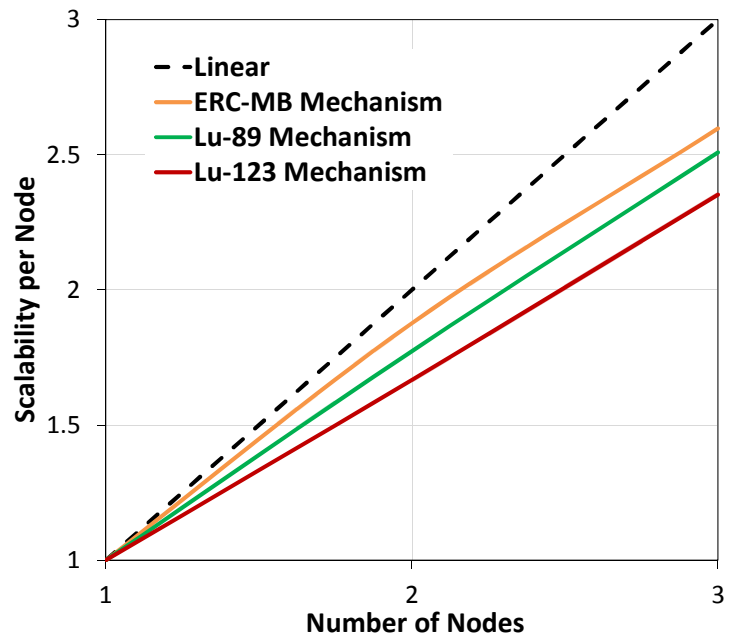
Computational Cost & Scalability

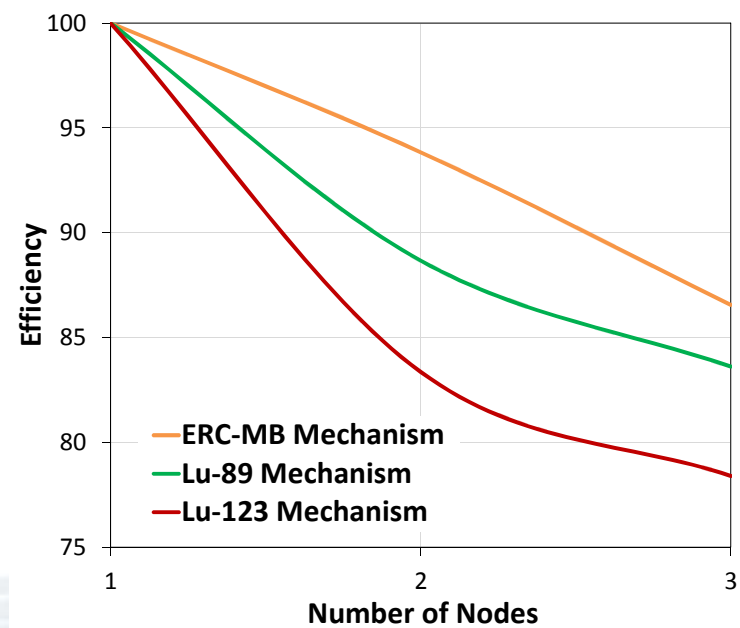
	Computational Time (for one node)
Lu-123 species	74 hours
Lu-89 species	38 hours
ERC-MB	13 hours

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





Summary & Future Work

- Reduced biodiesel mechanisms with (MD+MD9D+NHPT) as surrogates were developed and validated with 0D and 1D data from University of Connecticut
  - ✓ 89 species, 364 reactions
  - ✓ 123 species, 394 reactions
- Significant differences between methyl butanoate and methyl decanoate surrogate predictions were observed
- 123 species mechanism predicted the lift-off length, ignition delay, and species profiles fairly well under engine-like conditions
- Scalability studies were performed with all the mechanisms. Scalability and efficiency was lower with larger mechanisms
- **Full-cycle engine simulations** against CAT single-cylinder engine data with biodiesel to further validate these mechanisms
- Recently, the NHPT, MD, MD9D reaction pathways have been updated at LLNL. Use of these **updated reaction pathways,** has already improved ignition delay and flame lift-off length results.

