

Validation of Reduced Chemical Kinetic Mechanisms for Engine Simulations

Sibendu Som

Argonne National Laboratory

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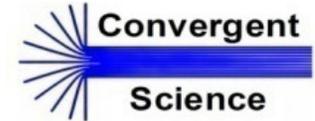
Presentation at: Workshop on Techniques for High-Pressure Combustion

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**



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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

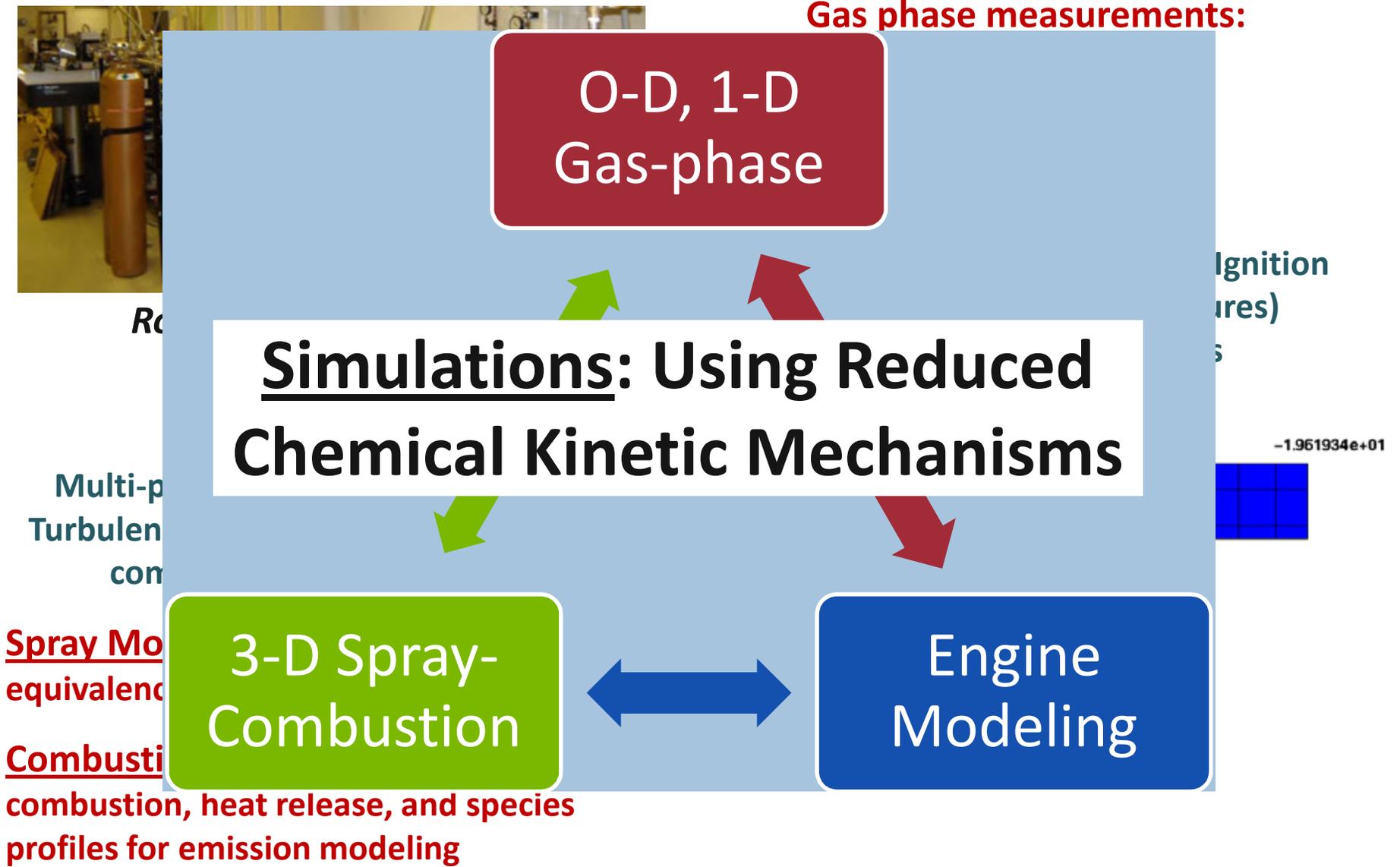
□ Robust validation against 3-D spray-combustion data

□ Bringing it all together: Engine simulations

□ Summary & Future Work

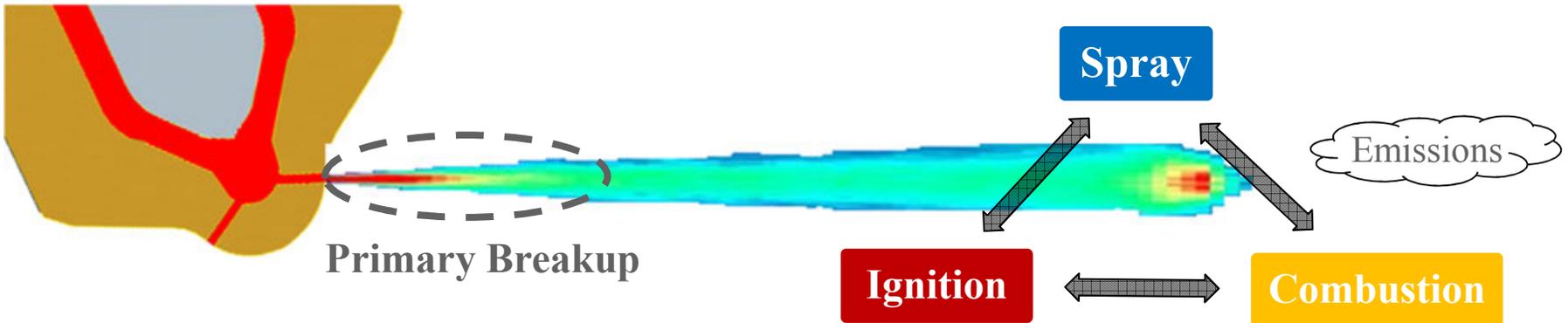


From Shock Tubes to Engines

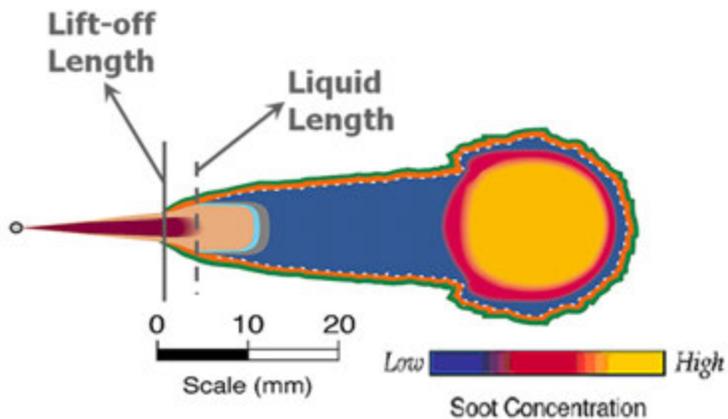


3-D Integrated Modeling Approach

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:

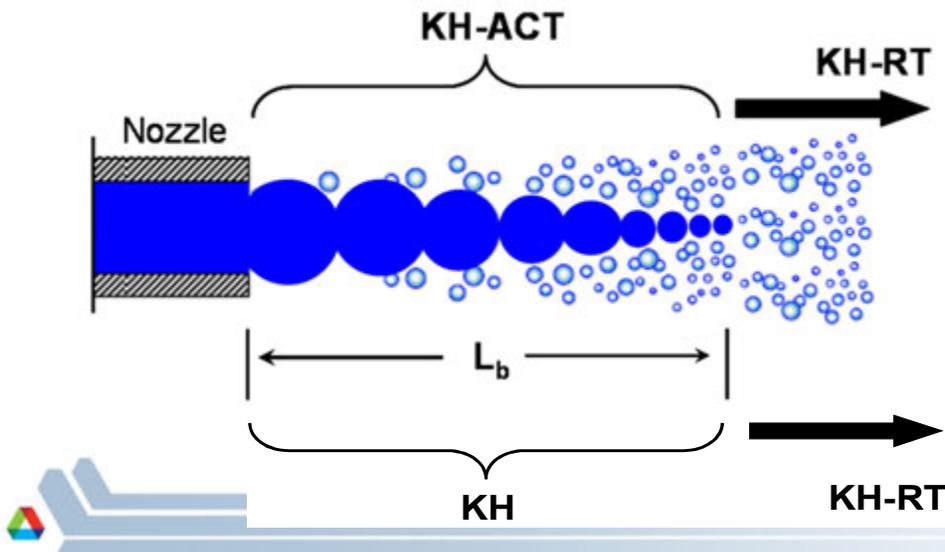
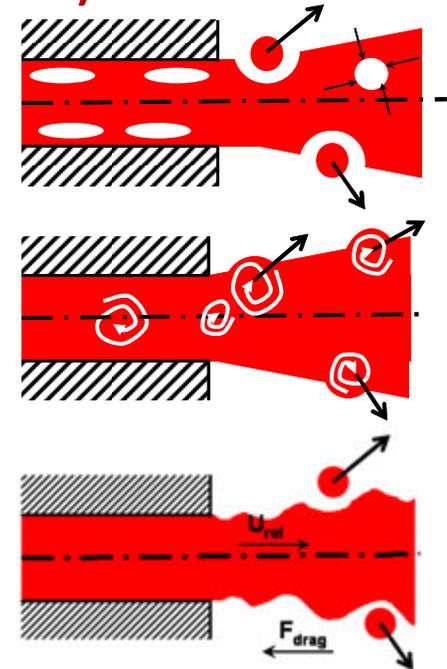
Constant-volume vessel (Sandia National Laboratory)

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- 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

Accurately predict fuel distribution)
 (equivalence ratio)!!)

