

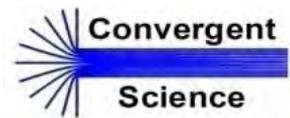
# Validation of Reduced Chemical Kinetic Mechanisms for Engine Simulations

**Sibendu Som**

Argonne National Laboratory

August 31<sup>st</sup> 2011

Presentation at: Workshop on Techniques for High-Pressure Combustion

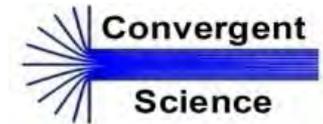


# Collaborators

Douglas E. Longman, Dr. Raghu Sivaramakrishnan, Dr. Mike Davis, Dr. Wei Liu at **Argonne National Laboratory**



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



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



Dr. Bill Pitz, Dr. Mani Sarathy at **Lawrence Livermore National Laboratory**



# Acknowledgements

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

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

Ms. Anita I. Ramirez at **University of Illinois at Chicago** for sharing engine data



# Outline

## □ Introduction

- From shock tubes to engines
- 3D Integrated modeling approach

## □ 3-D modeling set-up

- Sample spray validation

## □ Development of reduced reaction mechanisms

- N-heptane and n-dodecane: Diesel surrogates
- Methyl Decanoate + Methyl Decenoate: Biodiesel surrogate

## □ Validation against idealized combustion system data

## □ Robust validation against 3-D spray-combustion data

## □ Bringing it all together: Engine simulations

## □ Summary & Future Work



# From Shock Tubes to Engines

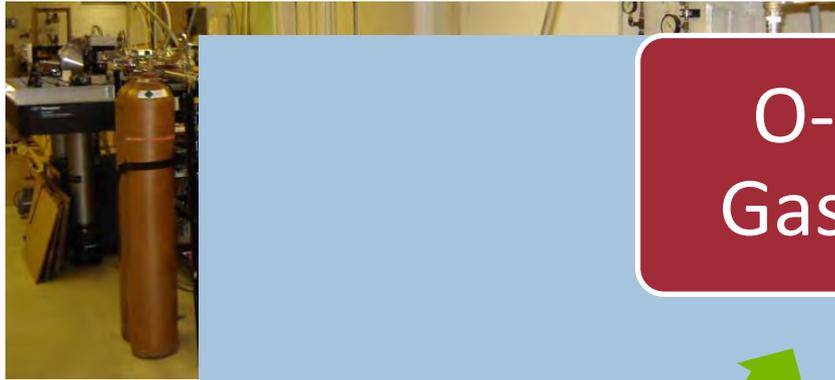
Gas phase measurements:

O-D, 1-D  
Gas-phase

Simulations: Using Reduced  
Chemical Kinetic Mechanisms

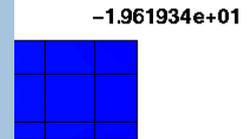
3-D Spray-  
Combustion

Engine  
Modeling



Re

Ignition  
(res)



Multi-p  
Turbulen  
com

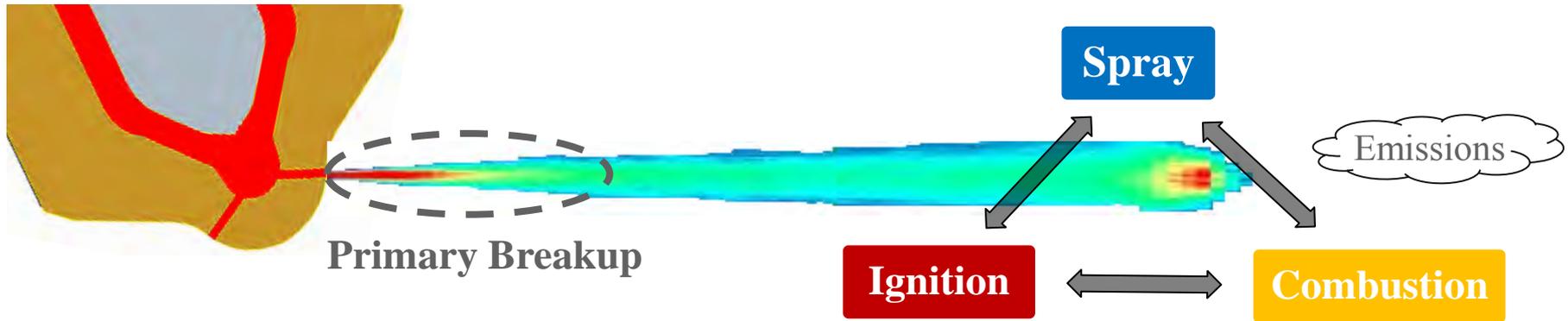
Spray Mo  
equivalenc

Combusti  
combustion, heat release, and species  
profiles for emission modeling

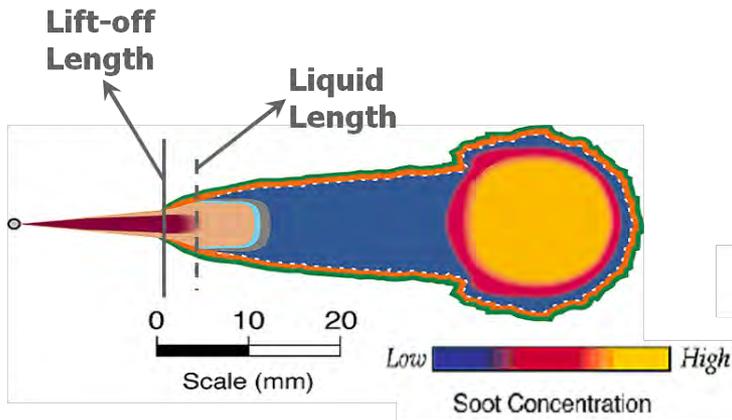


# 3-D Integrated Modeling Approach

## Inner Nozzle Flow



## Conceptual Combustion Model from Sandia National Laboratory



- ❑ Detailed inner-nozzle flow modeling
- ❑ Spray Modeling: **KH-ACT** primary breakup model  
Aerodynamics, Cavitation, Turbulence

Validation: **X-ray radiography** data

- ❑ **Detailed Chemistry:**
  - n-heptane – Diesel surrogate
  - n-dodecane – Diesel surrogate
  - Methyl Decanoate – Biodiesel surrogate

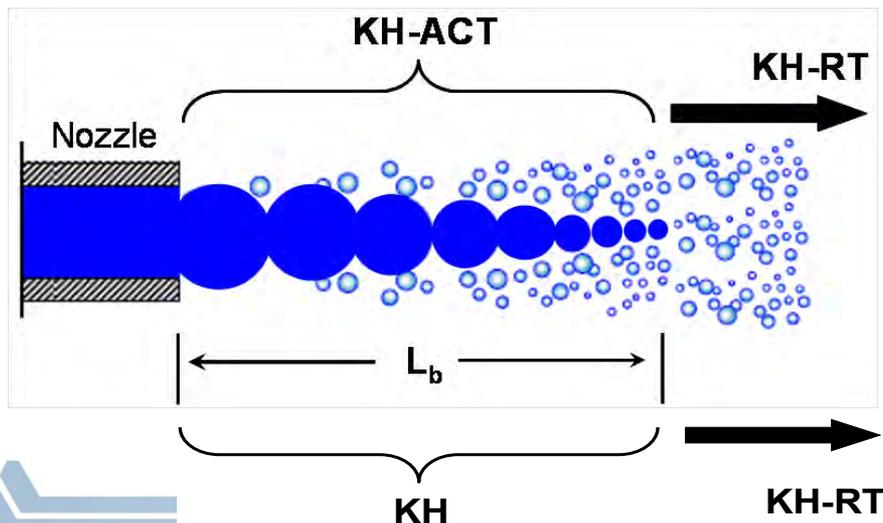
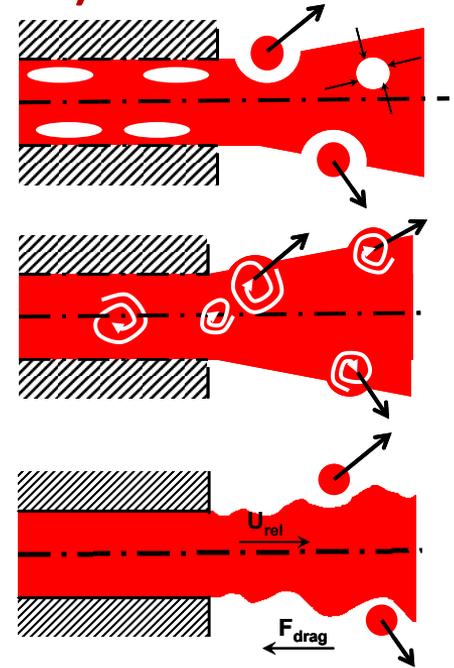
Validation:

Constant-volume vessel (Sandia National Laboratory)  
Engine data (Argonne National Laboratory)

# 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  $k-\epsilon$  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

Accurately predict fuel distribution  
(equivalence ratio)!!

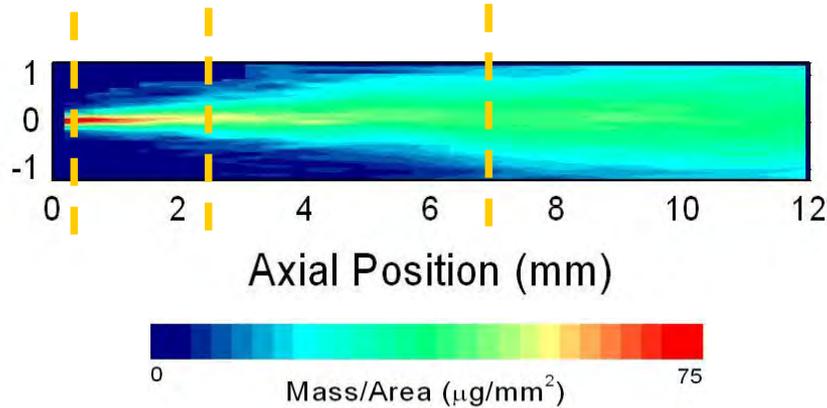
# 3-D Modeling Set-up

<b>Modeling Tool</b>	CONVERGE Source code access for spray and combustion modeling
<b>Dimensionality and type of grid</b>	3D, structured with Adaptive Mesh Resolution
<b>Spatial discretization approach</b>	2 <sup>nd</sup> order finite volume
<b>Smallest and largest characteristic grid size(s)</b>	Base grid size: 2mm or 4mm Finest grid size: 0.125mm, 0.25mm <u>Gradient based AMR</u> on the velocity and temperature fields. <u>Fixed embedding</u> in the near nozzle region to ensure the finest grid sizes
<b>Total grid number</b>	350K-450K for 0.25mm – RANS simulations 1.5-1.7 million for 0.125mm – LES case
<b>Parallelizability</b>	Good scalability up to 48 processors