Collaborators

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

Acknowledgements

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

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

Prof. Rolf Reitz and Ms. Jessica Brakora at University of Wisconsin for sharing the ERC-Bio mechanism

Upcoming Presentations

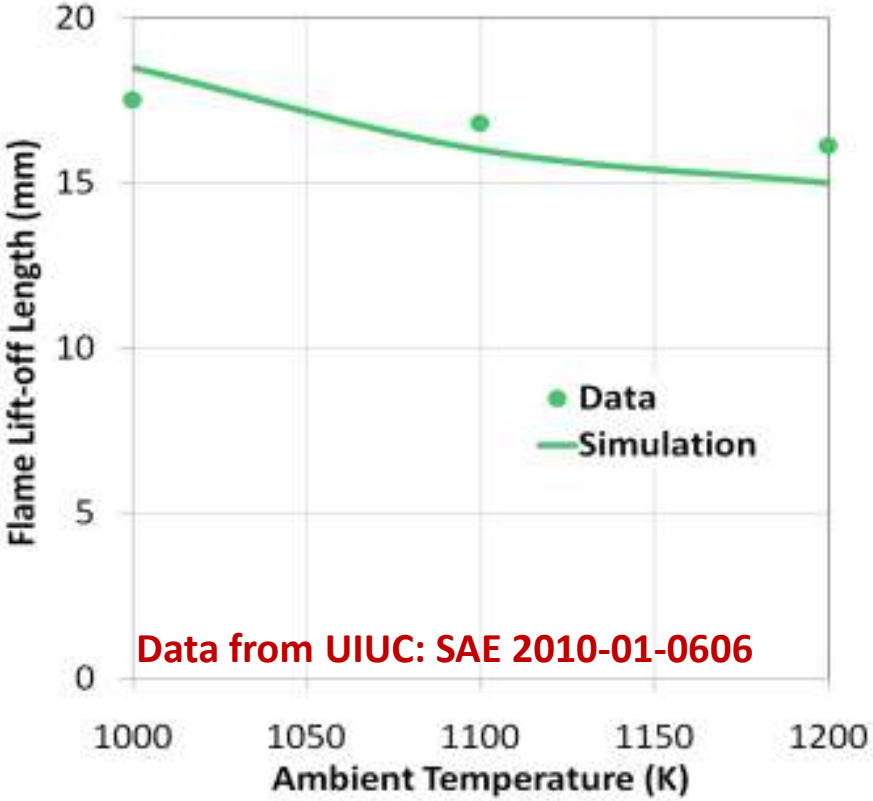
S. Som, D.E. Longman. **Co-ordination of Spray A simulation efforts**, ECN Workshop: May 2011, Ventura CA.

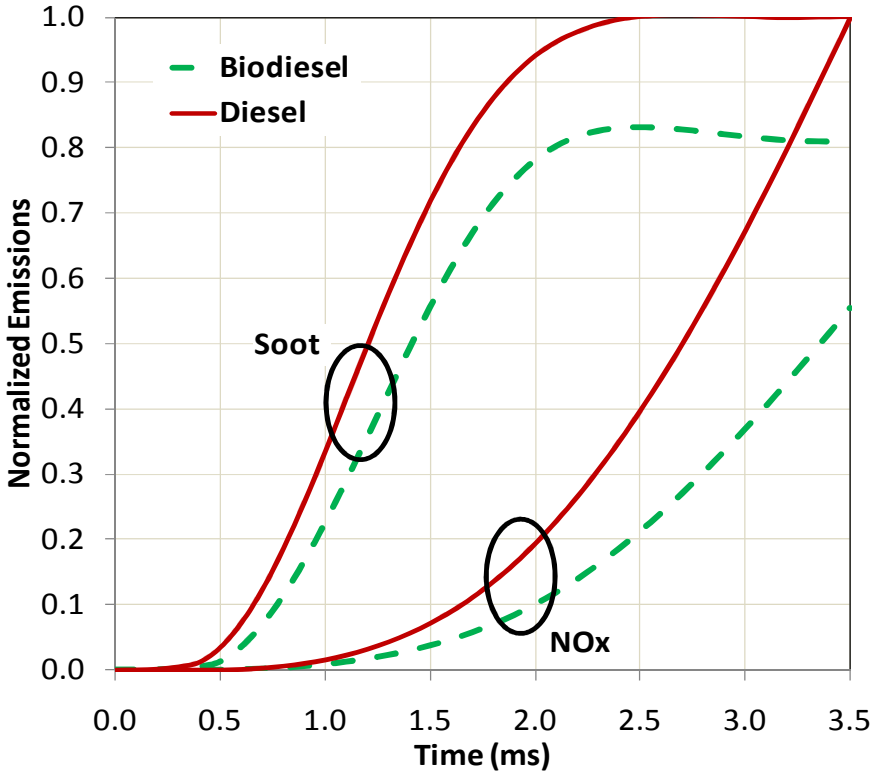
S. Som, D.E. Longman, Z. Luo, M. Plomer, T. Lu, E. Pomraning, P.K. Senecal. **Simulating flame lift-off characteristics of biodiesel fuel using detailed chemical-kinetic and LES turbulence models**, ASME-ICE: October 2011, Morgantown WV.