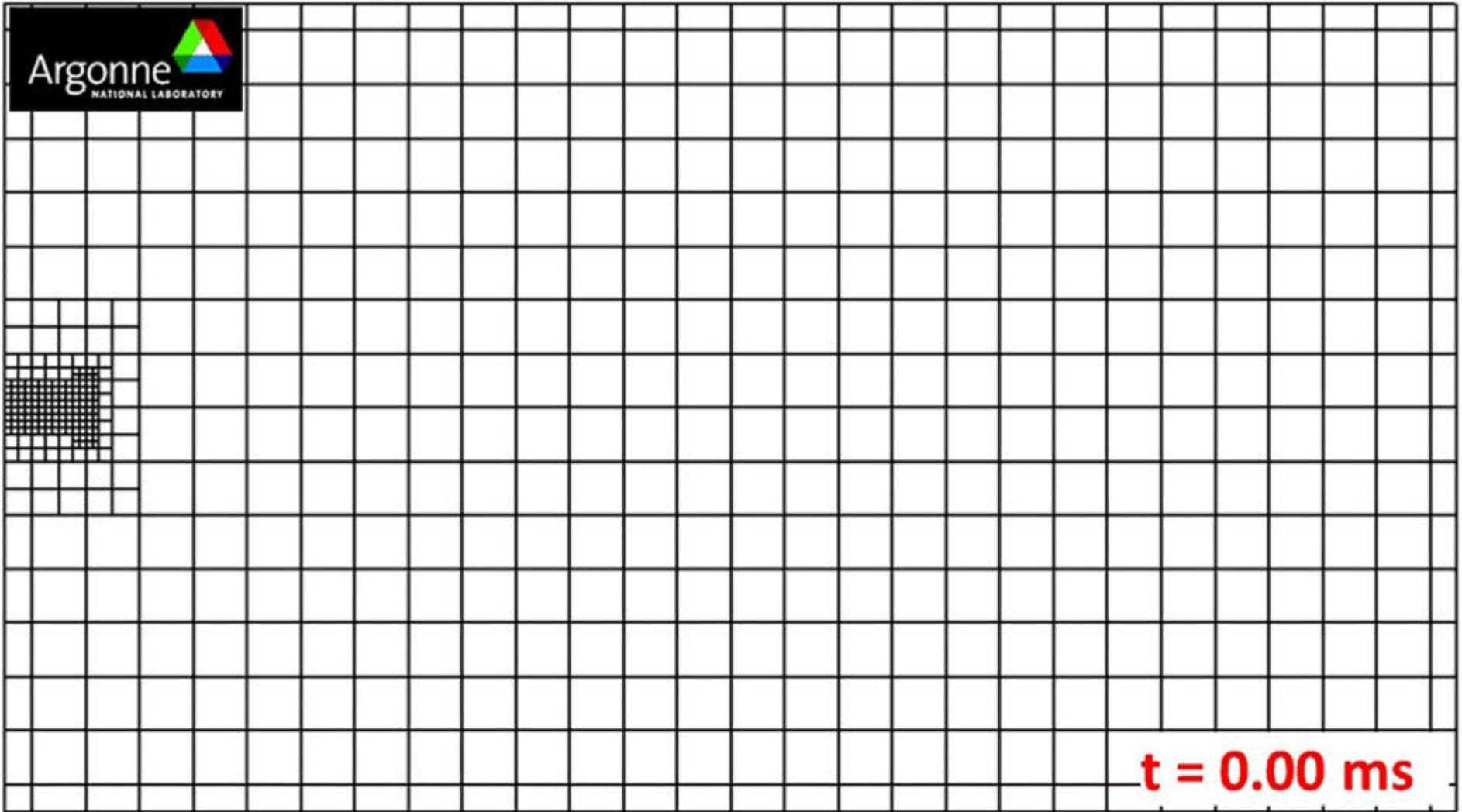
3-D Modeling Set-up

Modeling Tool	CONVERGE Source code access for spray and combustion modeling
Dimensionality and type of grid	3D, structured with Adaptive Mesh Resolution
Spatial discretization approach	2 nd order finite volume
Smallest and largest characteristic grid size(s)	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
Total grid number	350K-450K for 0.25mm – RANS simulations 1.5-1.7 million for 0.125mm – LES case
Parallelizability	Good scalability up to 48 processors

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



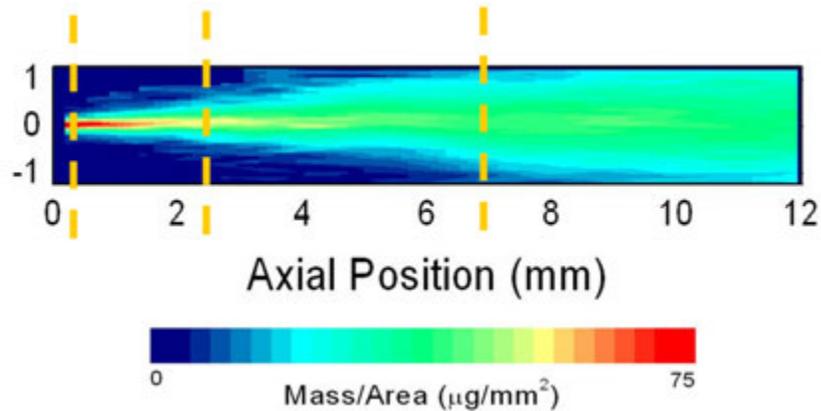
Adaptive Mesh Generation



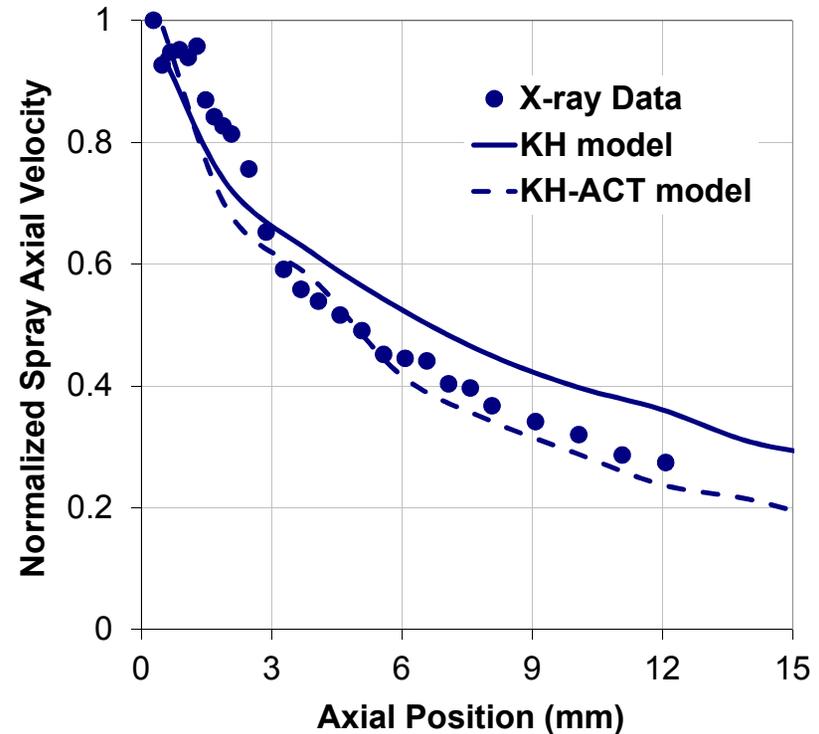
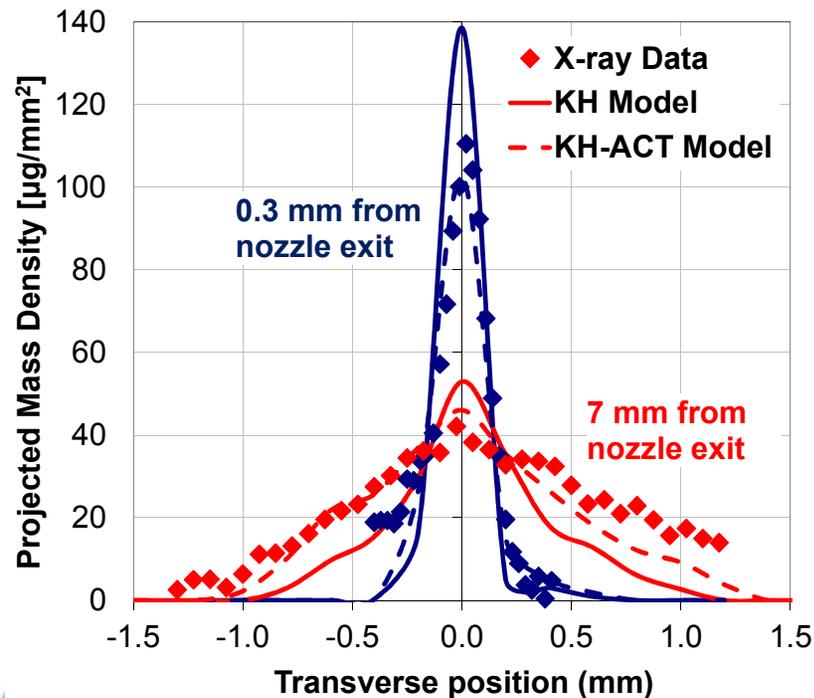
Base Grid Size = 2 mm, Minimum Grid Size = 0.25 mm)



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)**

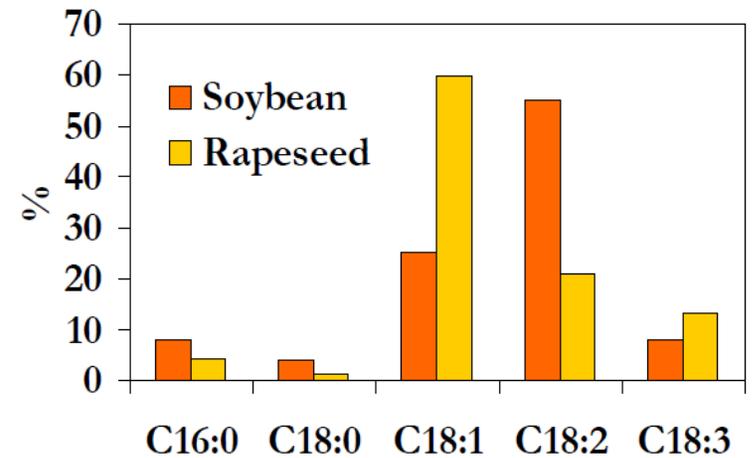
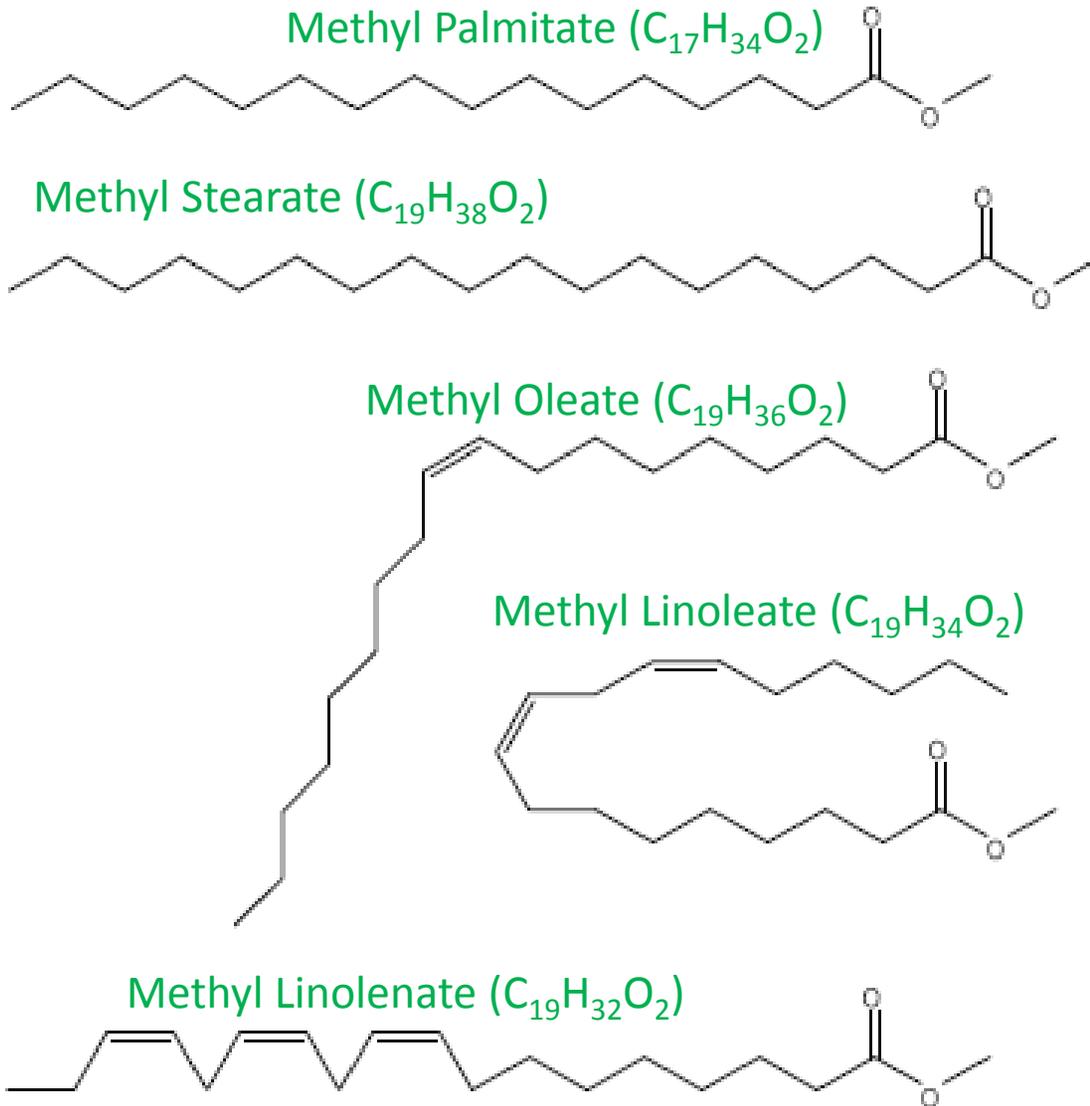
Methyl Decanoate (MD)