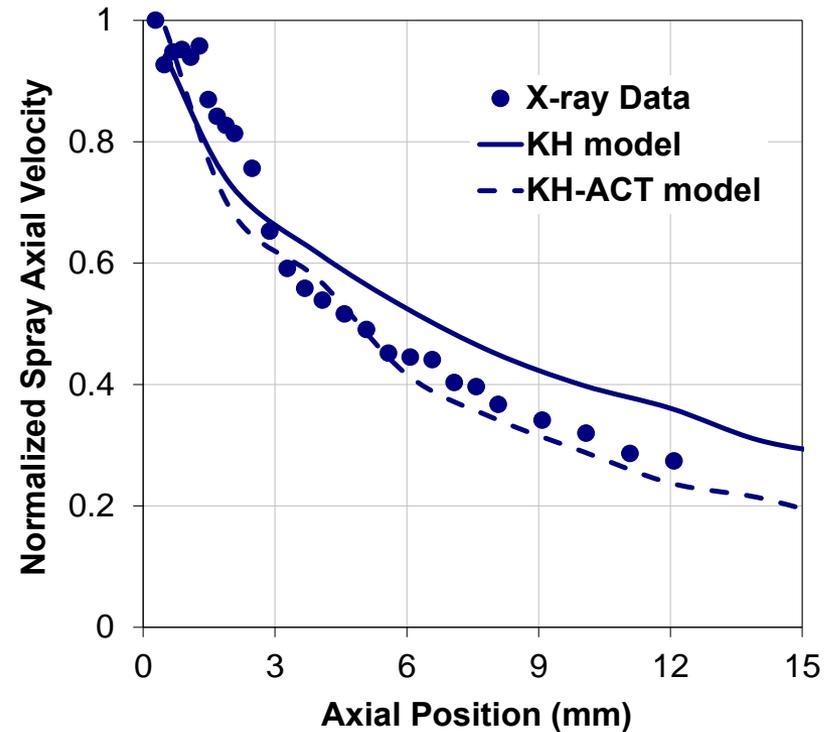
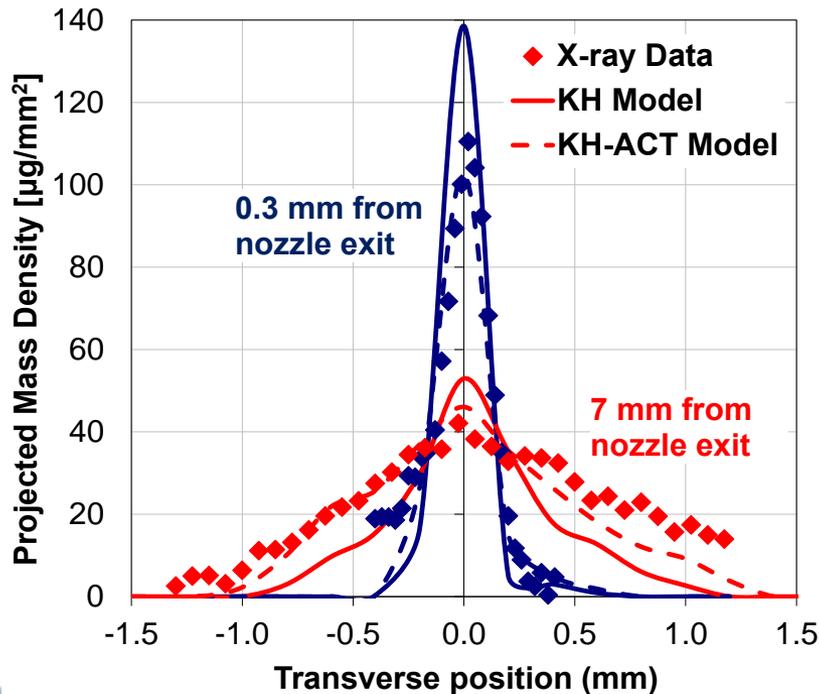
<b>Turbulence and scalar transport model(s)</b>	RNG k- $\epsilon$ , LES-Smagorinsky
<b>Spray models</b>	Breakup: KH-RT with breakup length concept Collision model: NTC, O'Rourke Coalescence model: Post Collision outcomes Drag-law: Dynamic model
<b>Time step</b>	Variable based on spray, evaporation, combustion processes
<b>Turbulence-chemistry interactions model</b>	Direct Integration of detailed chemistry well-mixed (no sub-grid model)
<b>Time discretization scheme</b>	PISO (Pressure Implicit with Splitting of Operators)



# 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
- ❑ Spray Dispersion accurately captured by only the KH-ACT model. KH model under-predicts spray spreading

**Accurate fuel distribution (equivalence ratio) is critical for reliable combustion predictions!**

# Development of Reduced Reaction Mechanisms

**Biodiesel surrogates:  
(from LLNL)**

**Methyl Decanoate (MD)**

**Methyl 9 Decenoate (MD9D)**

**n-Heptane (NHPT)**

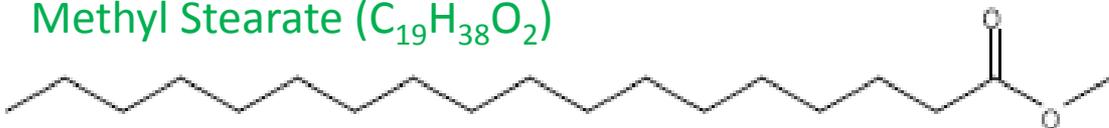


# Composition of Biodiesels

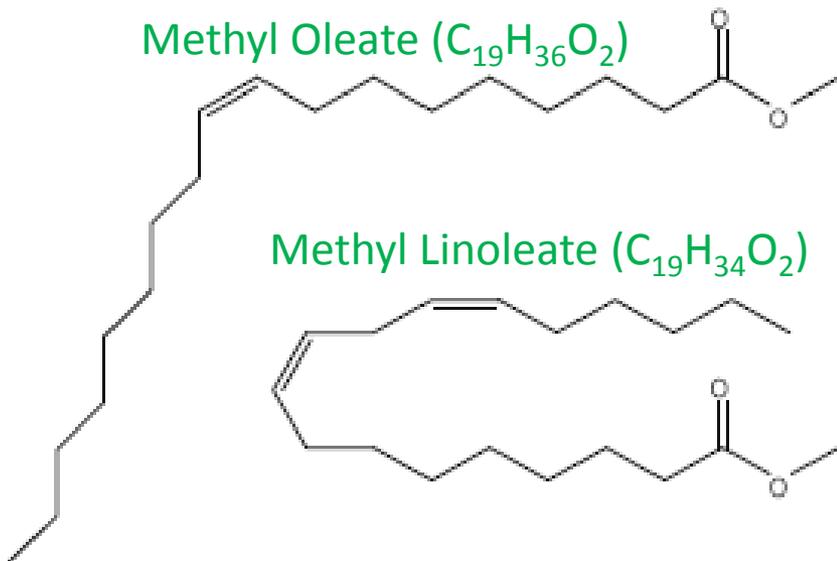
Methyl Palmitate ( $C_{17}H_{34}O_2$ )



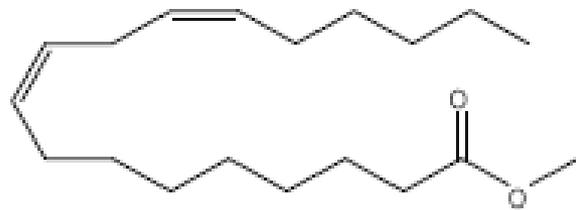
Methyl Stearate ( $C_{19}H_{38}O_2$ )



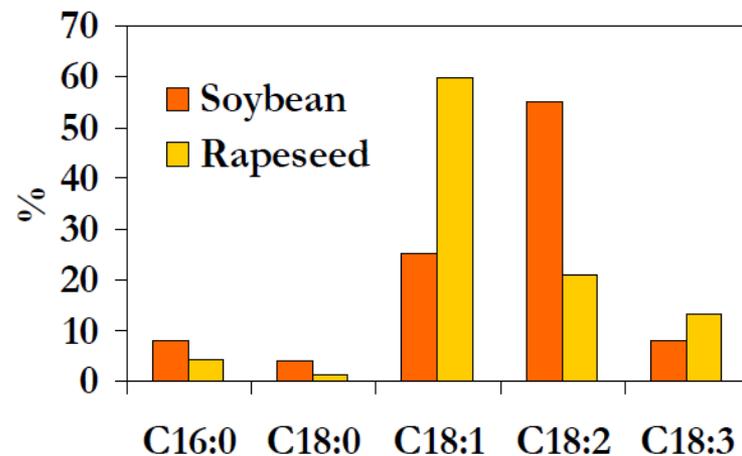
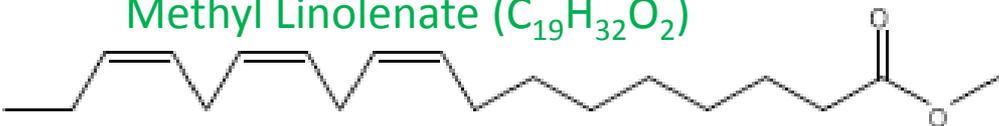
Methyl Oleate ( $C_{19}H_{36}O_2$ )



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

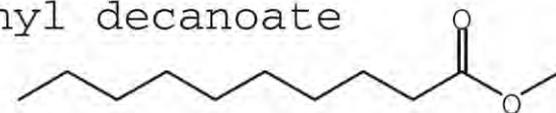


Methyl Linolenate ( $C_{19}H_{32}O_2$ )

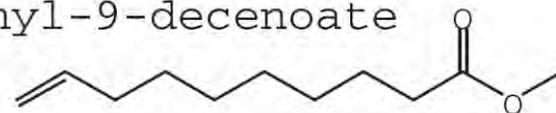


**Biodiesel is a mixture of long-chain, oxygenated, unsaturated components**

methyl decanoate



methyl-9-decenoate



n-heptane,  $n-C_7H_{16}$

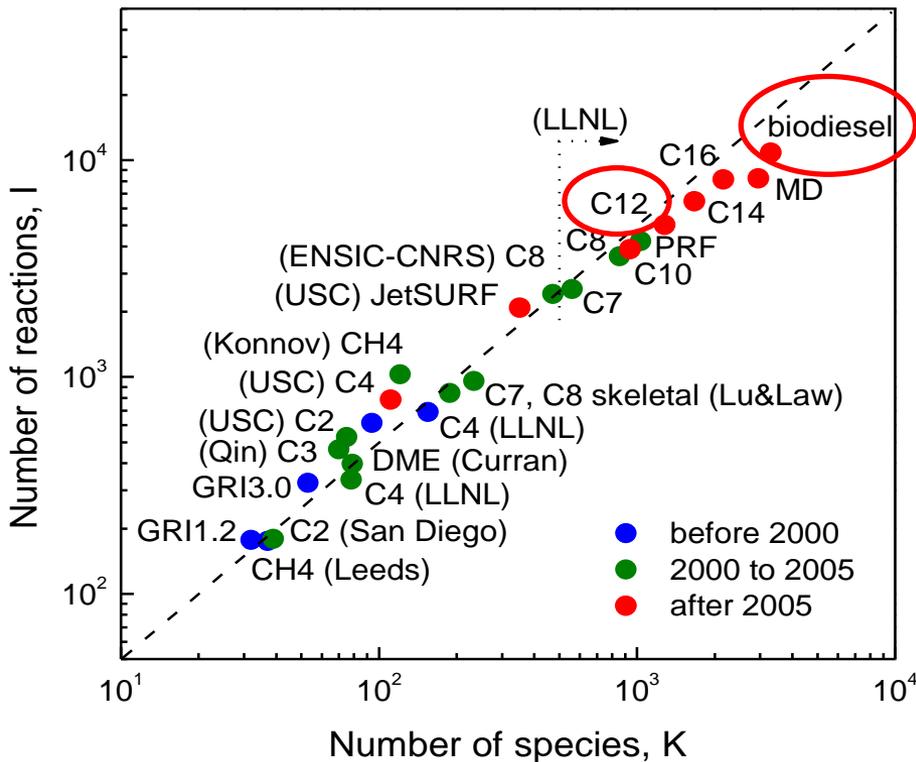
# Detailed Mechanisms in Engine Simulations\*