Thank You!

ssom@anl.gov
dlongman@anl.gov
tlu@engr.uconn.edu

Methyl Butanoate as Surrogate





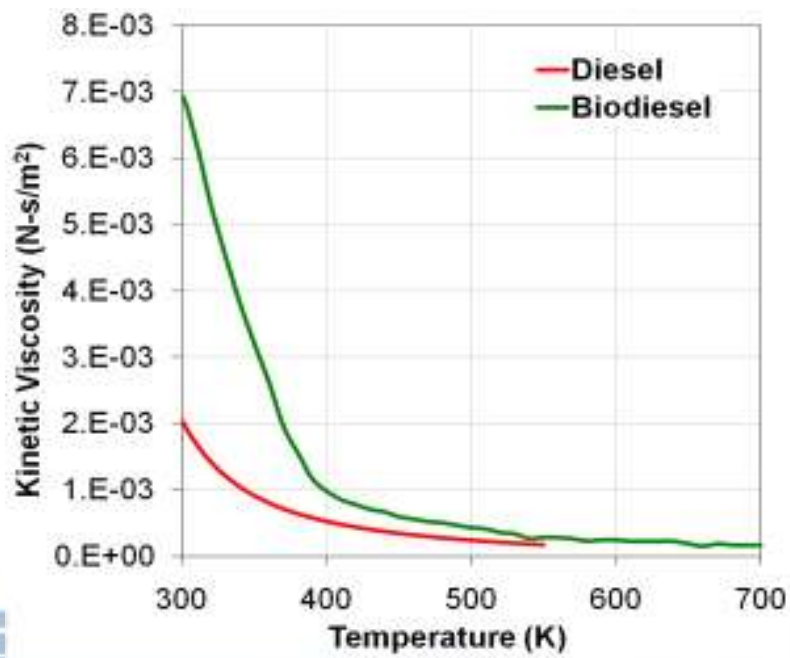
- Diesel surrogate (n-heptane): 42 species, 168 reaction mechanism from Chalmers University
- Biodiesel surrogate (methyl butanoate): 41 species, 150 reaction mechanism {Brakora et al. SAE 2008-01-1378}

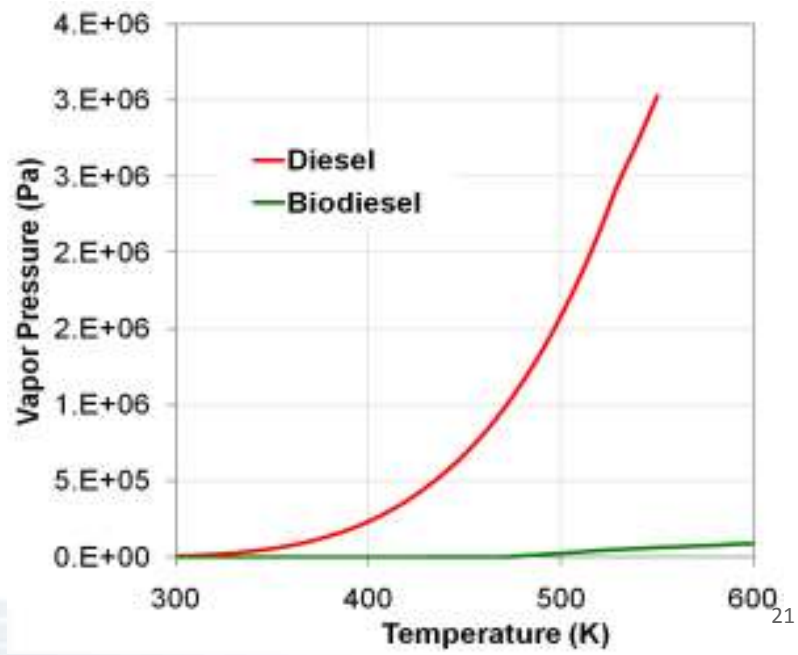
- Lower soot emission trends with biodiesel well captured
- Biodiesel surrogate not able to capture the accurate NOx trends!