Methyl 9 Decenoate (MD9D)

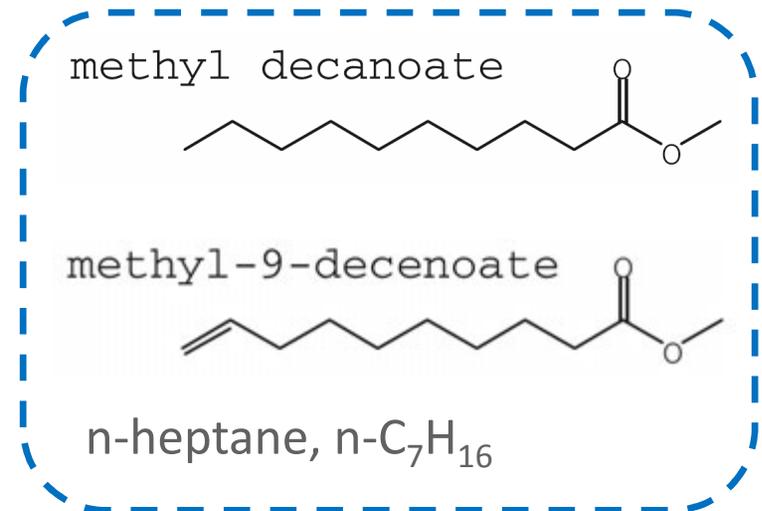
n-Heptane (NHPT)



Composition of Biodiesels



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



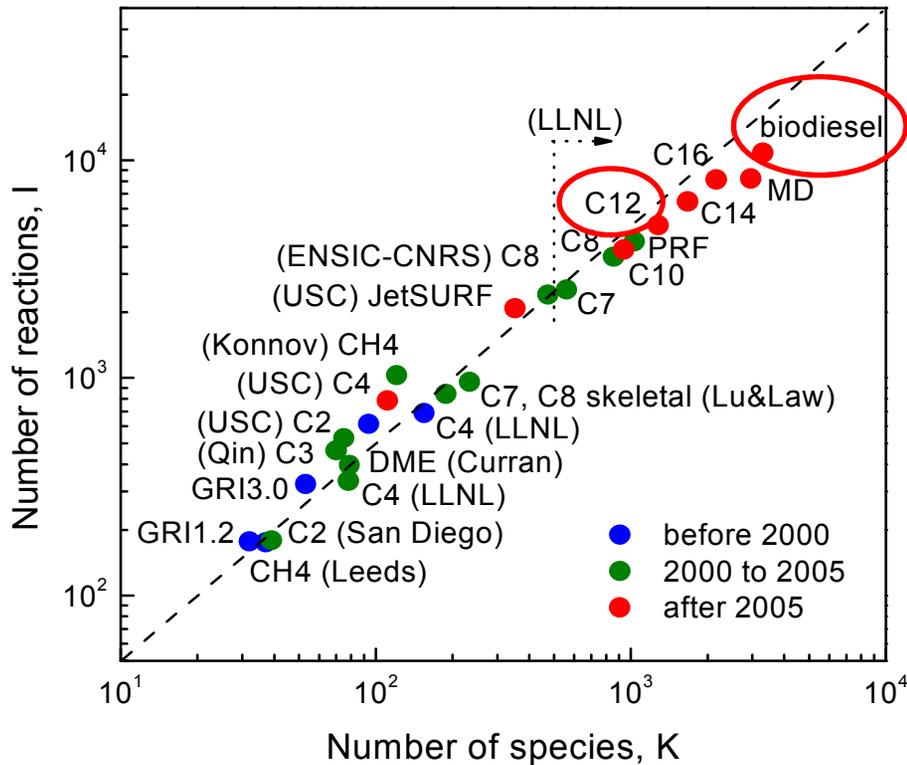
Detailed Mechanisms in Engine Simulations*

Large mechanism sizes

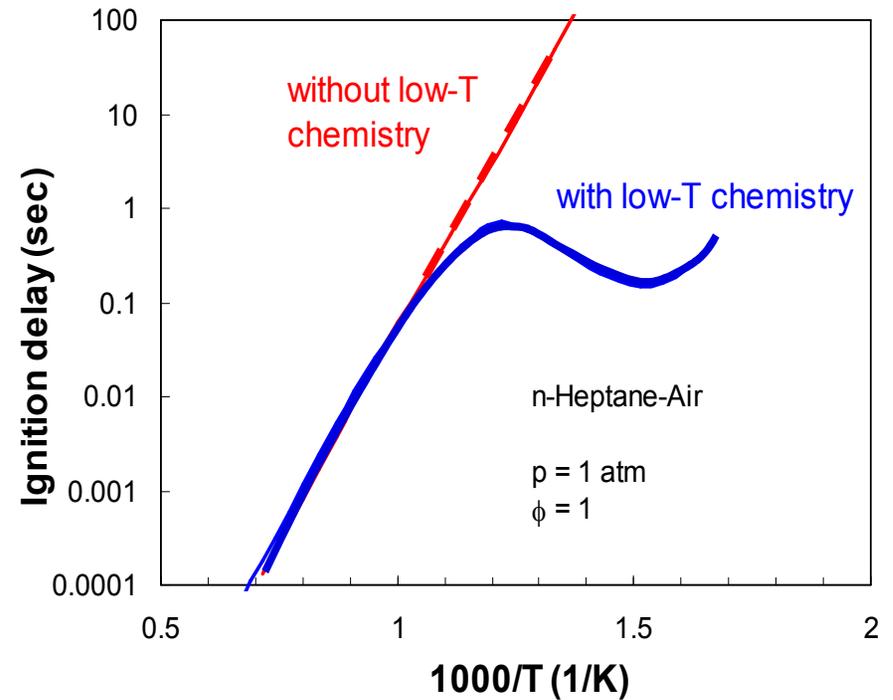
3329 species; 10,806 reactions (Biodiesel)

2115 species; 8157 reactions (C12)

From Lawrence Livermore (LLNL)



Detailed chemistry is important

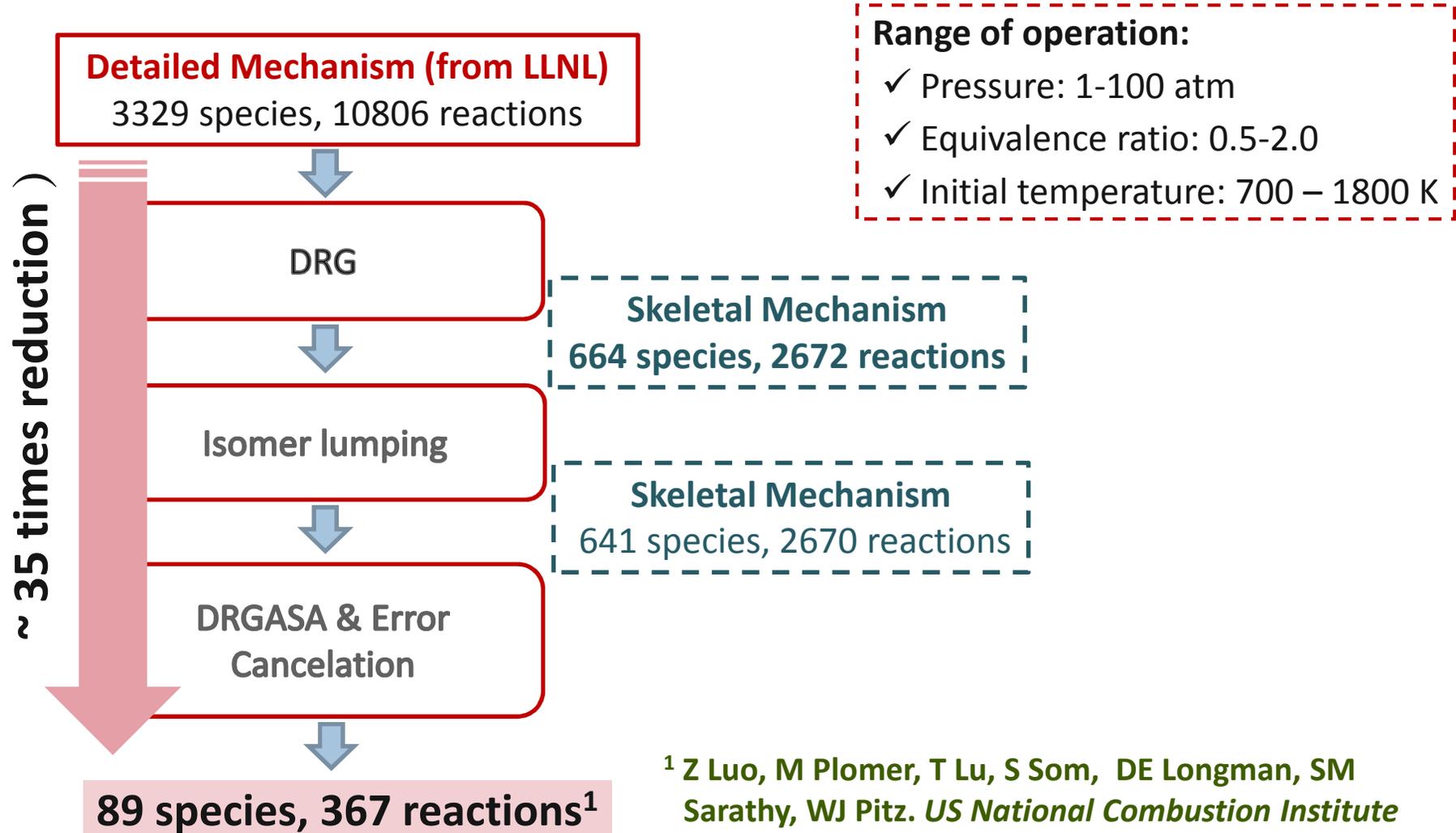


Mechanism reduction needed for CFD simulations with large mechanisms

* Lu and Law, 2009

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

Mechanism Reduction Methodology



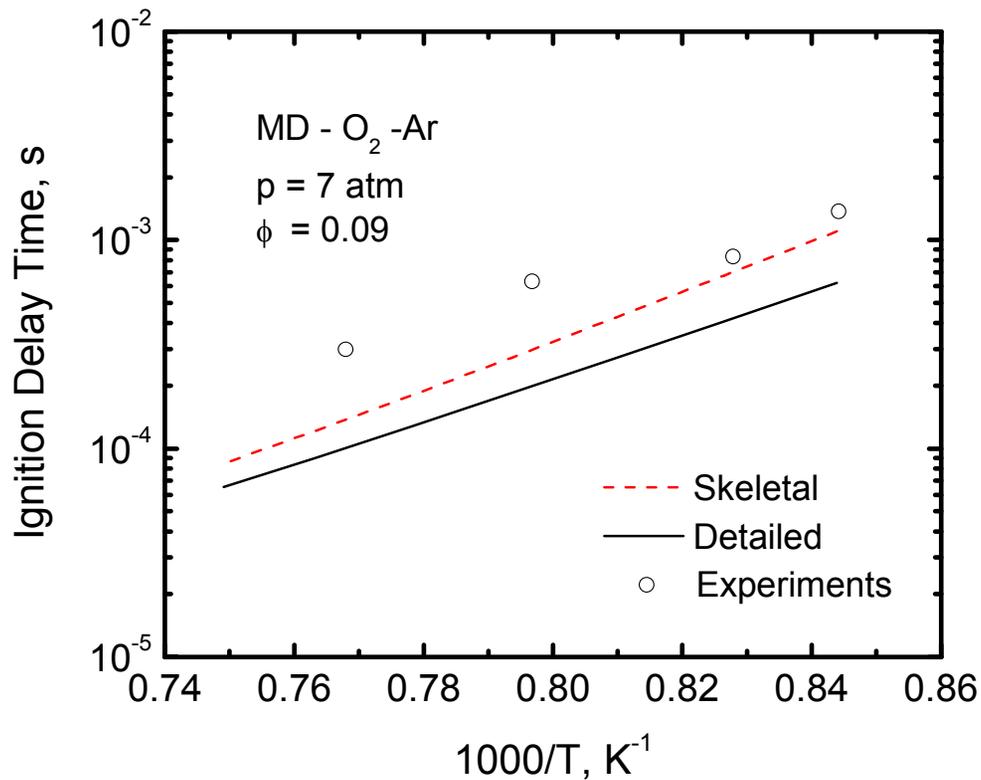
¹ Z Luo, M Plomer, T Lu, S Som, DE Longman, SM Sarathy, WJ Pitz. *US National Combustion Institute meeting, March 2011*