## Large mechanism sizes

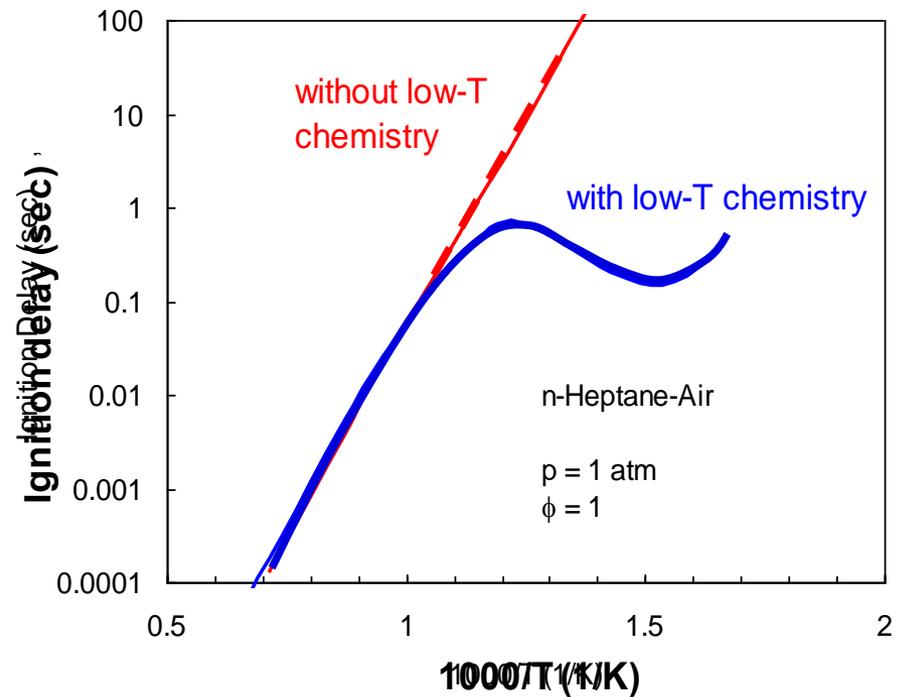
3329 species; 10,806 reactions (Biodiesel)

2115 species; 8157 reactions (C12)

From Lawrence Livermore (LLNL)



## Detailed chemistry is important

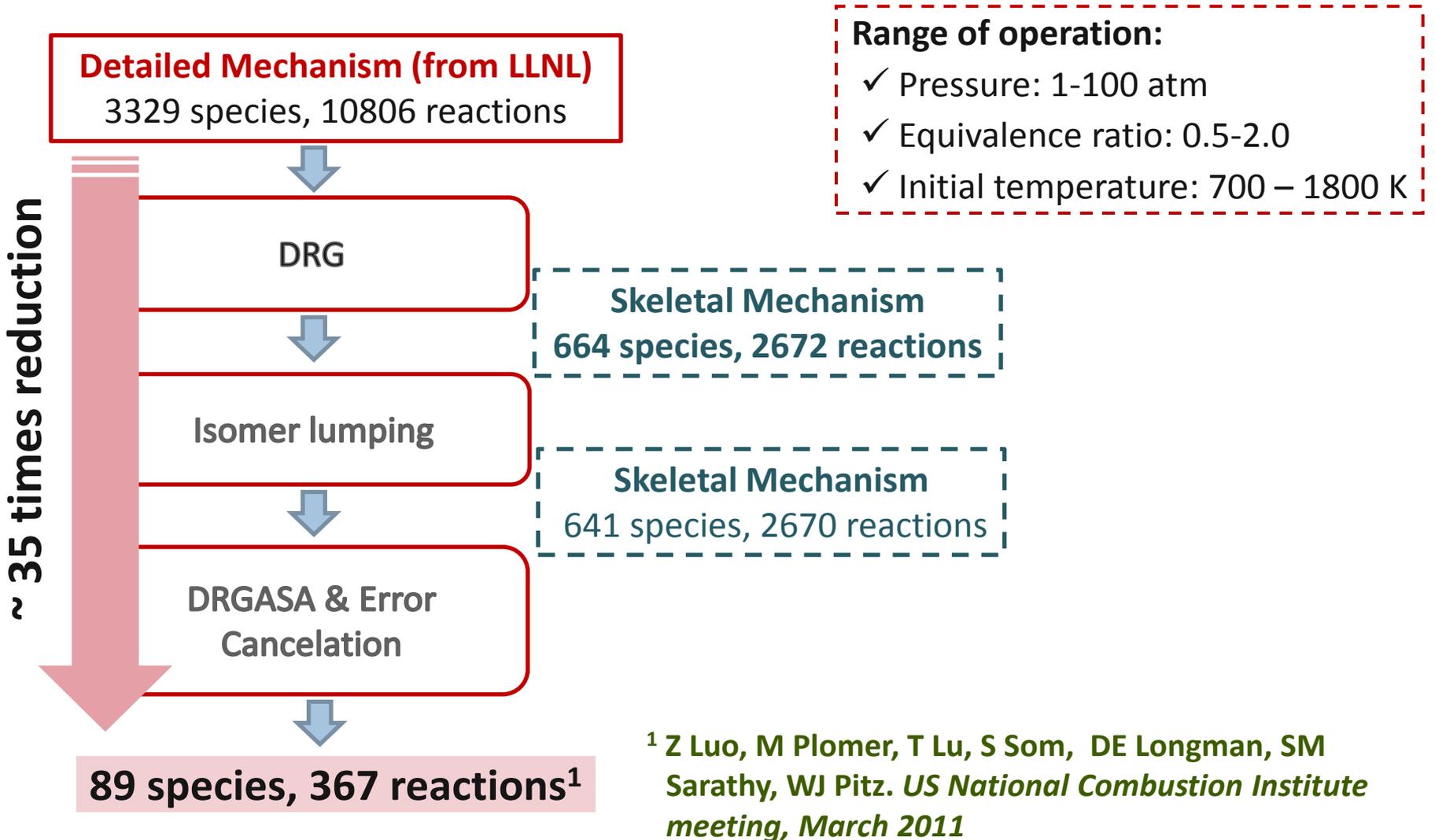


Mechanism reduction needed for CFD simulations with large mechanisms

\* Lu and Law, 2009

Computational time:  $N^2 \sim N^3$

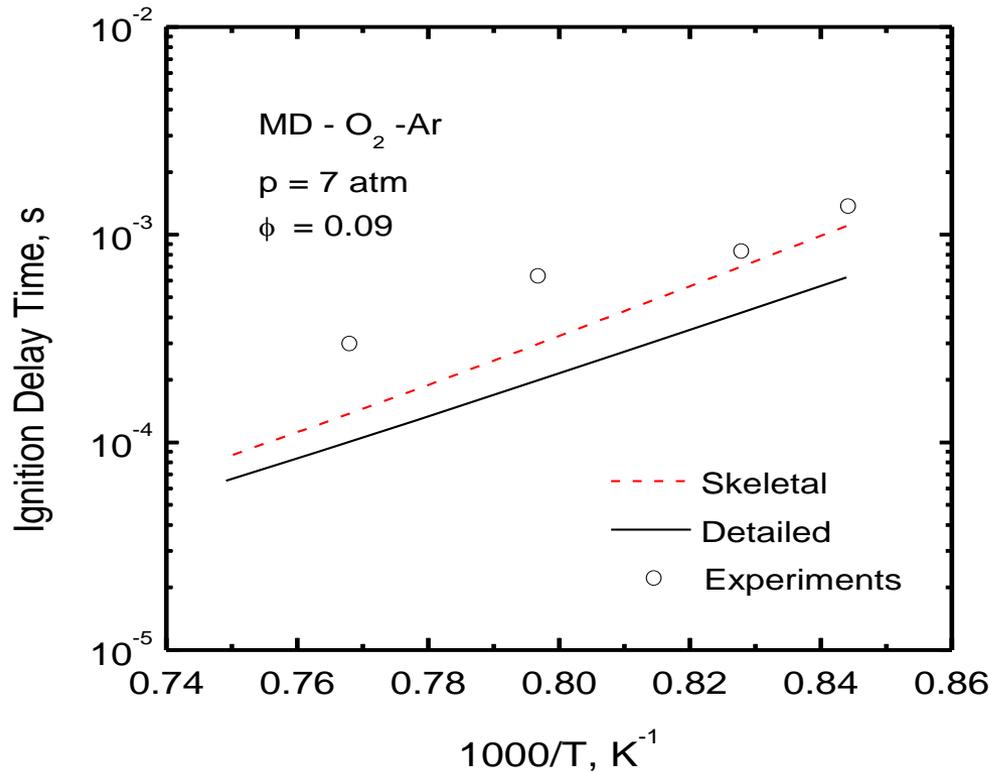
# Mechanism Reduction Methodology



# Validation against Idealized Combustion Systems: Biodiesel

## Shock-Tube

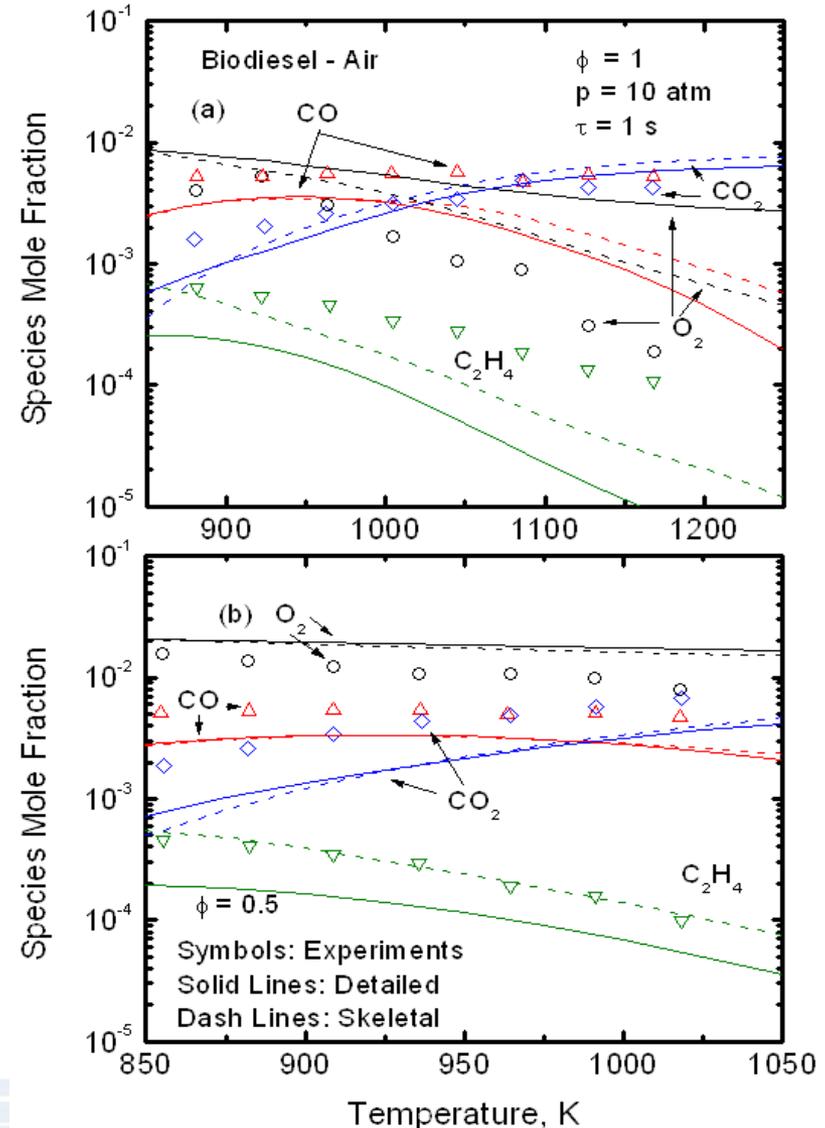
Haylett et al. 2011



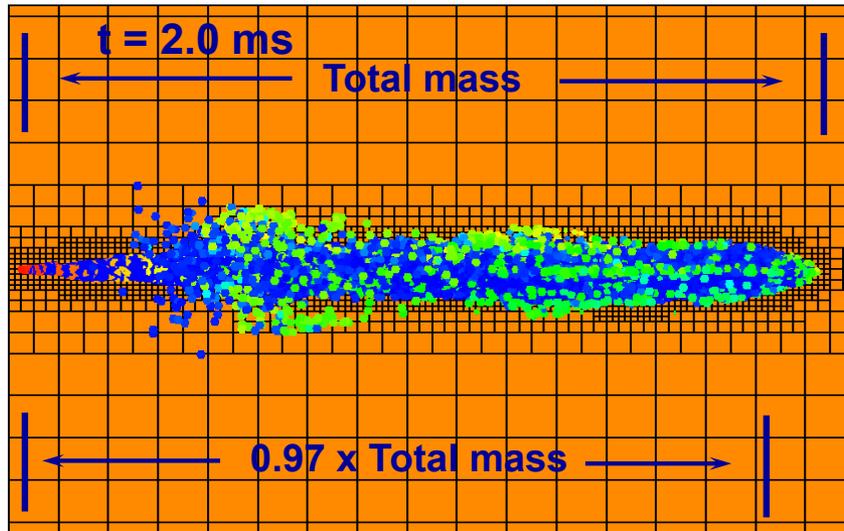
89 species mechanism is able to predict ignition and species characteristics very well!