Differences in Fuel Properties*

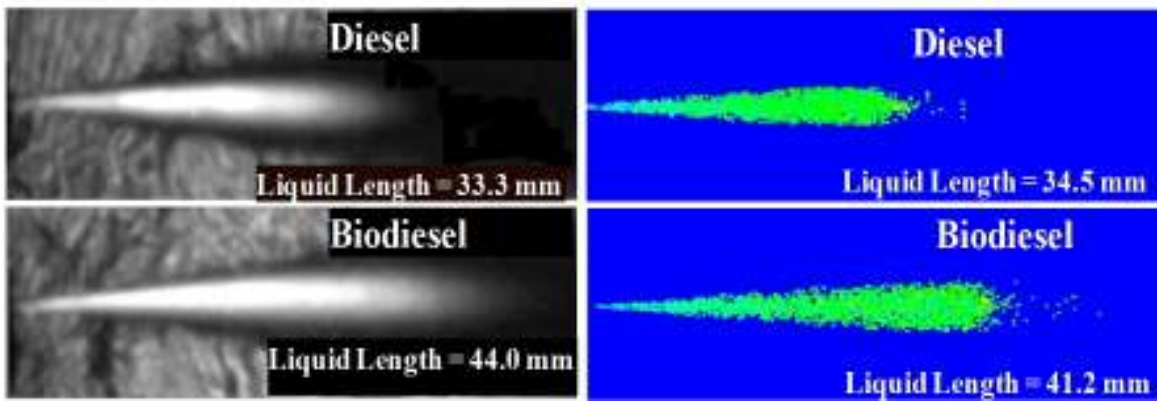
Fuel Property	Diesel	Biodiesel (SME)
Carbon Content [wt %]	87	76.74
Hydrogen Content [wt %]	13	12.01
Oxygen Content [wt %]	0	11.25
Density @ 15°C (kg/m3)	**820**	**877.2**
Surface Tension @ 25°C (N/m)	**0.020**	**0.0296**
Heat of Combustion (MJ/Kg)	**42.0**	**37.4**
Heat of Vaporization (KJ/Kg)	**361.0**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