Validation against Idealized Combustion Systems: Biodiesel

Shock-Tube)

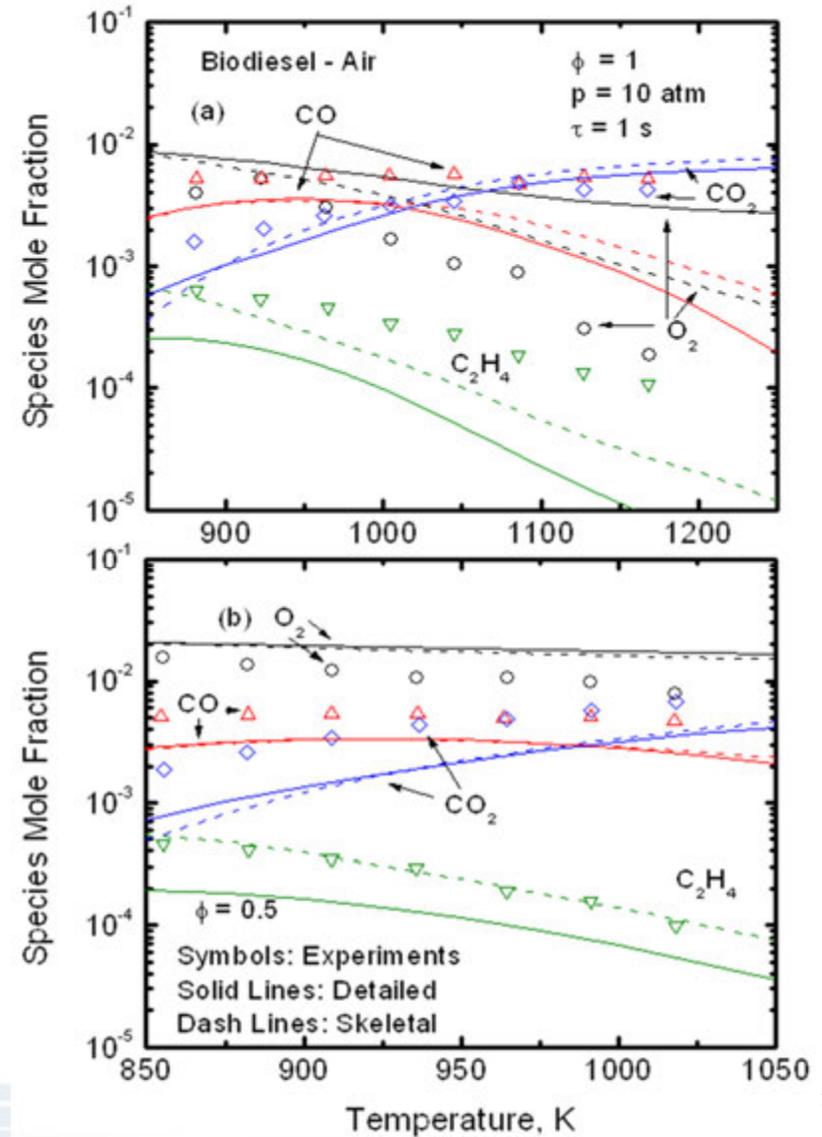
Haylett et al. 2011)



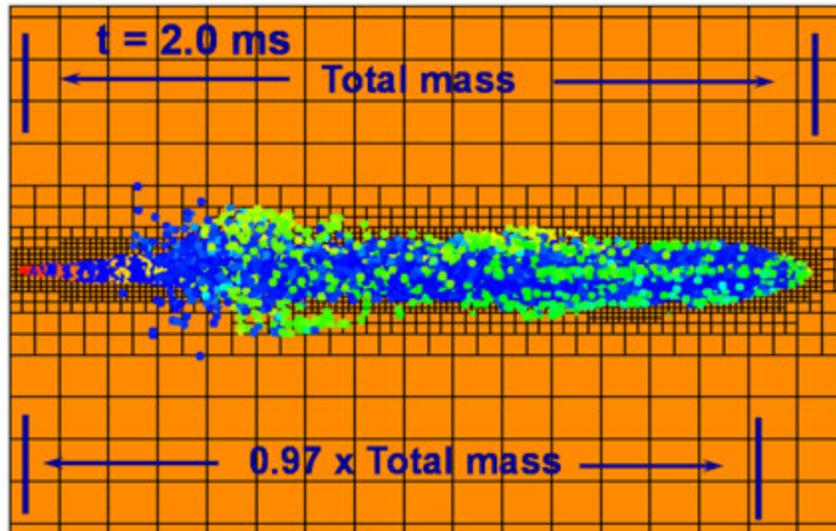
89 species mechanism is able to predict ignition and species characteristics very well!

Jet-Stirred Reactor (JSR)

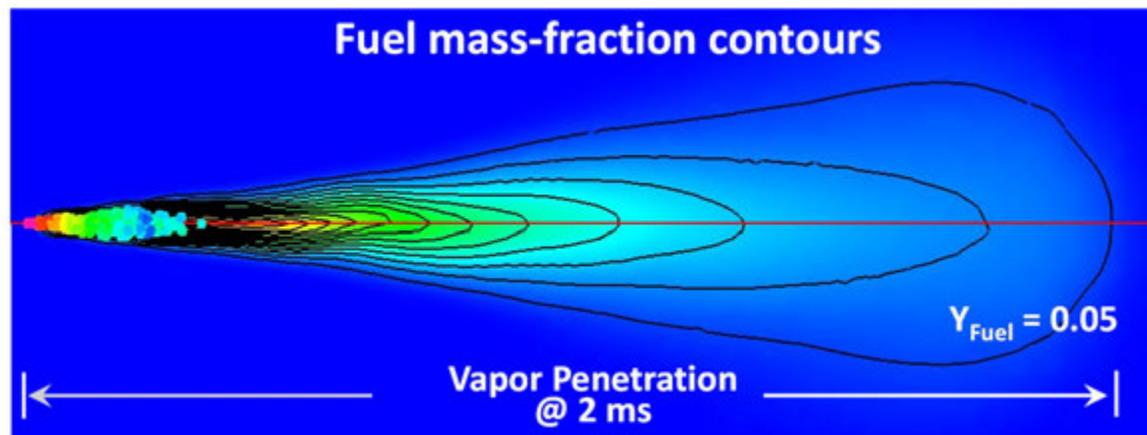
Dagaut et al. PCI 2007



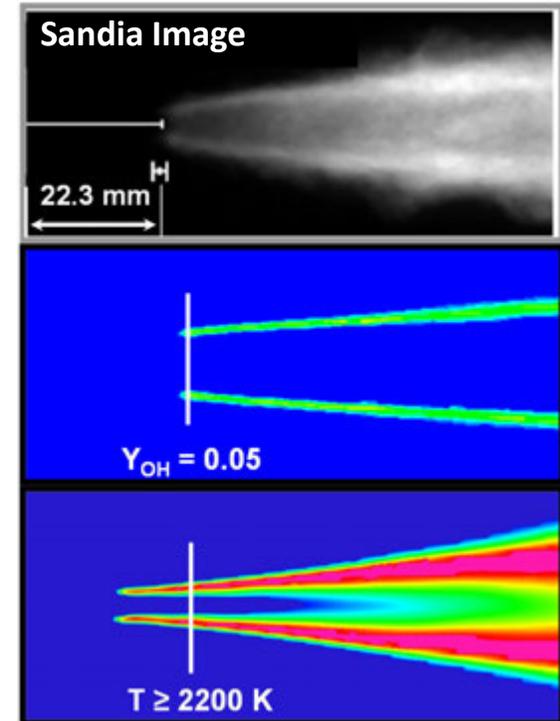
3D Simulations: Some Definitions



Spray penetration @ 2 ms)



Lift-off length)



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



Biodiesel: Case set-up

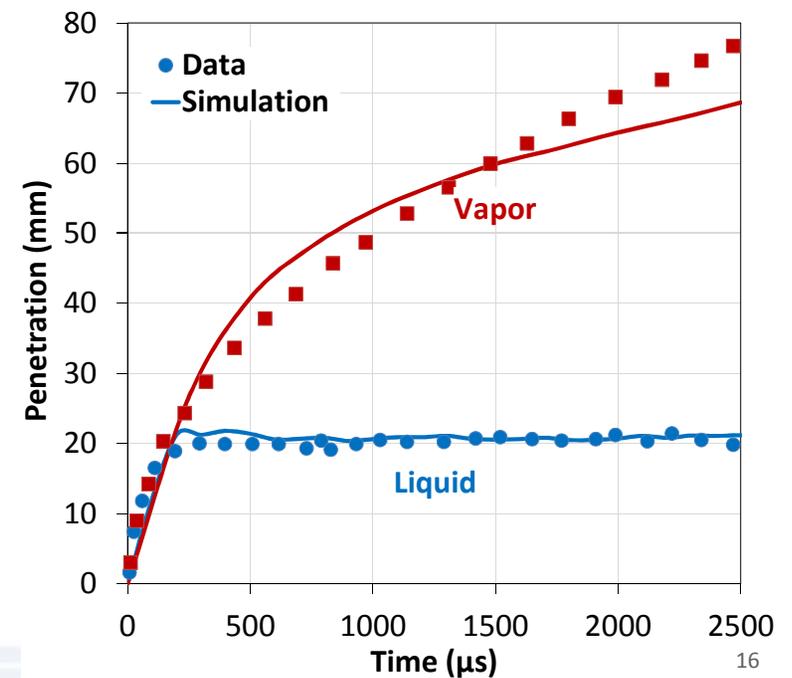
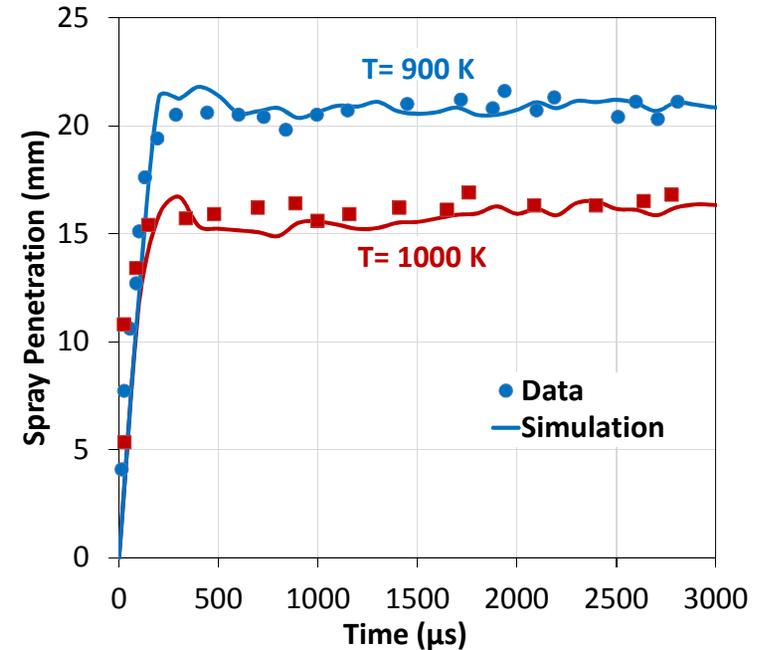
Injection & Ambient conditions for Biodiesel studies at Sandia*

Parameter	Quantity
Injection System	Bosch Common Rail
Nozzle Description	Single-hole, mini-sac
Duration of Injection [ms]	7.5
Orifice Diameter [μm]	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 [kg/m^3]	22.8
Chamber Temperature [K]	900, 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!