## Jet-Stirred Reactor (JSR)

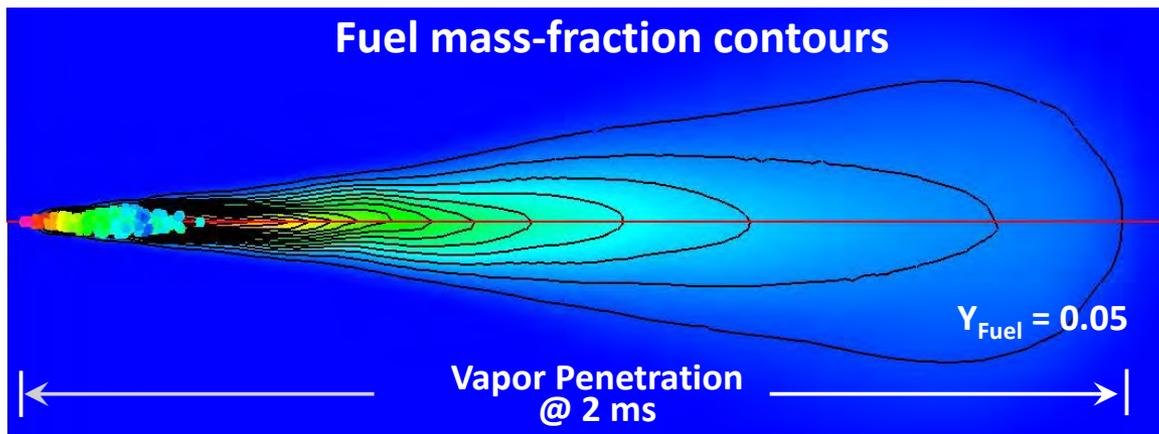
Dagaut et al. PCI 2007



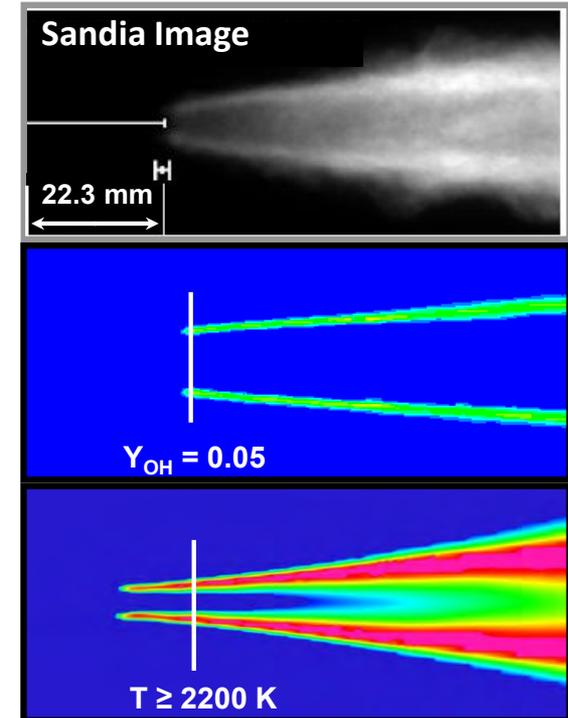
# 3D Simulations: Some Definitions



**Spray penetration @ 2 ms**



## Lift-off length



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

# Biodiesel: Case set-up

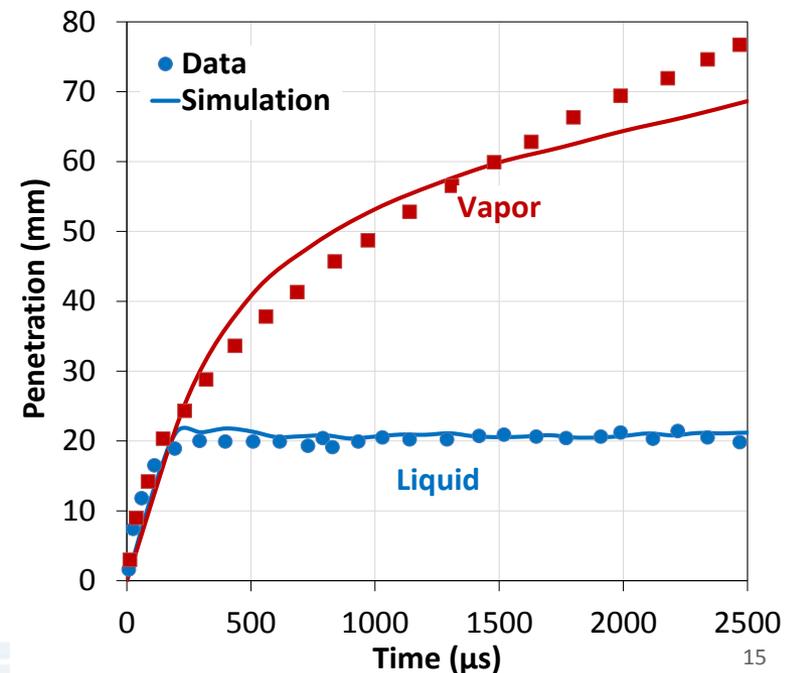
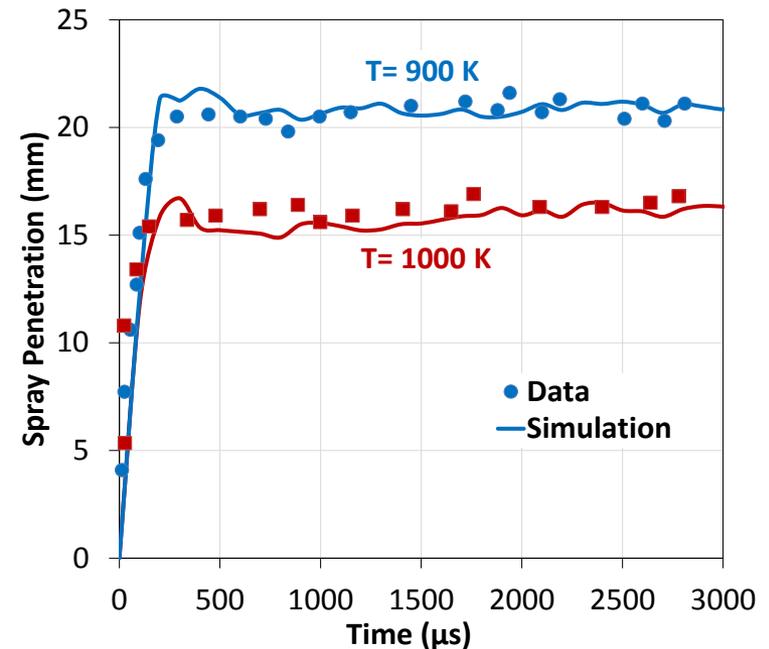
## Injection & Ambient conditions for Biodiesel studies at Sandia\*

Parameter	Quantity
Injection System	Bosch Common Rail
Nozzle Description	Single-hole, mini-sac
Duration of Injection [ms]	7.5
Orifice Diameter [ $\mu\text{m}$ ]	90
Injection Pressure [Bar]	1400
Fill Gas Composition (mole-fraction)	$\text{N}_2=0.7515$ , $\text{O}_2=0.15$ , $\text{CO}_2=0.0622$ , $\text{H}_2\text{O}=0.0363$
Chamber Density [ $\text{kg}/\text{m}^3$ ]	22.8
Chamber Temperature [K]	900, 1000
Fuel Density [ $\text{kg}/\text{m}^3$ ]	877
Fuel Injection Temperature [K]	363

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

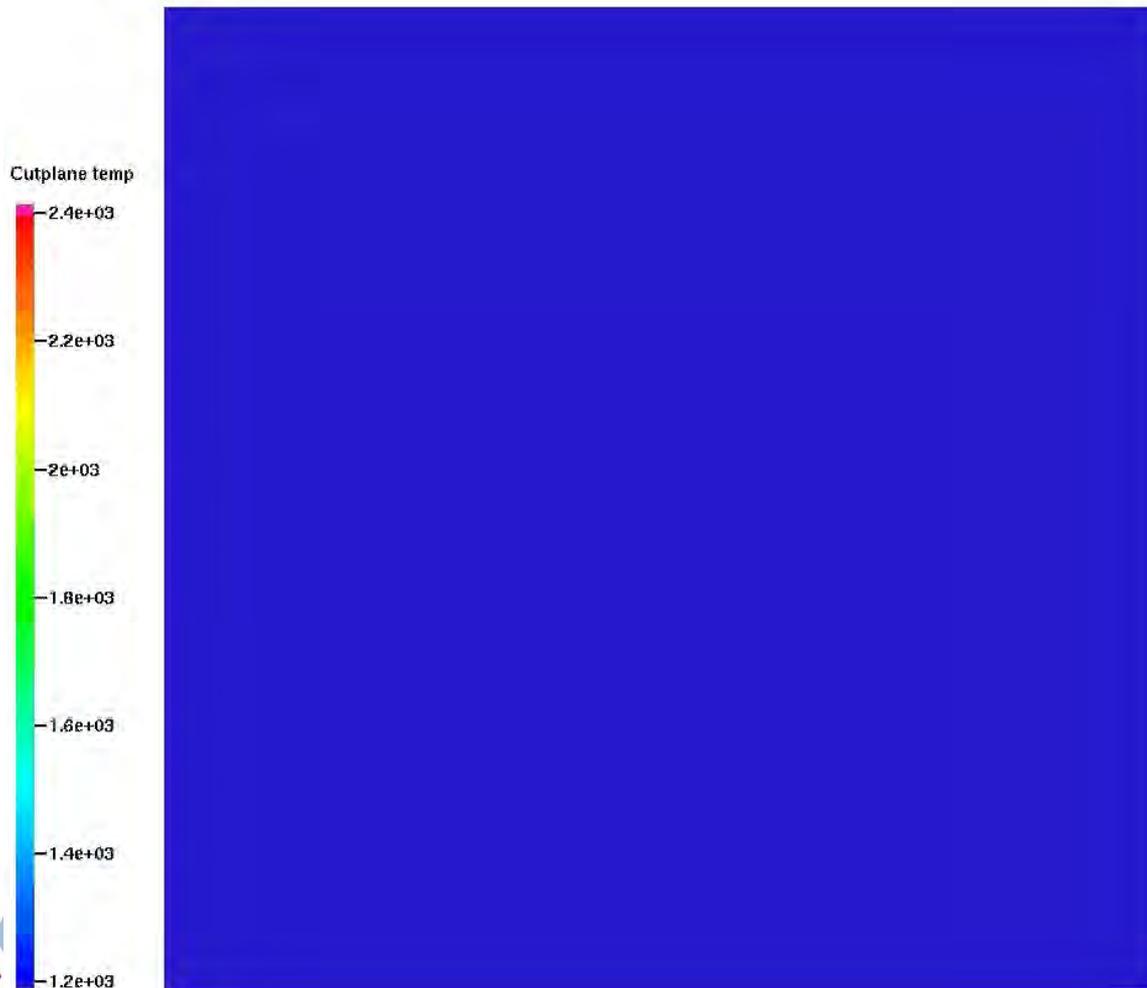
JG Nerva, CL Genzale, JMG Oliver, LM Pickett.  
Fundamental Spray and Combustion Measurements of Biodiesel under Diesel steady conditions. *Under preparation*