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



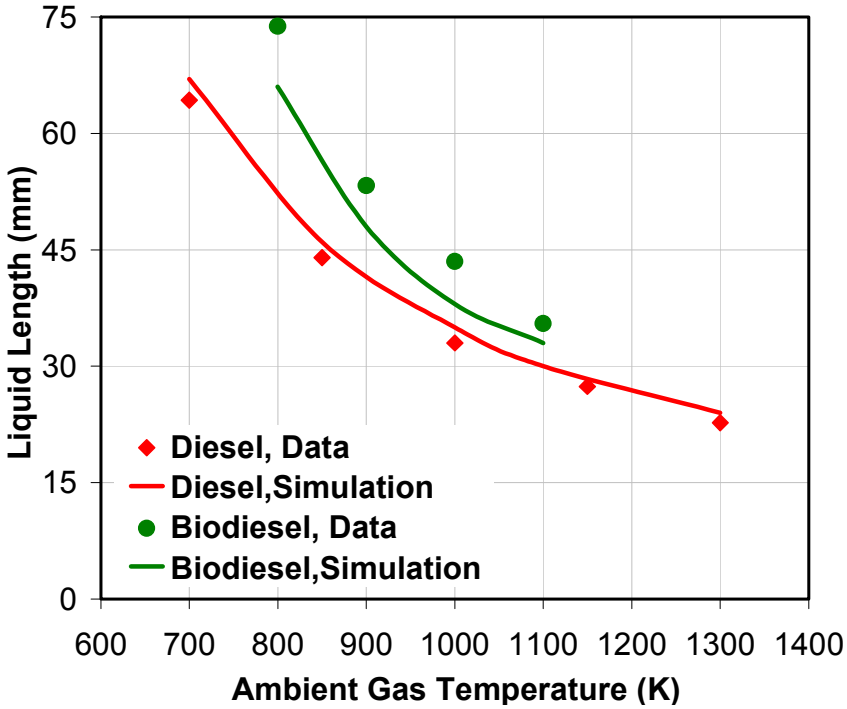


Evaporating Sprays: Liquid Length

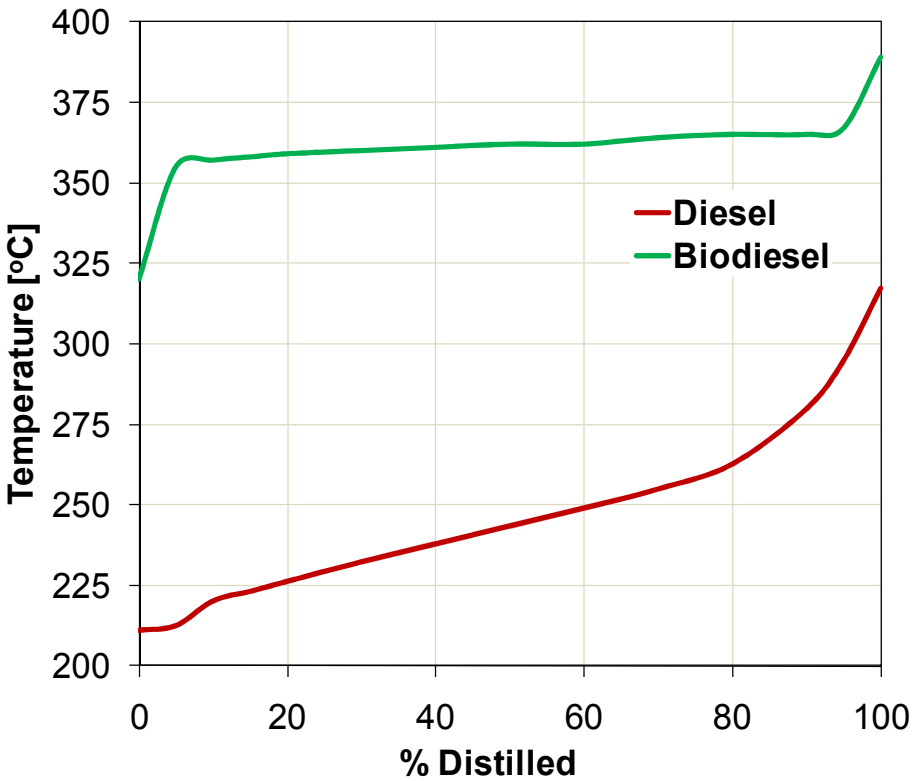


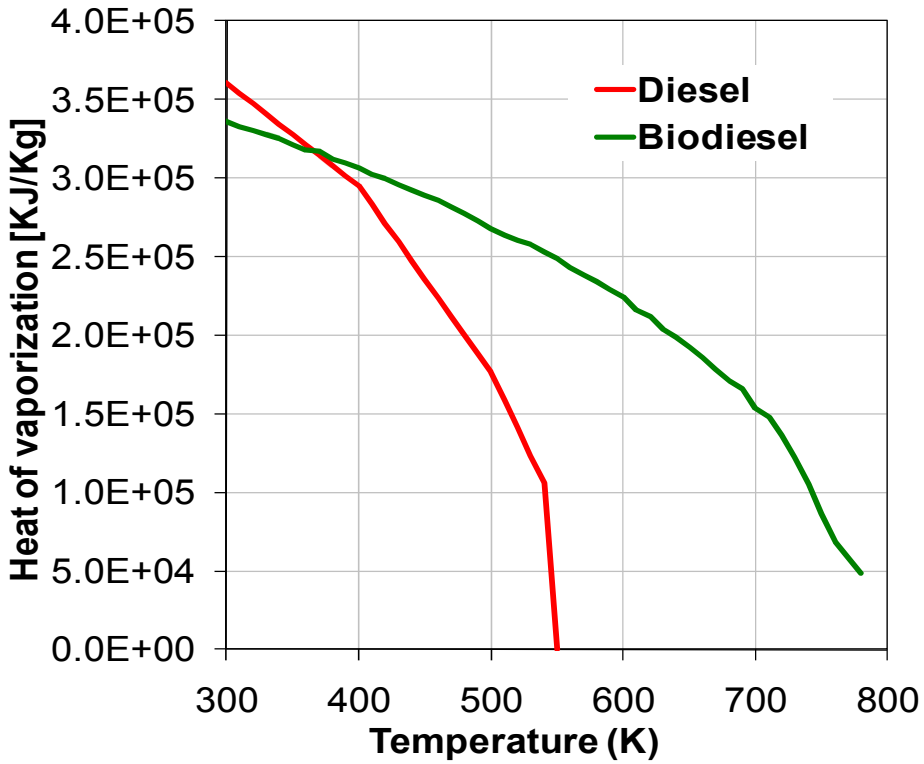
Data from:
1) DL Siebers: SAE 980809
2) BS Higgins, CJ Mueller, DL Siebers: SAE 1999-01-0519