Spray-Combustion Simulation: Biodiesel

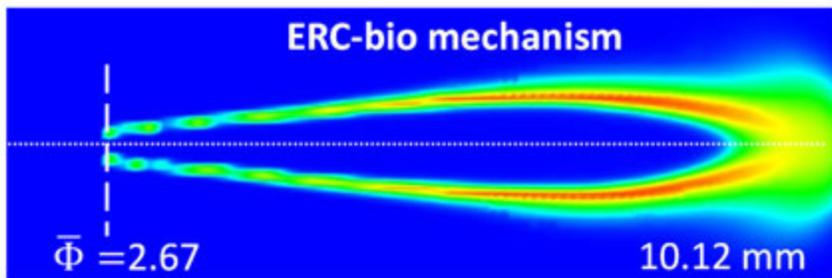
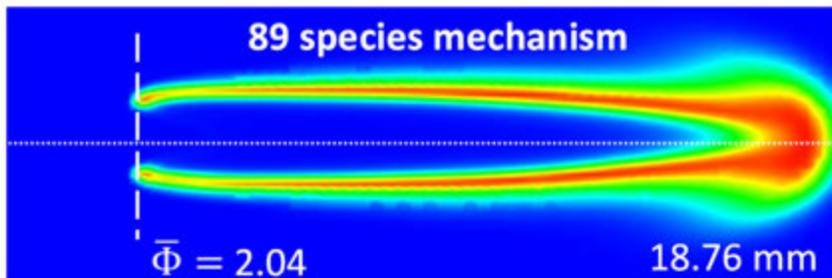
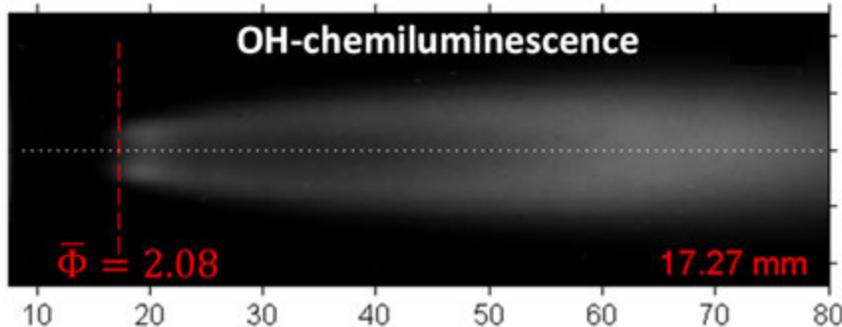
- ✓ 3D simulations: results on a cut-plane are animated
- ✓ Total of 350K-450K grid points for resolving a 108 mm (each side) cube
- ✓ 0.25 mm minimum grid size
- ✓ 85 hours on 8 processors in the Fusion (Argonne) cluster



- ❑ Liquid Length = 15.4 mm
- ❑ Ignition delay = 391 μ s
- ❑ Lift-off length = 18.76 mm

Validation of Biodiesel Reaction Mechanisms

@ T = 1000 K)



CSE is further assessing the ERC-bio mechanism!

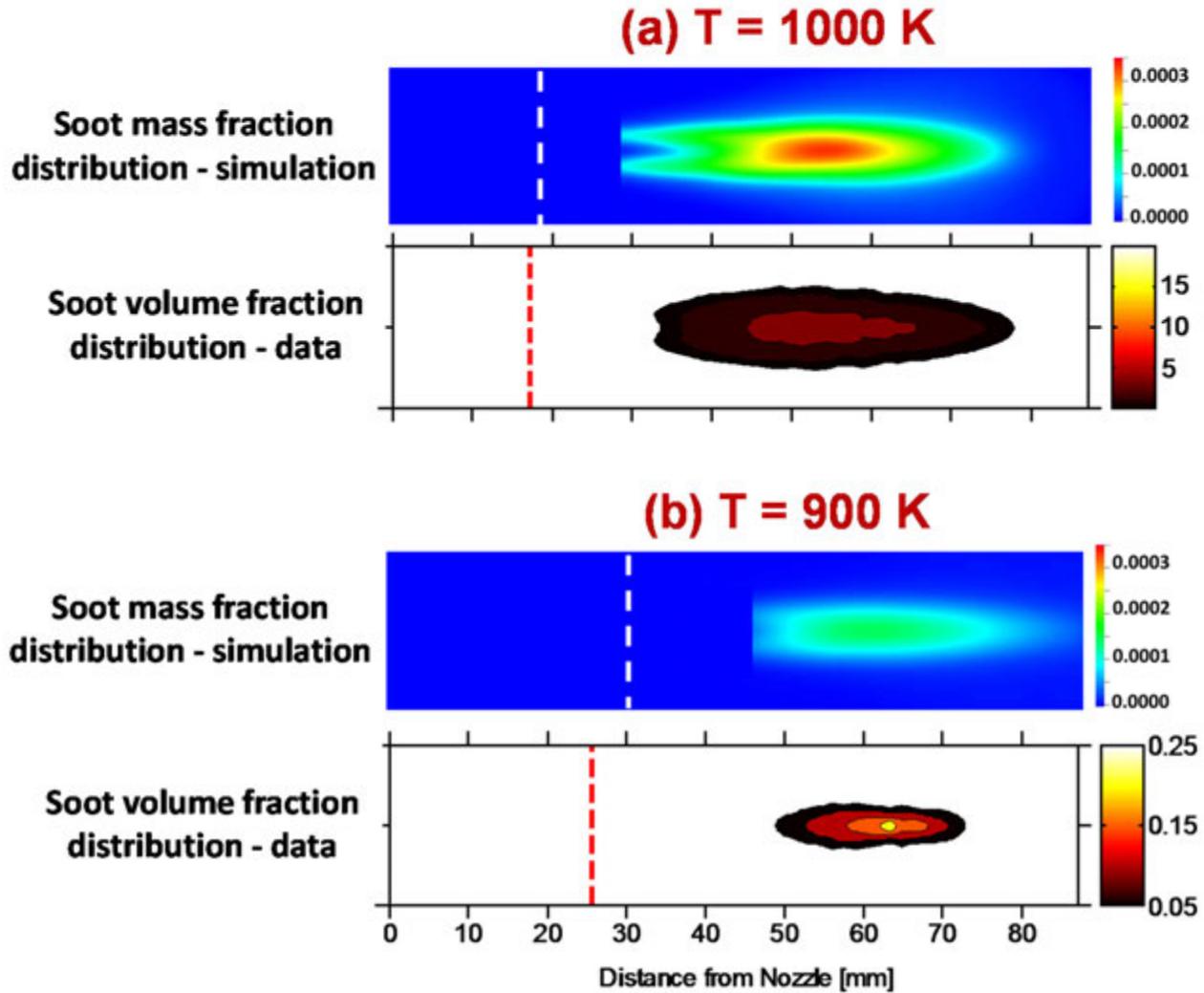
- ❑ Data from Sandia National Laboratory
- ❑ Simulations plot OH contours at a cut-plane
- ❑ ERC-bio mechanism: (Methyl Butanoate + NHPT) 41 species and 150 reactions. SAE Paper No. 2008-01-1378
- ❑ ERC-bio mechanism (using MB as a surrogate) under predicts lift-off length and ignition delay and consequently 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 (μs)
Sandia Data	396
89 species	391
ERC-Bio mechanism	220