**Non-reacting spray characteristics well predicted by the simulations!**



# Spray-Combustion Simulation: Biodiesel

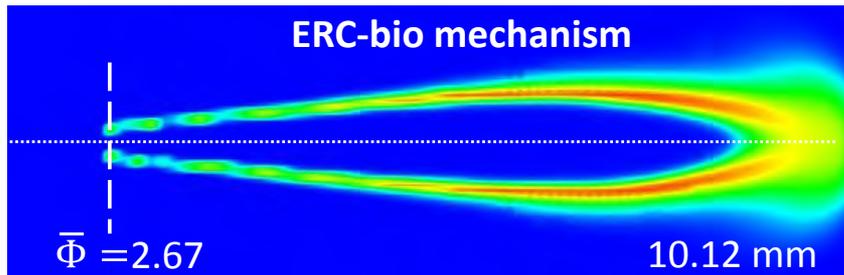
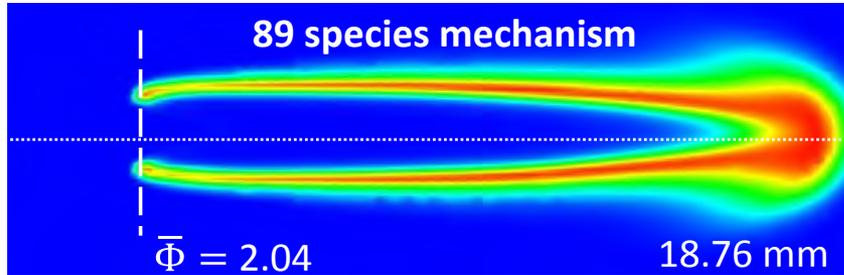
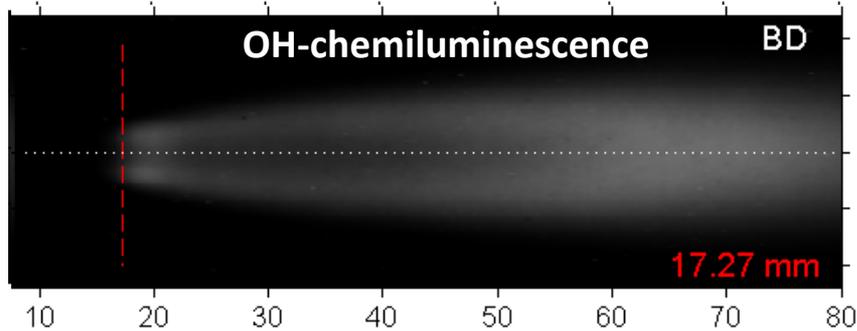
- ✓ 3D simulations: results on a cut-plane are animated
- ✓ Total of 350K-450K grid points for resolving a 108 mm (each side) cube
- ✓ 0.25 mm minimum grid size
- ✓ 85 hours on 8 processors in the Fusion (Argonne) cluster



- ❑ Liquid Length = 15.4 mm
- ❑ Ignition delay = 391  $\mu$ s
- ❑ Lift-off length = 18.76 mm

# Validation of Biodiesel Reaction Mechanisms

**@ T = 1000 K**



**CSE is further assessing the ERC-bio mechanism!**

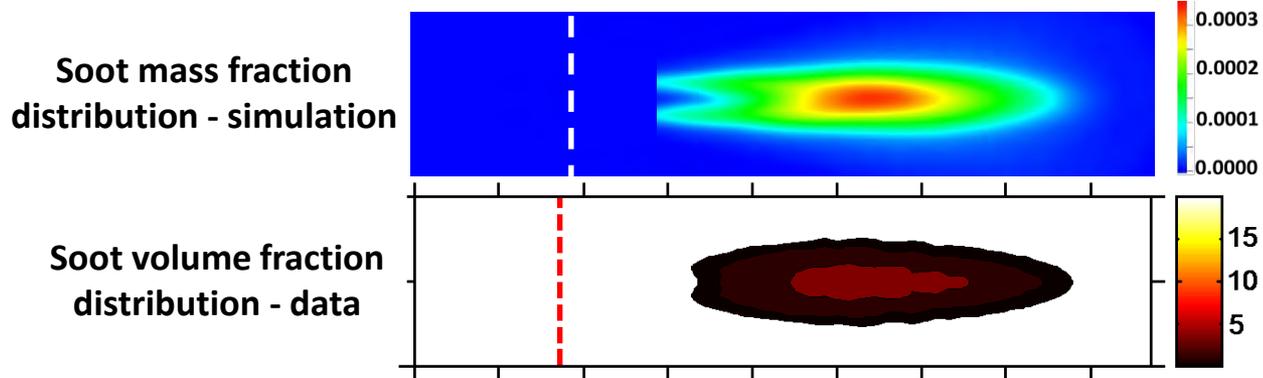
- ❑ Data from Sandia National Laboratory
- ❑ Simulations plot OH contours at a cut-plane
- ❑ ERC-bio mechanism: (Methyl Butanoate + NHPT) 41 species and 150 reactions. SAE Paper No. 2008-01-1378
- ❑ ERC-bio mechanism (using MB as a surrogate) under predicts lift-off length and ignition delay and consequently over-predicts equivalence ratio
- ❑ 89 species mechanism (using MD as a surrogate) captures ignition delay, flame lift-off length, and equivalence ratio very well

@ T = 1000 K	Ignition Delay ( $\mu\text{s}$ )
Sandia Data	396
89 species	391
ERC-Bio mechanism	220

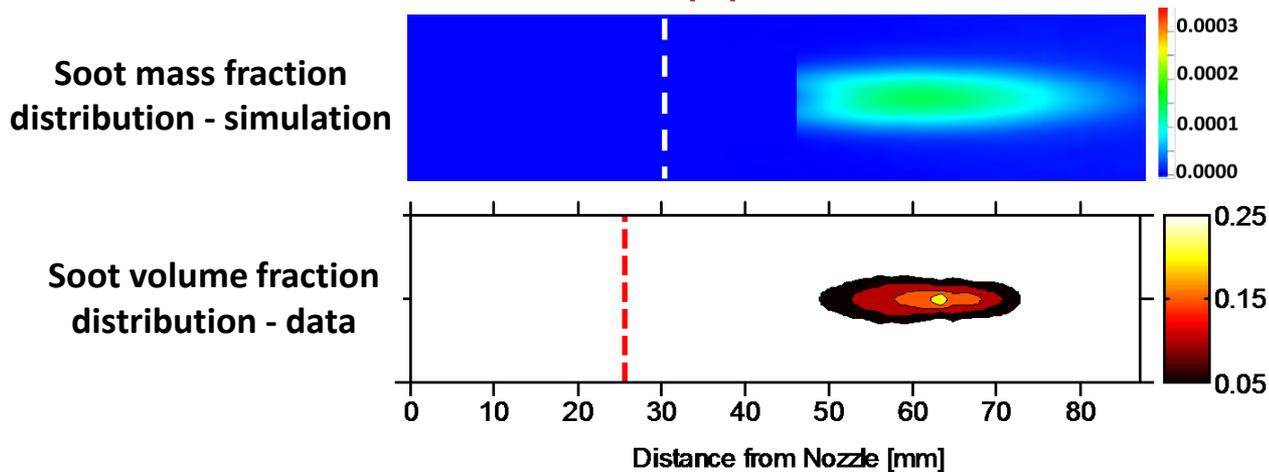
# Prediction of Soot Distribution

89 species mechanism

(a)  $T = 1000\text{ K}$



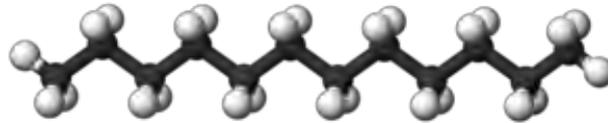
(b)  $T = 900\text{ K}$



$\text{C}_2\text{H}_2$  is used as a soot pre-cursor!

# Development of Reduced Reaction Mechanisms

Diesel surrogate:  
n-dodecane ( $nC_{12}H_{26}$ )



**n-Dodecane Mechanism (from LLNL)**

2115 species, 8157 reactions



**103 species, 370 reactions\***

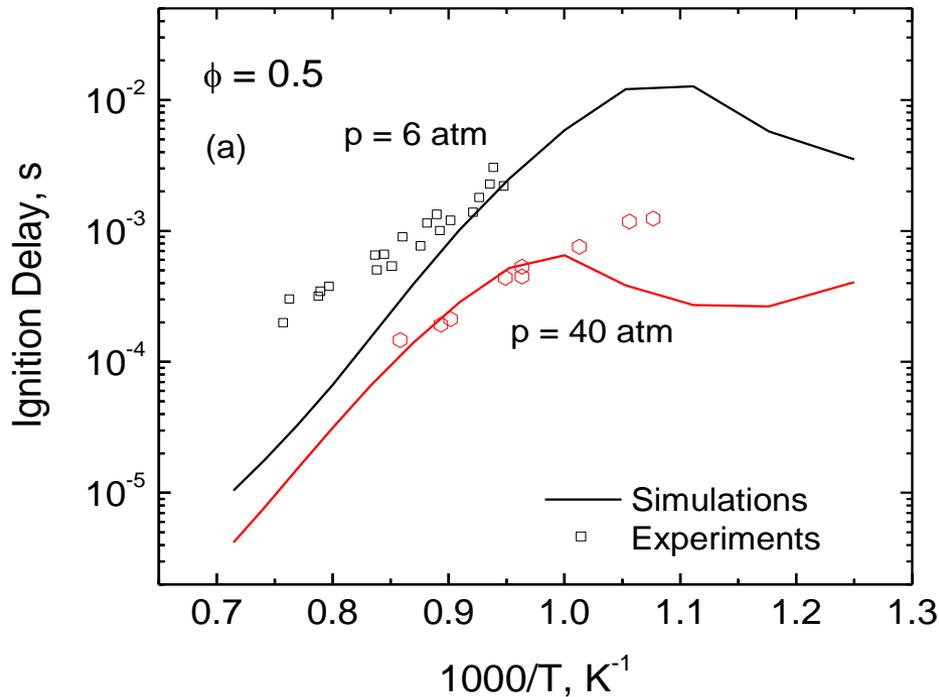
\* S. Som, D.E. Longman, Z. Luo, M. Plomer, T. Lu. *Eastern States Section of the Combustion Institute meeting, October 2011*