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?

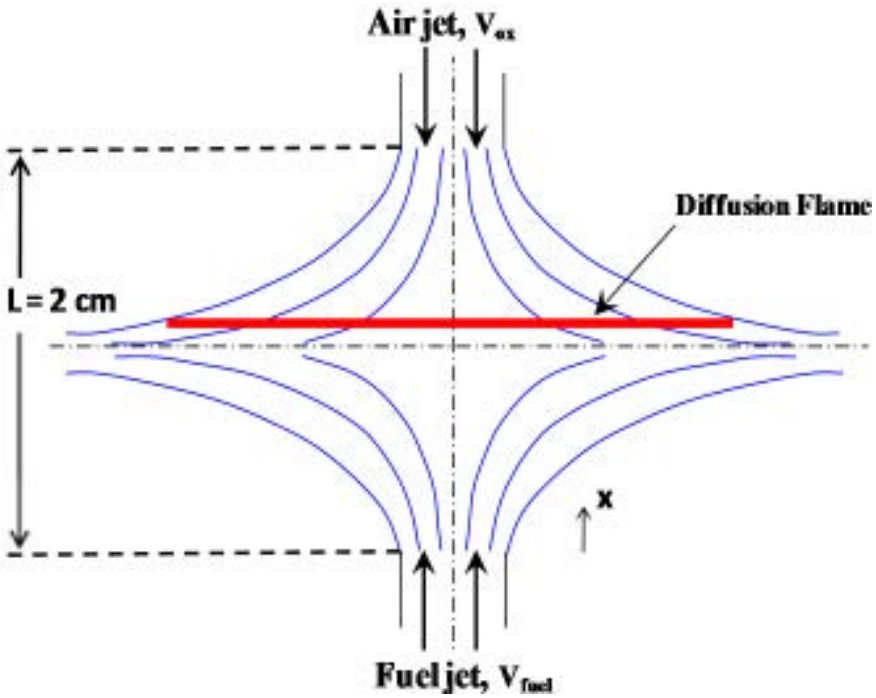




Slower breakup for biodiesel* is due to lesser amount of inner nozzle turbulence and cavitation. This results is increased spray penetration and reduction in spray cone-angle!