Prediction of Soot Distribution

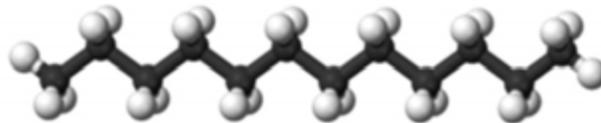
89 species mechanism



C_2H_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



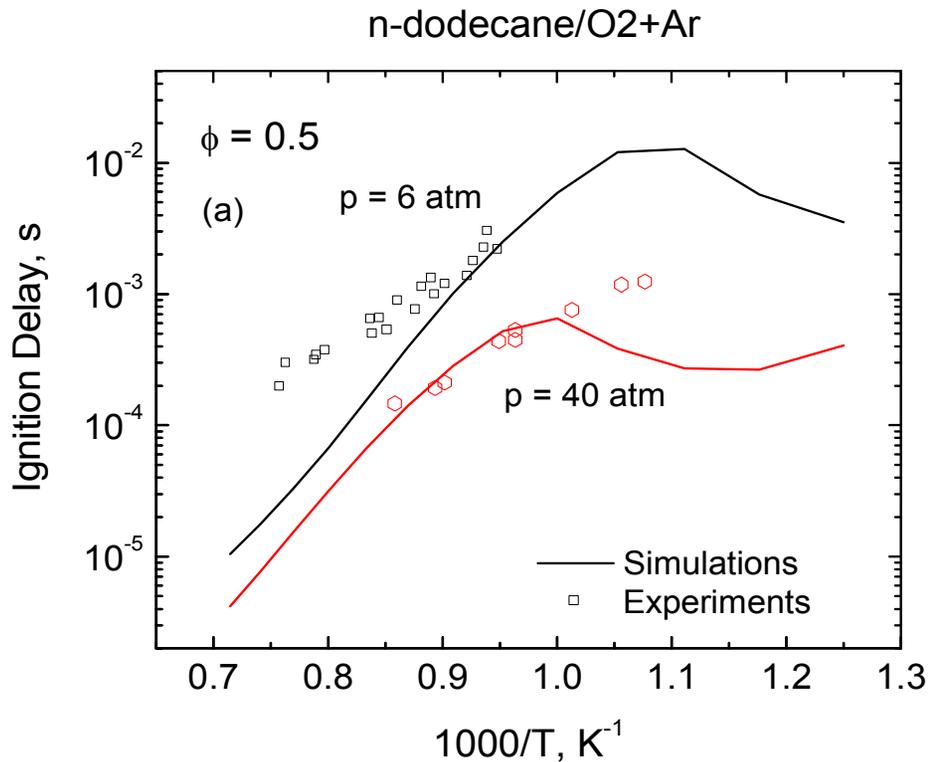
103 species, 370 reactions*

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



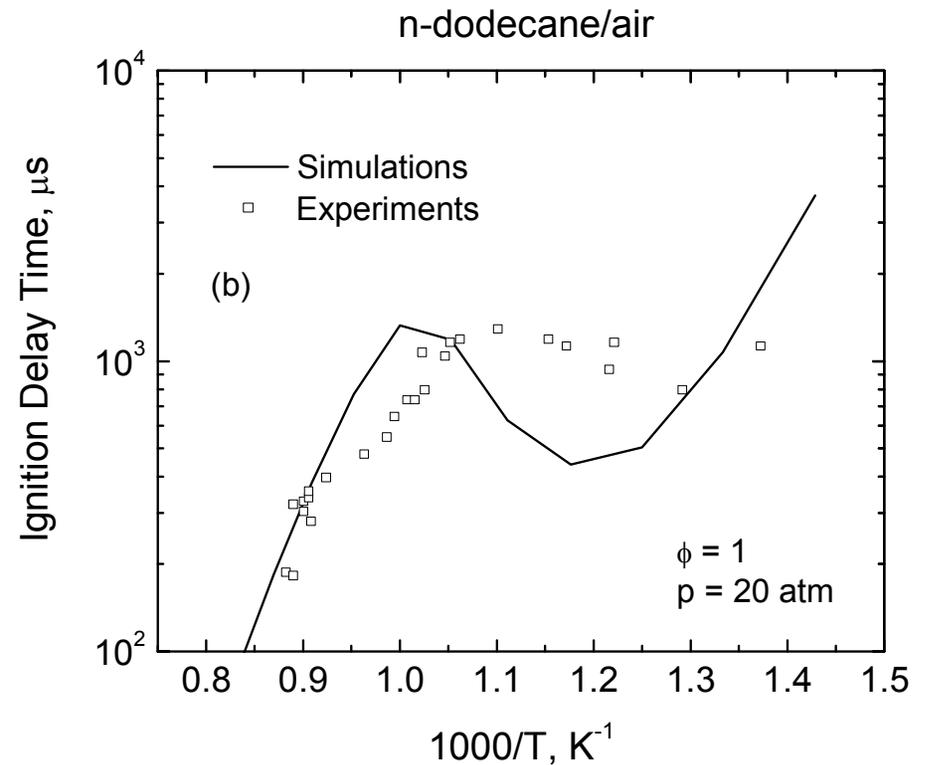
Validation against Shock Tube data

103 species, 370 reactions: n-dodecane reduced mechanism)



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

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



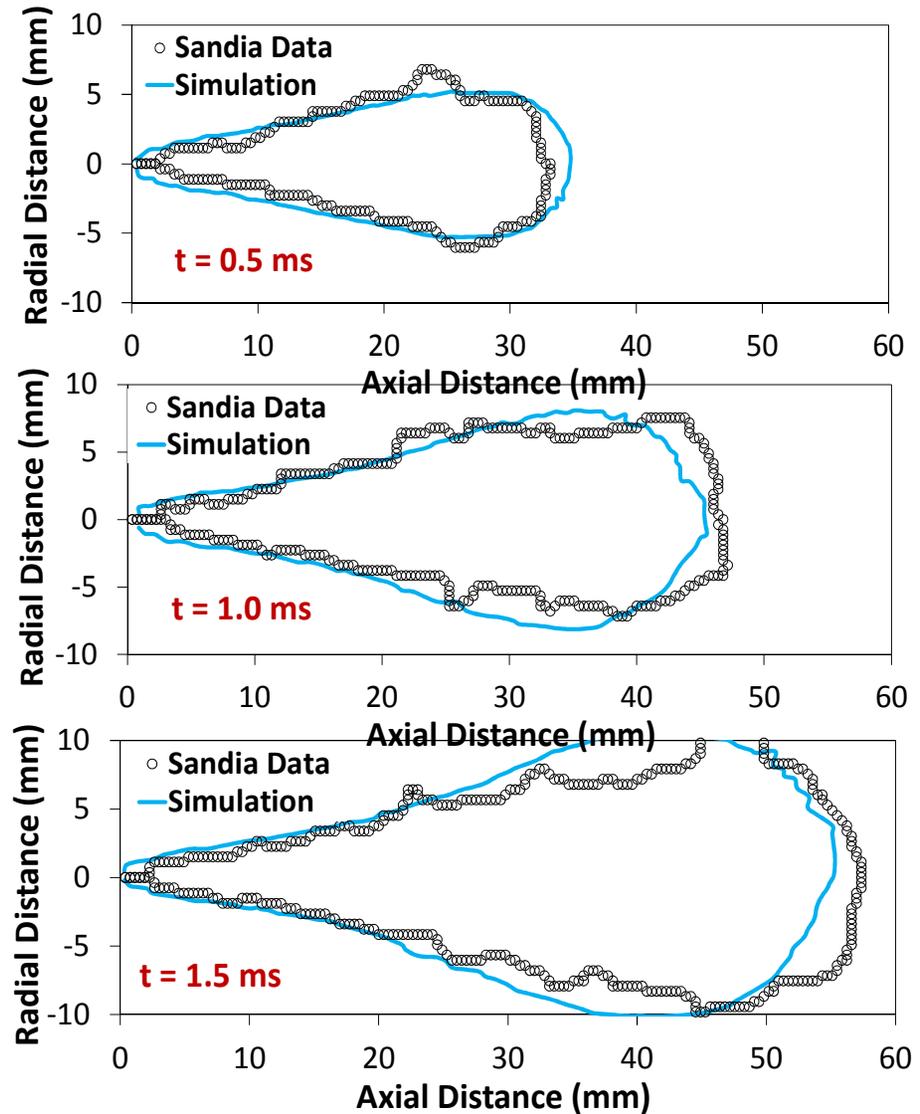
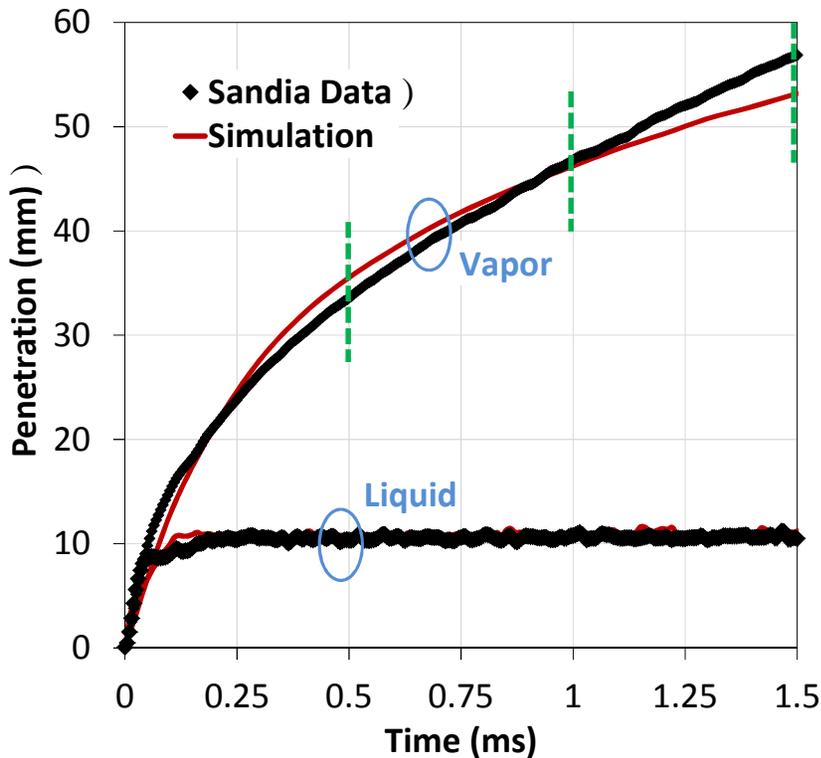
Experimental data from: Vasu et al. Proc. of
Combustion Institute 2009



3D Spray (non-combusting) Validation

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:)

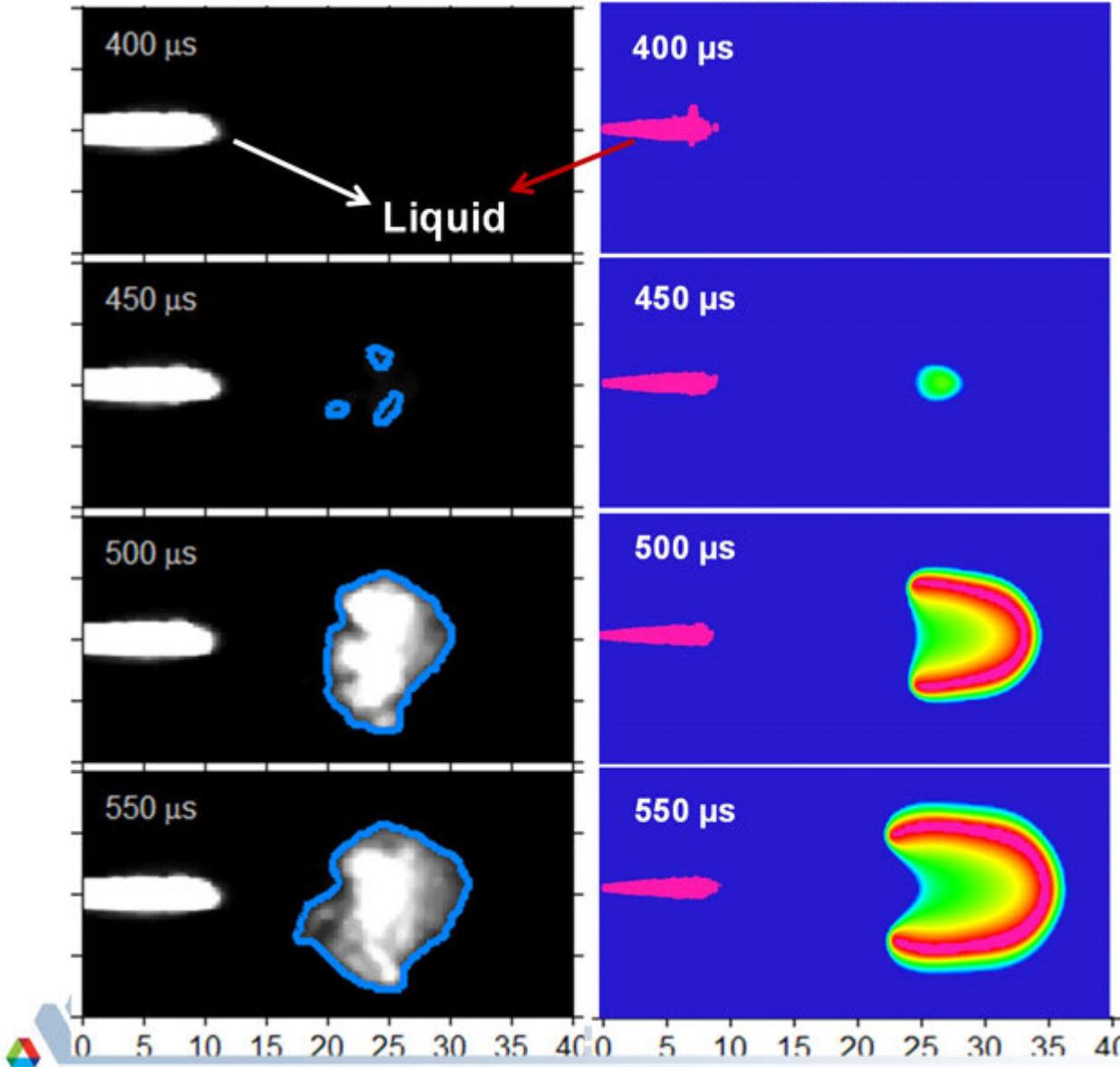
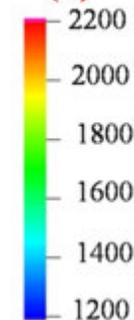
Natural Luminosity high-speed imaging for detection of ignition delay

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

Simulation:)