# Validation against Shock Tube data

103 species, 370 reactions: n-dodecane reduced mechanism

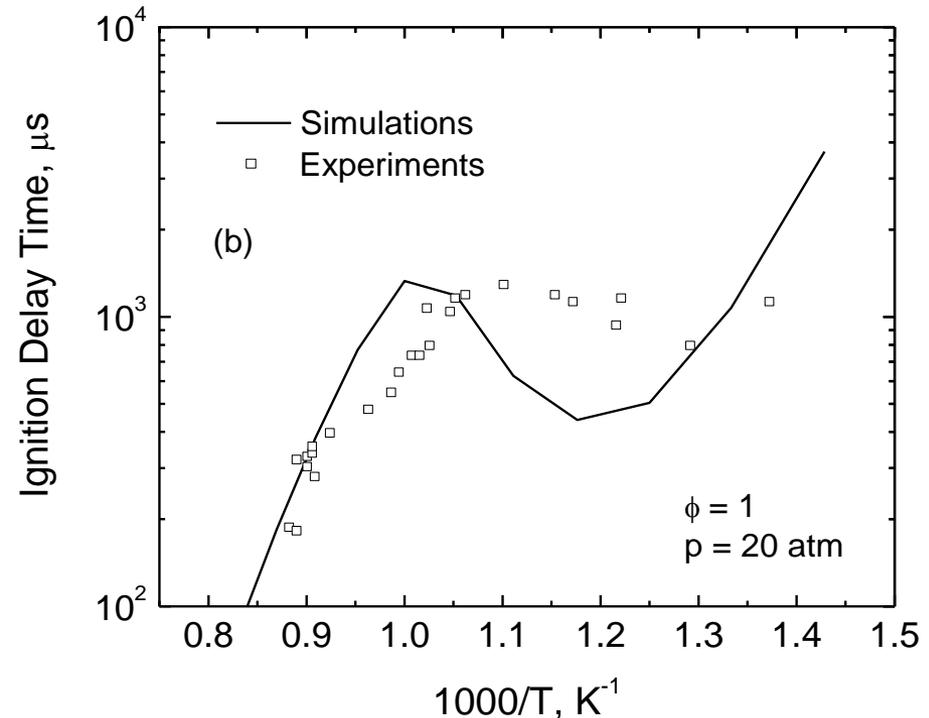
n-dodecane/O<sub>2</sub>+Ar



Black symbols: experimental data from:  
Davidson et al. Combustion and Flame 2008

Red symbols: experimental data from:  
Shen et al. Energy and Fuels 2009

n-dodecane/air

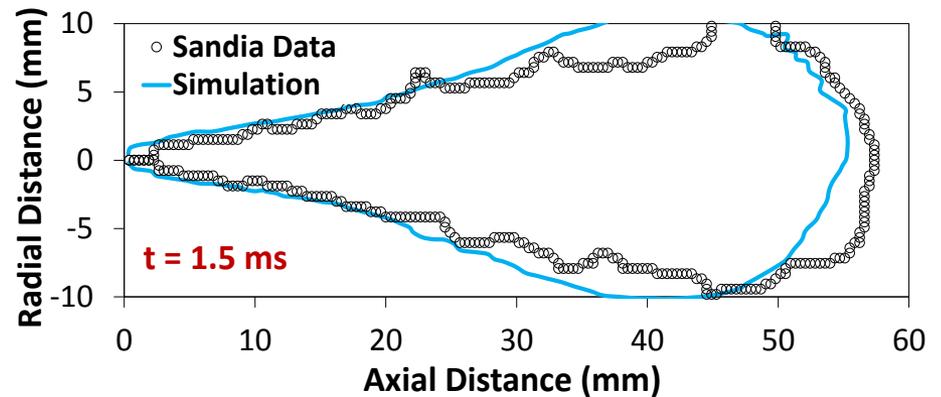
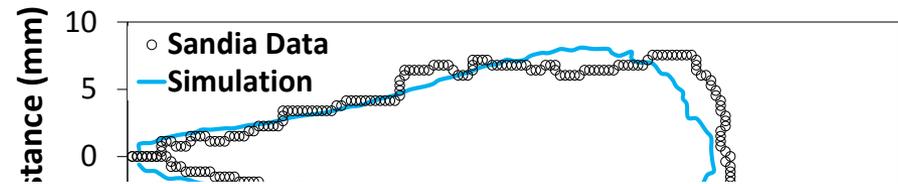
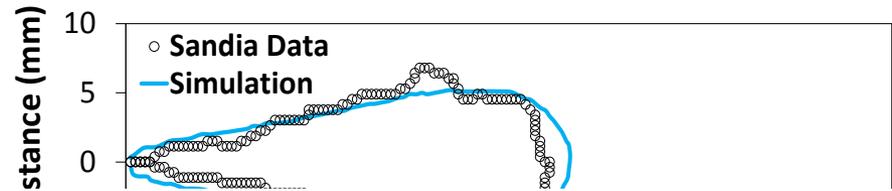
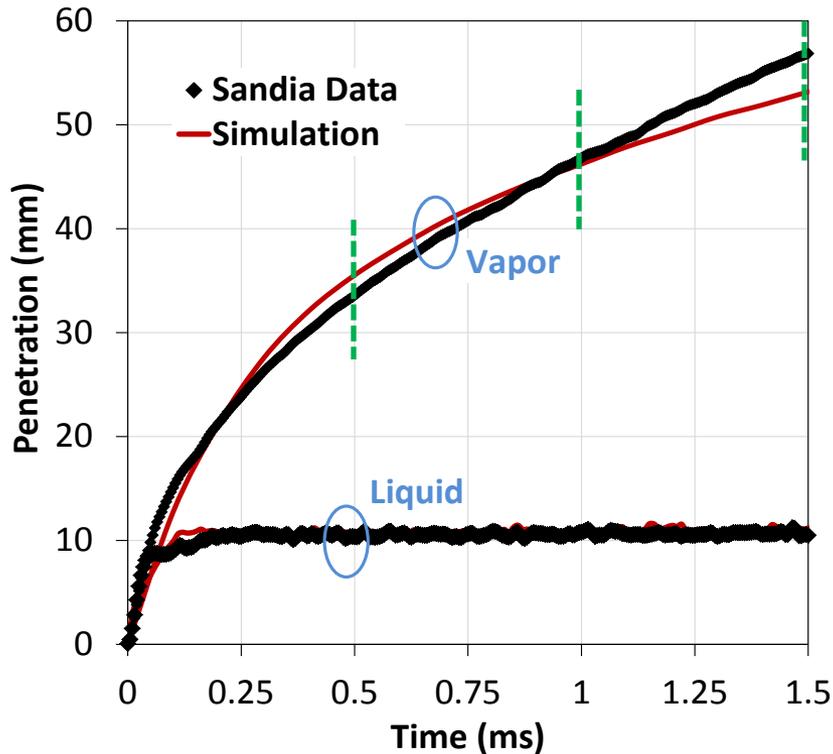


Experimental data from: Vasu et al. Proc. of  
Combustion Institute 2009

# 3D Spray (non-combustion)

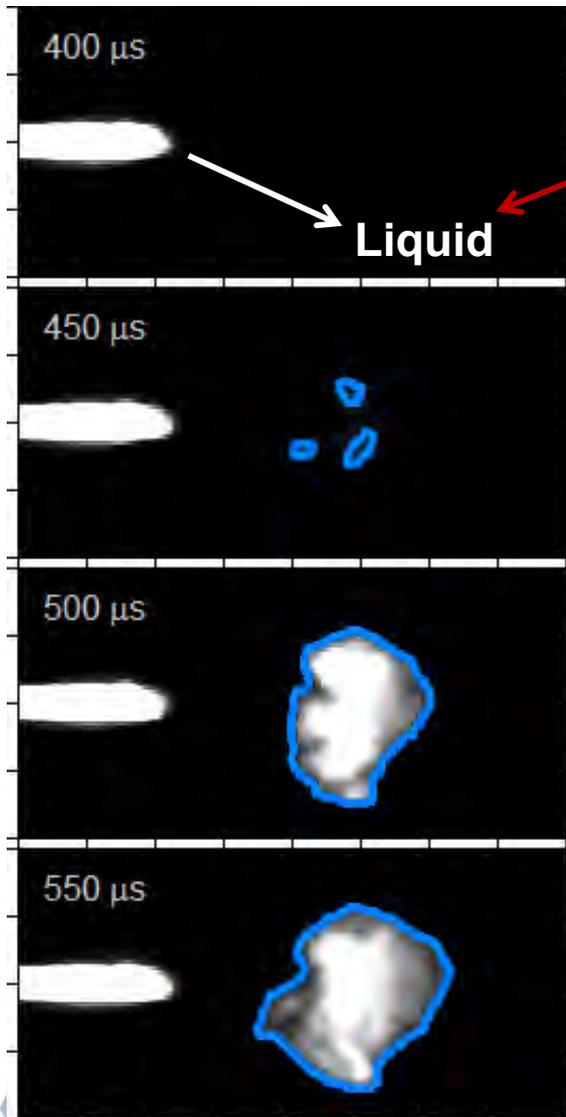
Data from Sandia National Laboratory:  
<http://www.sandia.gov/ecn/>

Simulation are able to capture the spray characteristics very well!

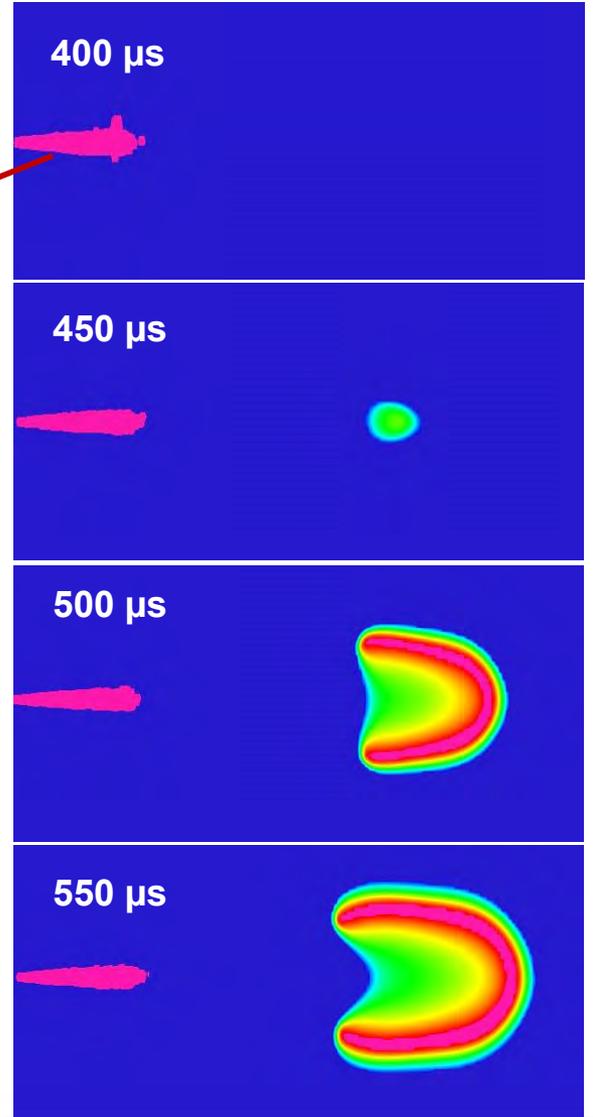


# Liquid Length and Ignition Location

## Sandia Data



## Simulation



## Experiments:

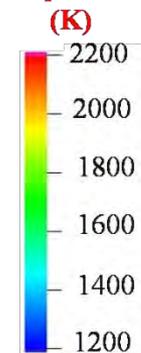
Natural Luminosity high-speed imaging for detection of ignition delay