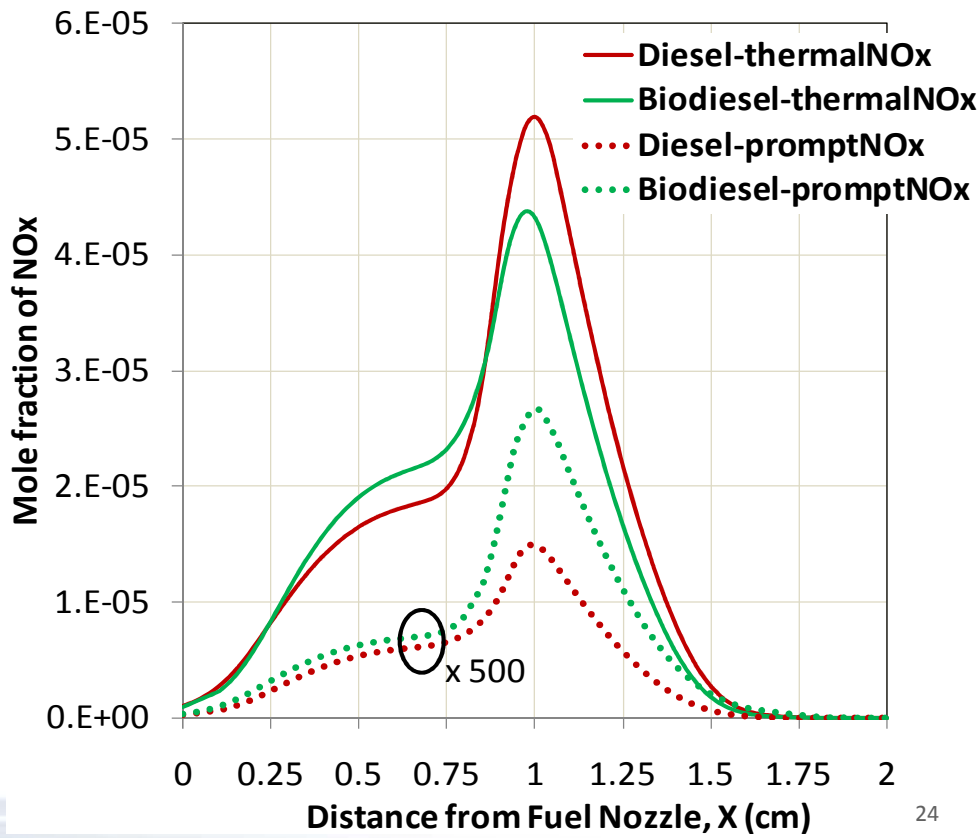
***S Som, DE Longman, AI Ramirez, SK Aggarwal. *FUEL* 2010**

Emission Characteristics in 1-D Configuration

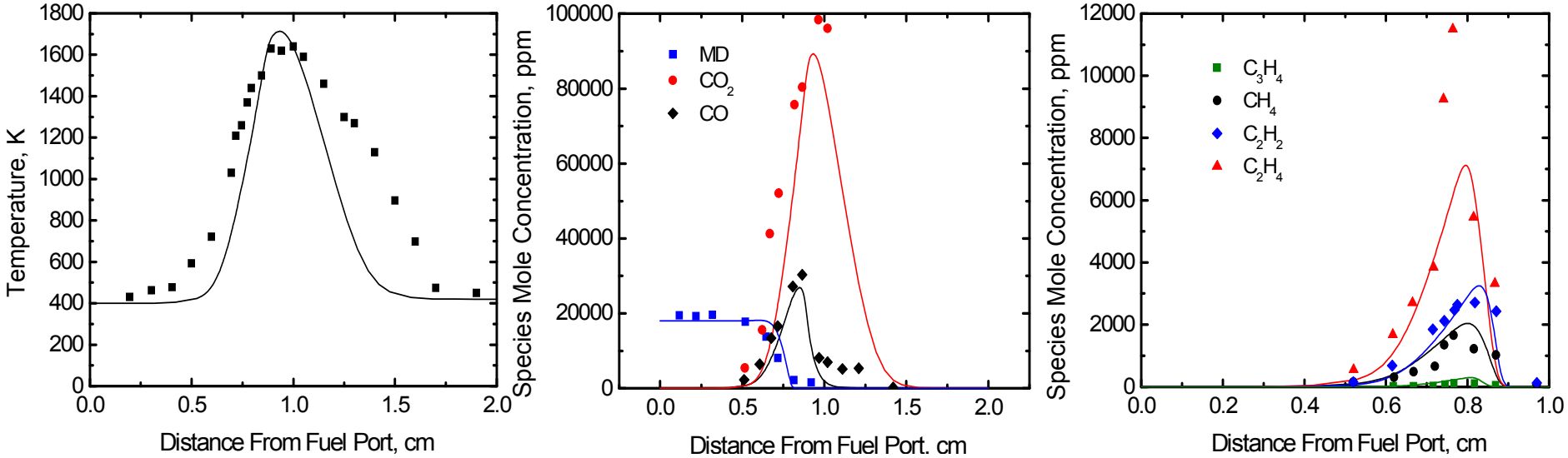


- Counter-flow configuration to study the NOx chemistry further
- GRI-3.0 NOx chemistry consisting of prompt, thermal, N_2O
- Simulations performed in CHEMKIN 4