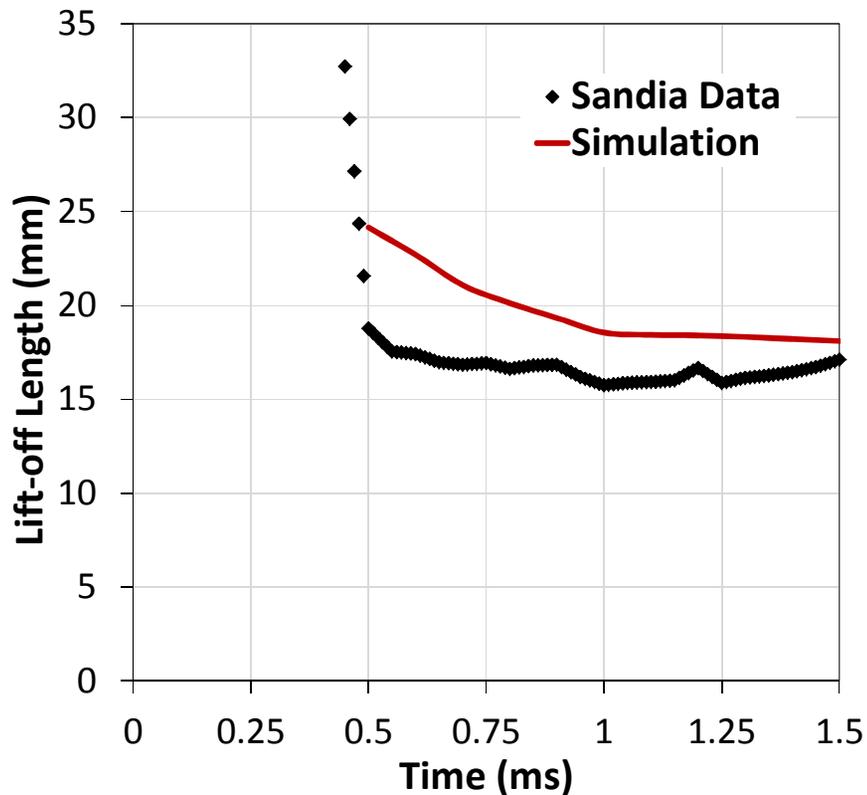
Temperature contours plotted to capture ignition location and delay

Temperature (K)

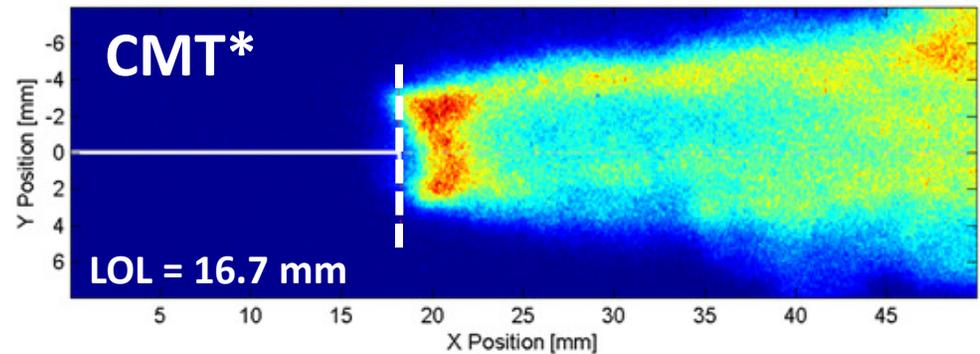


Ignition Delay and Flame lift-off Length

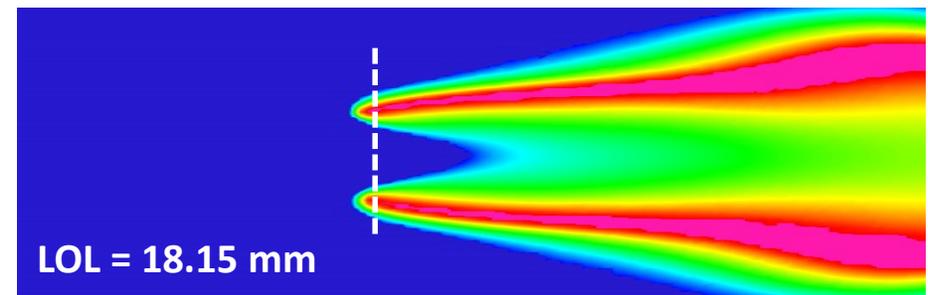
	Ignition Delay (ms)	Lift-off Length (mm)
Sandia Data	0.440	16.50
Simulation	0.425	18.15



OH chemiluminescence



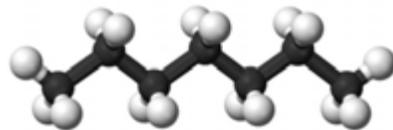
Simulation



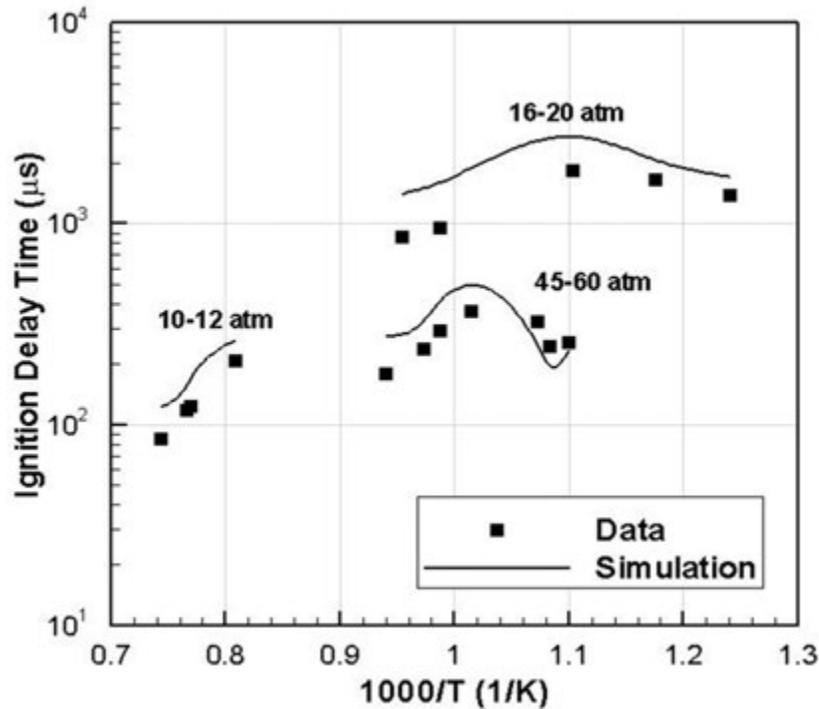
*<http://www.cmt.upv.es/ECN07.aspx>

Bringing it all together!

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

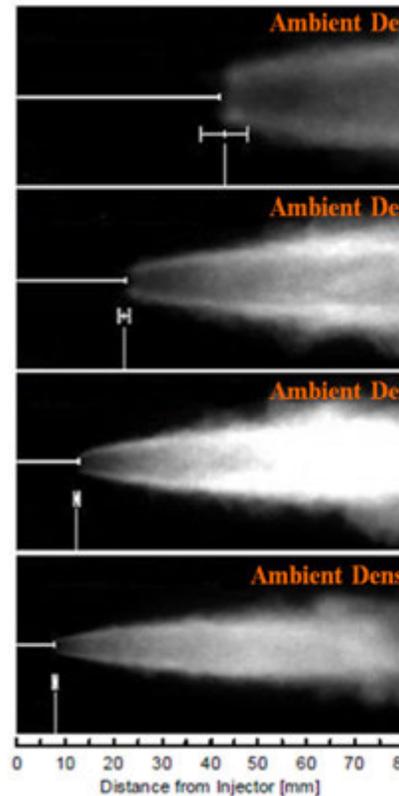


n-Heptane Mechanism Validation

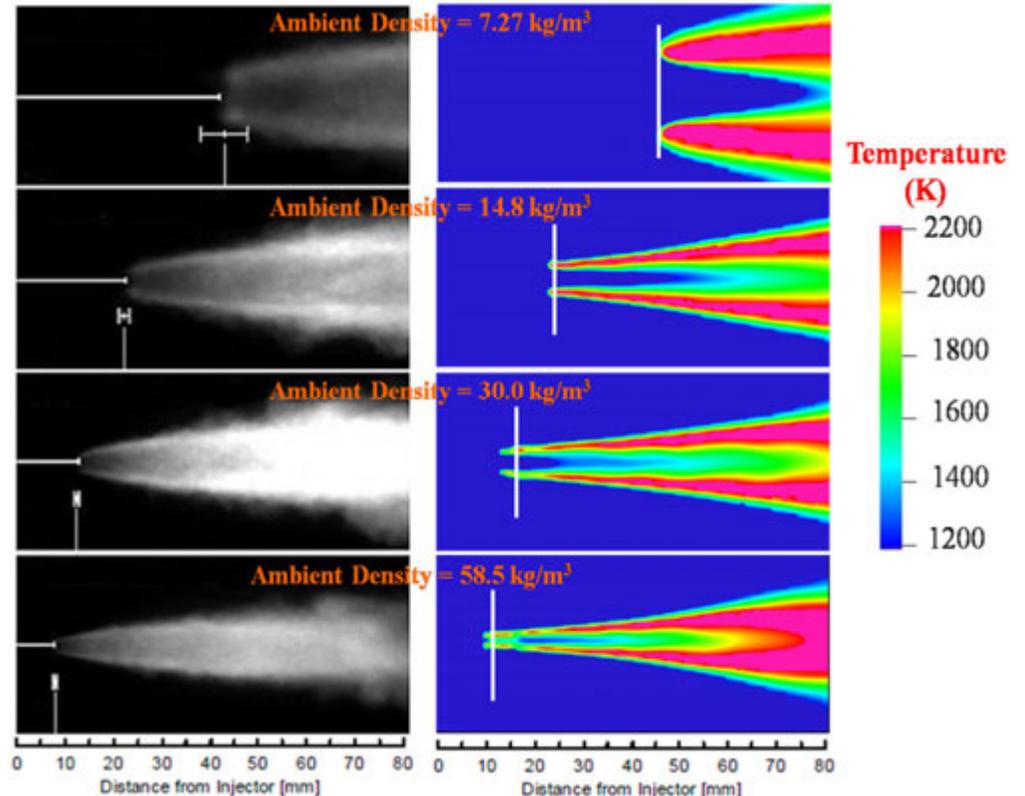


- ❑ Shock-tube data from Gauthier et al. Comb and Flame 2004
- ❑ n-heptane: 68 species, 168 reactions (Lu et al.): Comb. and Flame 2009
- ❑ Accurately captures NTC characteristics