<http://www.sandia.gov/ecn/>

## Simulation:

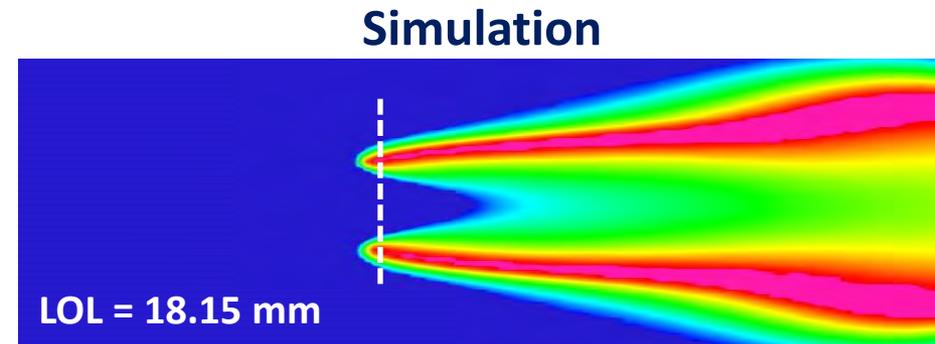
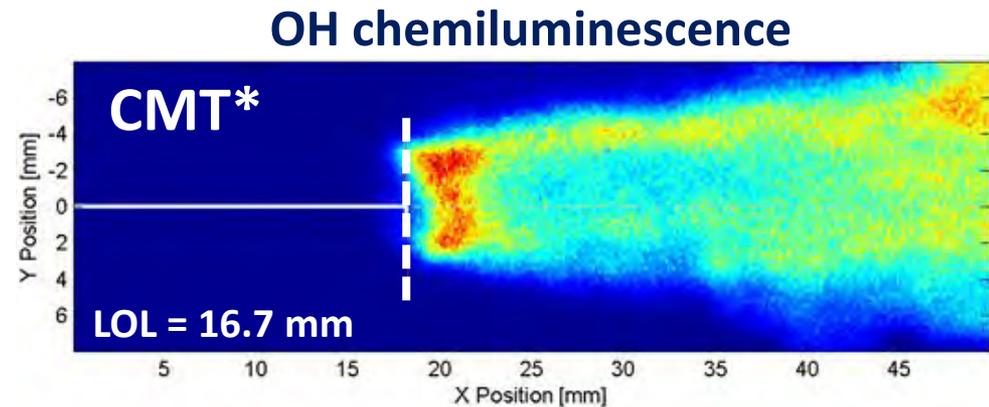
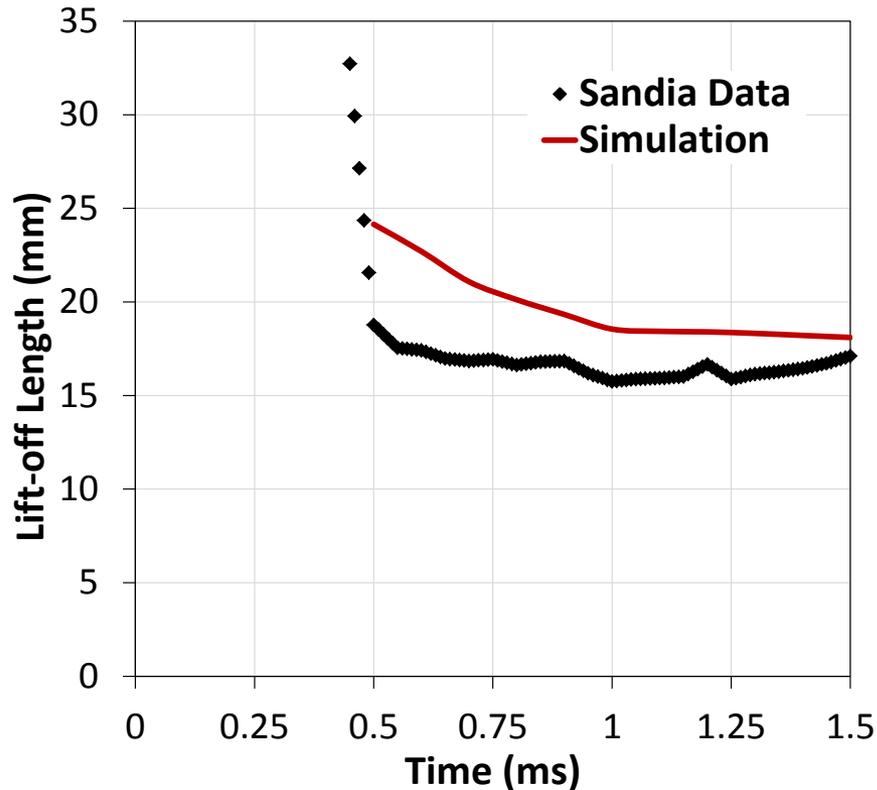
Temperature contours plotted to capture ignition location and delay

## Temperature (K)



# Ignition Delay and Flame lift-off Length

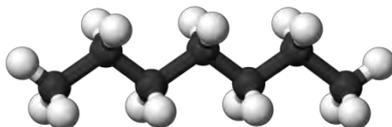
	Ignition Delay (ms)	Lift-off Length (mm)
Sandia Data	0.440	16.50
Simulation	0.425	18.15



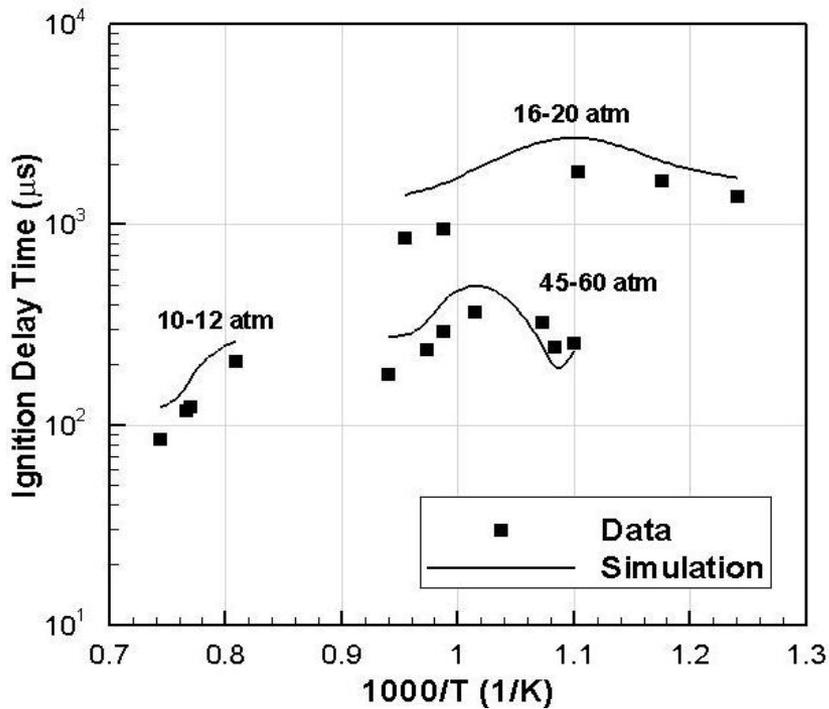
\*<http://www.cmt.upv.es/ECN07.aspx>

# Bringing it all together!

Diesel surrogates:  
n-heptane ( $nC_7H_{16}$ )



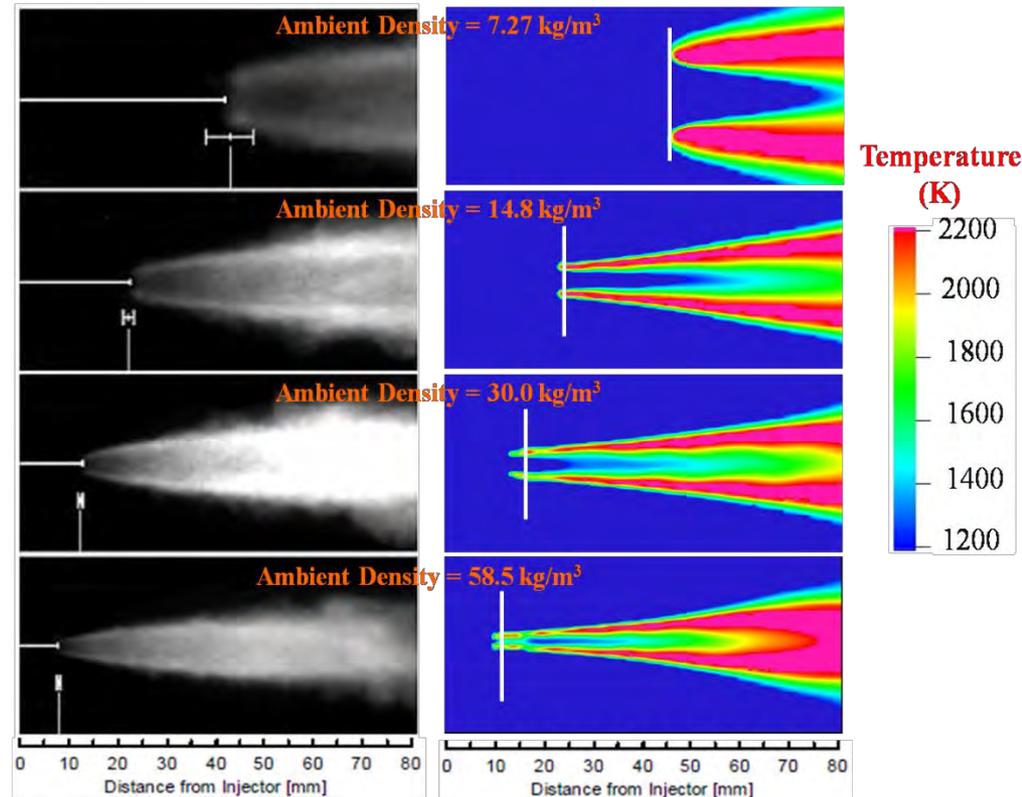
# n-Heptane Mechanism Validation



- Shock-tube data from Gauthier et al. Comb and Flame 2004
- n-heptane: 68 species, 168 reactions (Lu et al.): Comb. and Flame 2009
- Accurately captures NTC characteristics