- 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

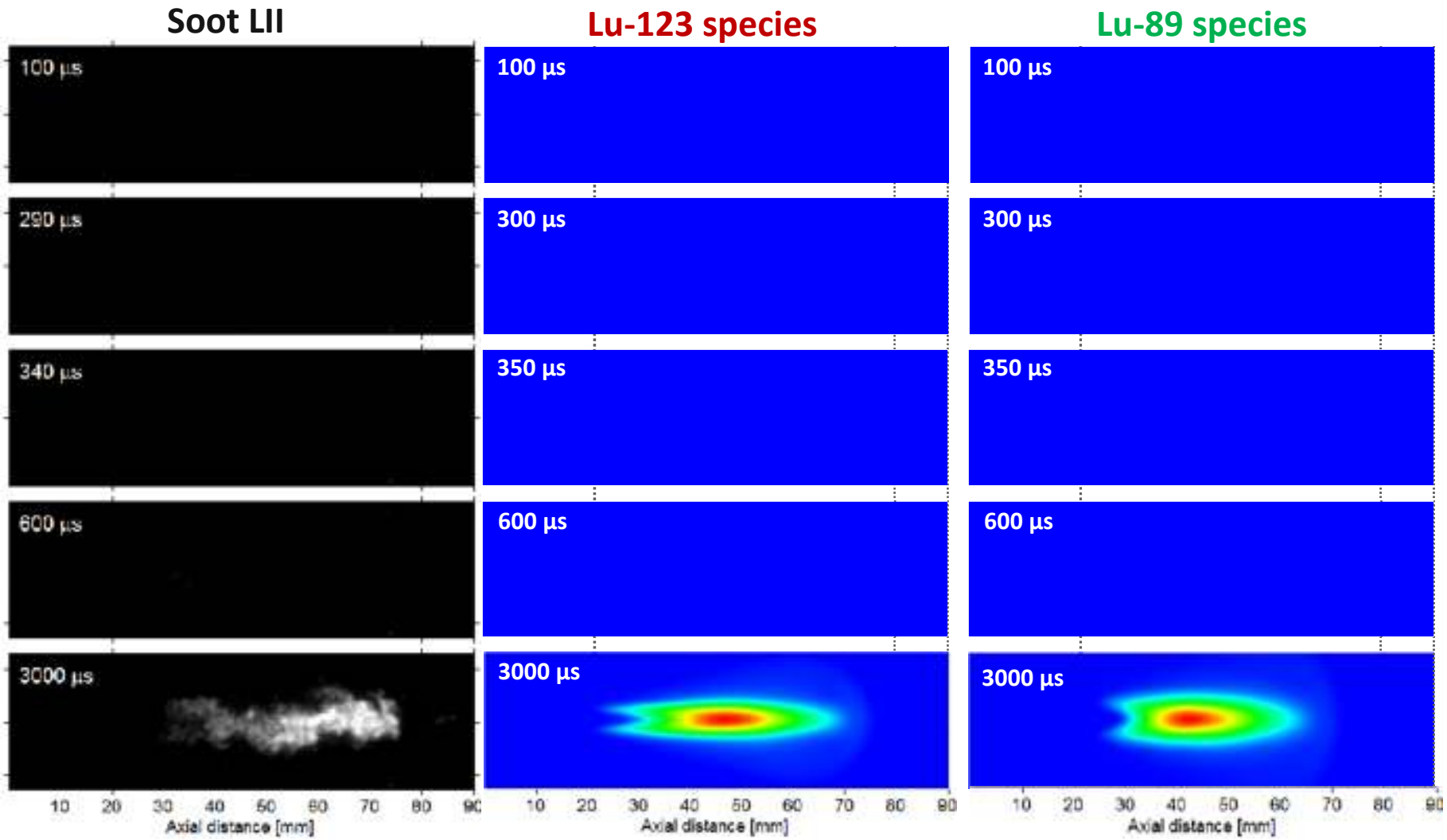


- Detailed Mechanism (Methyl Decanoate + Methyl Decenoate + N-heptane) from LLNL 2010: 3329 species, 10806 reactions
- Directed Relation Graph (DRG) reduction: 472 species, 2237 reactions
- Isomer lumping and DRG reduction: 242 species, 1819 reactions
- Sensitivity analysis aided DRG: 118 species, 83 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)**

Flame Structure with Different Mechanisms

Soot Validation with MD+MD9D+NHPT Mechanism



C_2H_2 used as a soot precursor