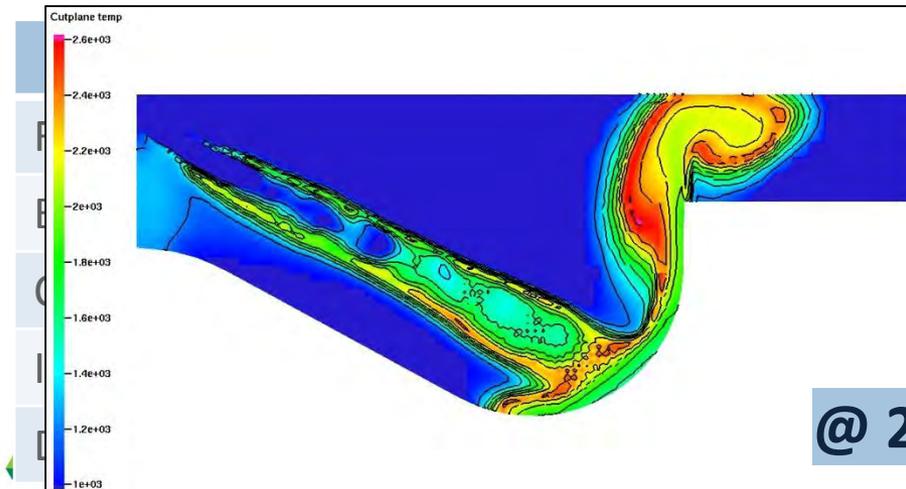
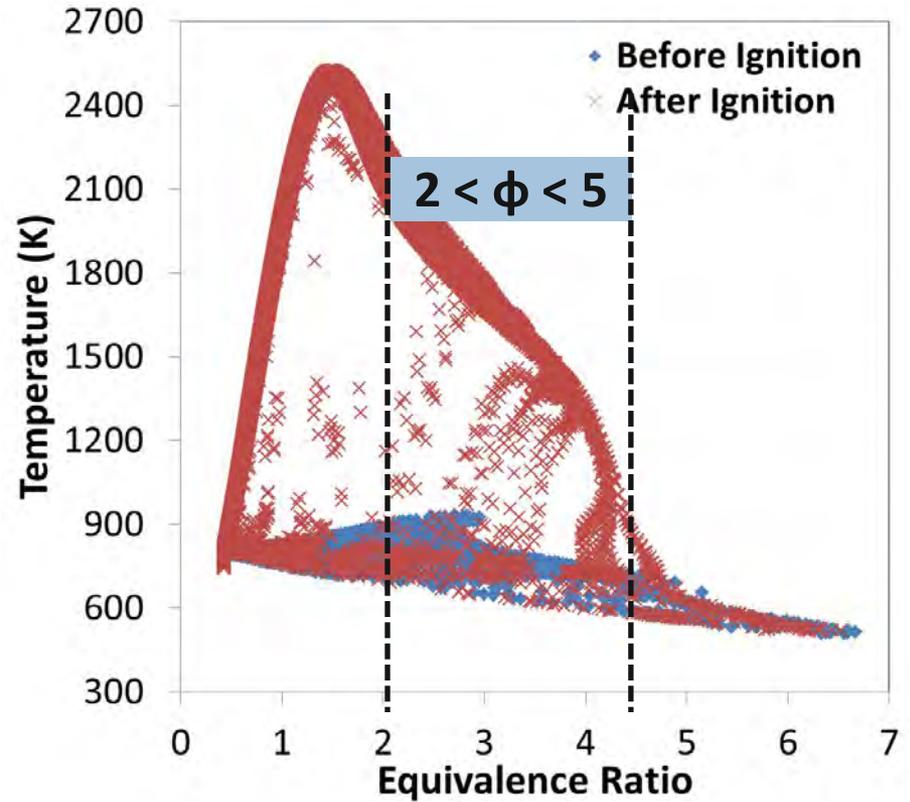
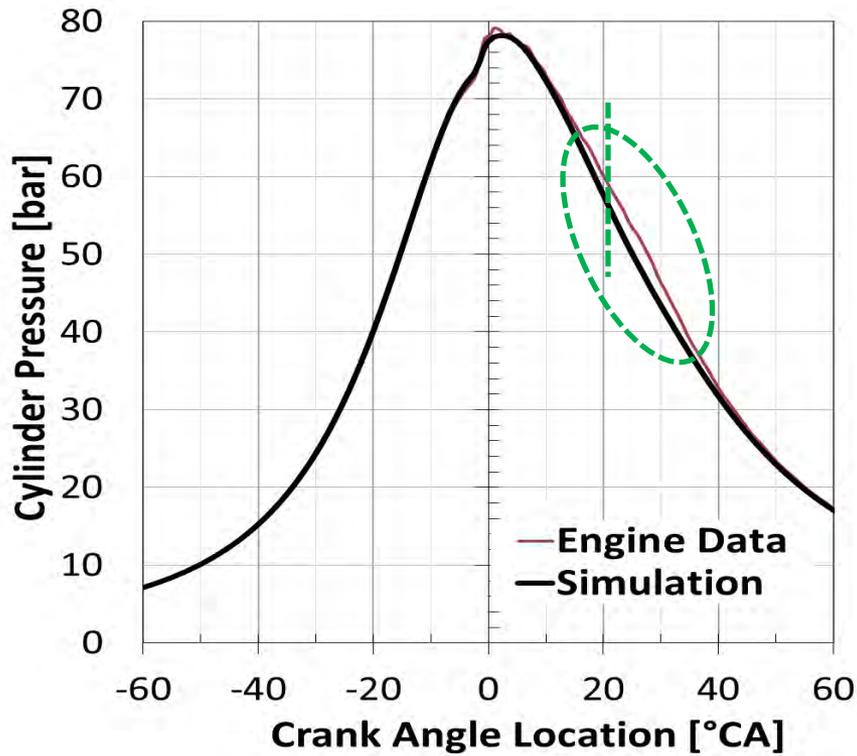
Data

Simulations

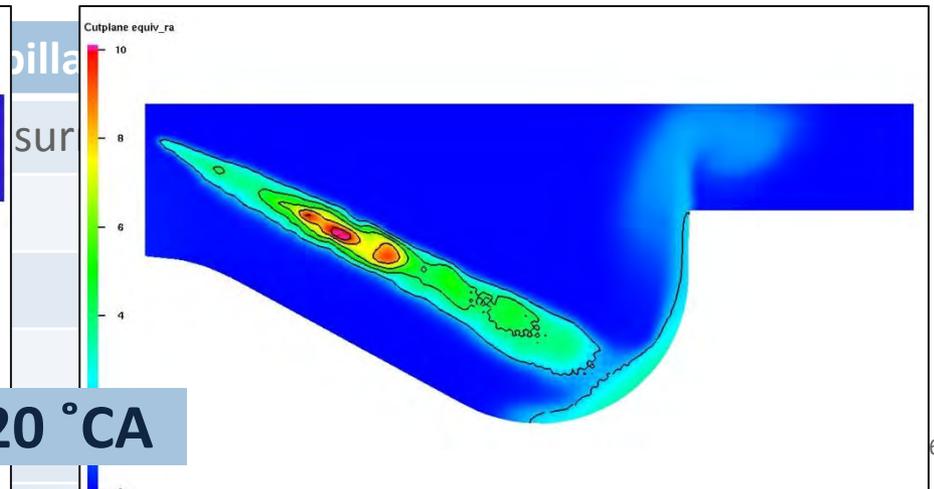


- Data from Sandia National Laboratory <http://www.sandia.gov/ecn/>
- Lift-off trends well predicted
- About 15% under-prediction at low ambient densities

# Engine Simulation



@ 20 °CA



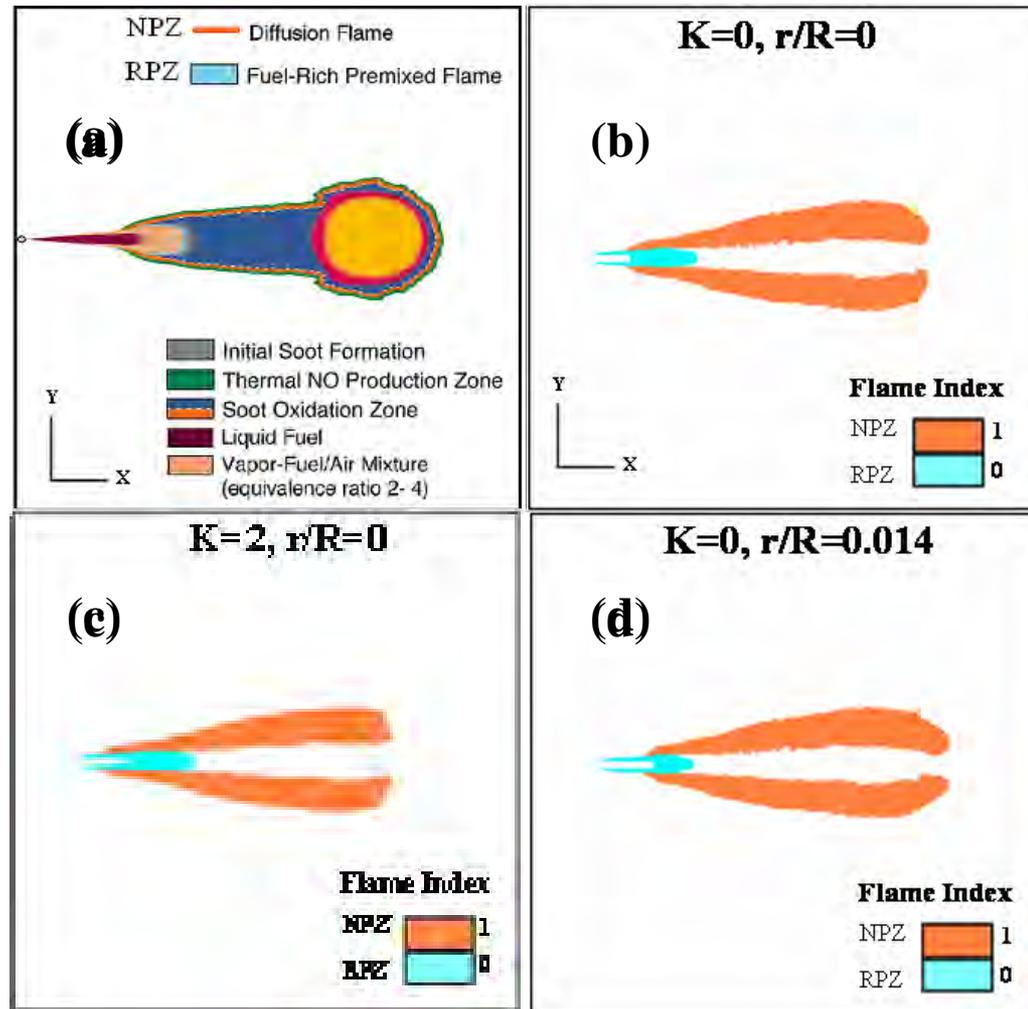
# Flame Index for Diesel Engine Applications

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

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

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

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



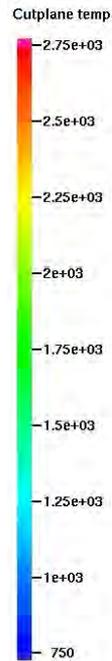
$K=0, r/R=0$ : Cylindrical Nozzle

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

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

# Summary

- ❑ Systematic mechanism reduction performed (starting from detailed mechanism from LLNL) for operation under compression ignition engine conditions
  - ✓ MD+MD9D+NHPT: Used as a biodiesel surrogate
  - ✓ n-dodecane and n-heptane: Used as diesel surrogates
- ❑ The reaction rates of these reduced mechanism are not tuned to match any specific data-set
- ❑ Robust validation performed against idealized combustion system data:
  - ✓ 0-D systems: Shock tube, Jet stirred reactor
  - ✓ 1-D system: Premix flame speed, counter flow diffusion flames
  - ✓ 3-D spray combustion system
- ❑ The reduced mechanism matched the experimental data very well under all the condition investigated
- ❑ Larger mechanisms and molecules were observed to predict ignition and combustion characteristics better compared to the smaller counterparts
- ❑ Engine simulations were performed using the systematically reduced reaction mechanisms. These mechanisms were able to capture 3-D ignition and combustion characteristics very well



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**Thank You!!**

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[http://www.transportation.anl.gov/engines/multi\\_dim\\_model\\_home.html](http://www.transportation.anl.gov/engines/multi_dim_model_home.html)



# Computational Cost & Scalability

	Computational Time (for one node)
ERC-bio mechanism	~ 19 hours
Lu et al. NHPT	~ 42 hours
89 species mechanism	~ 85 hours

Scalability per node =  $T_1/T_n$

Efficiency per node =  $T_1 \times 100 / nT_n$

$n$  = 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