Data



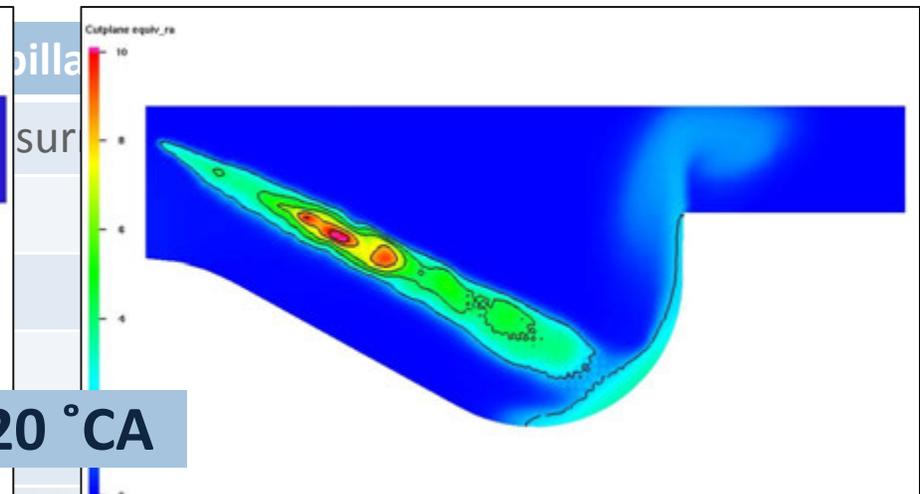
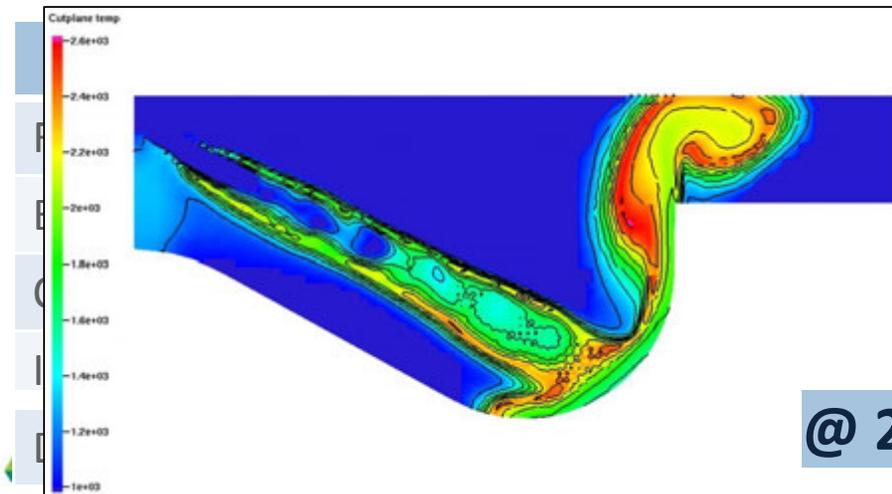
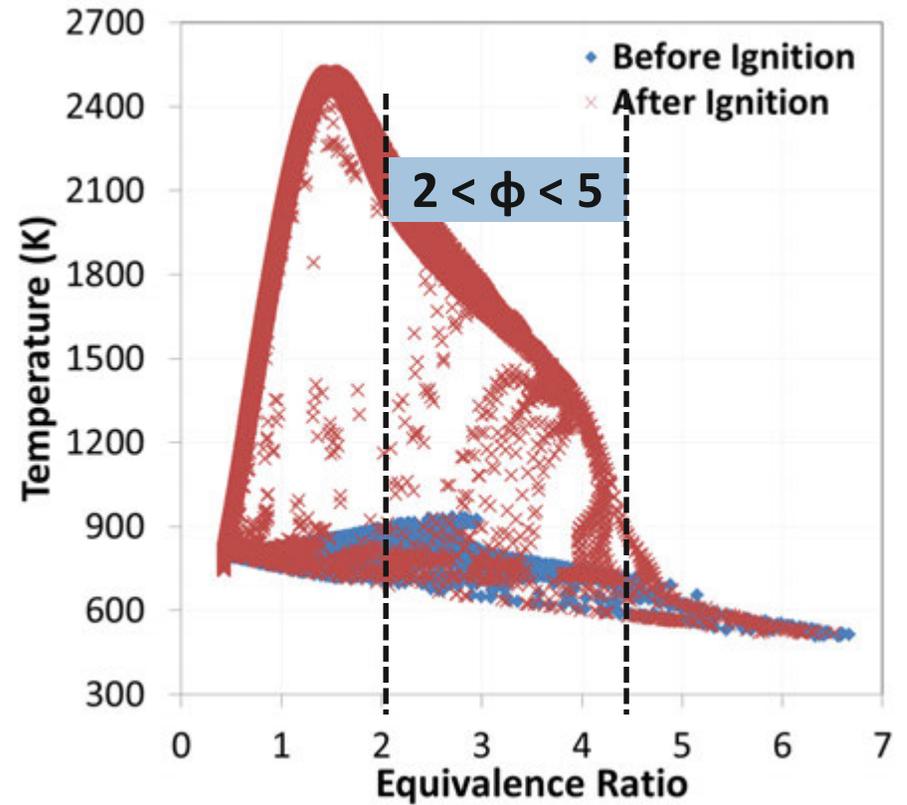
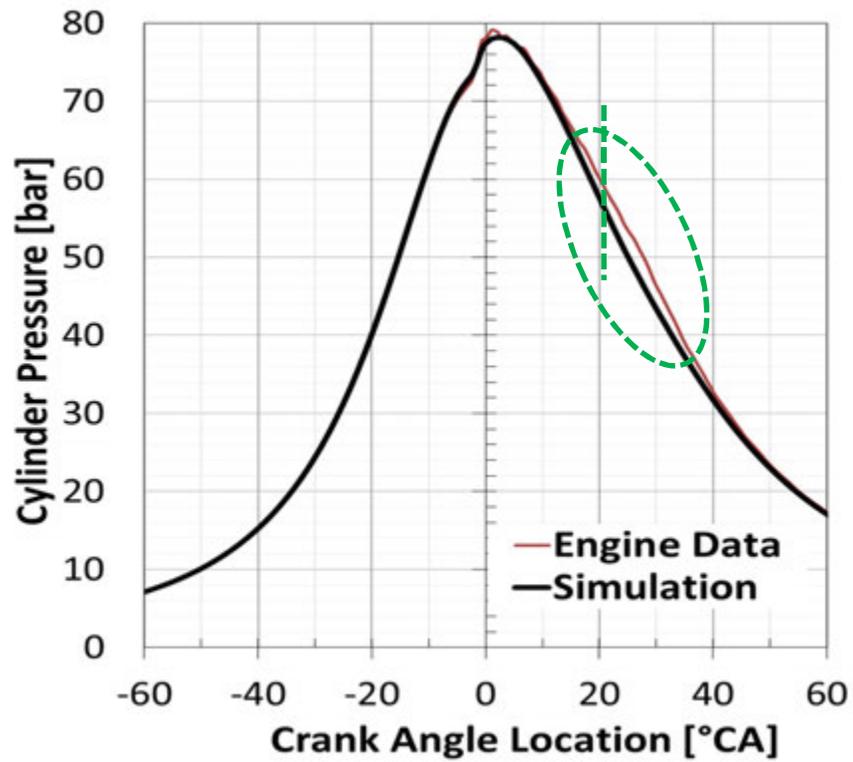
Simulations



- ❑ 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

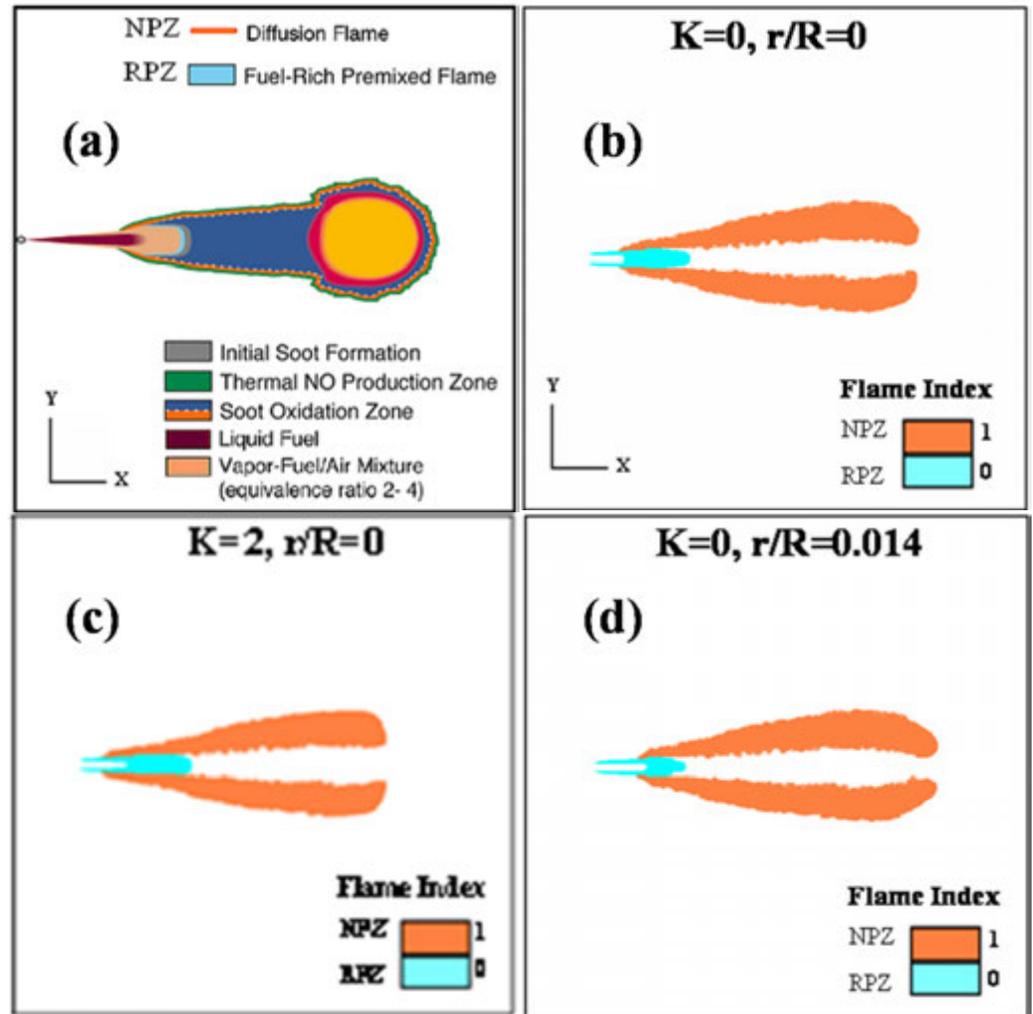
$$G_{CO.O_2} = \nabla Y_{CO} \cdot \nabla Y_{O_2}$$

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

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

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

- 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

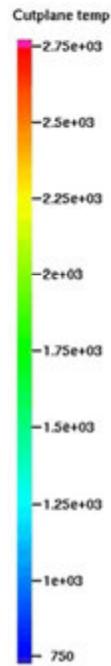
$K=2, r/R=0$: Conical Nozzle

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

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





Thank You!!

Contact: ssom@anl.gov

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

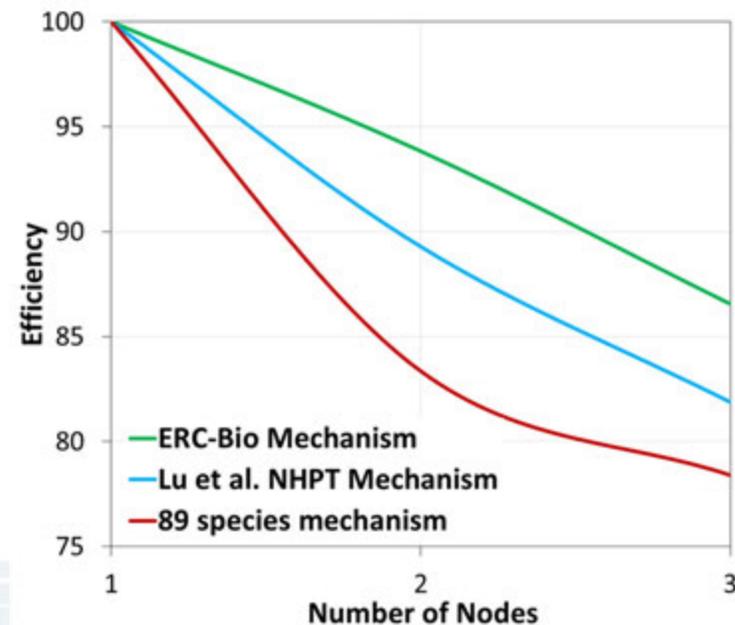
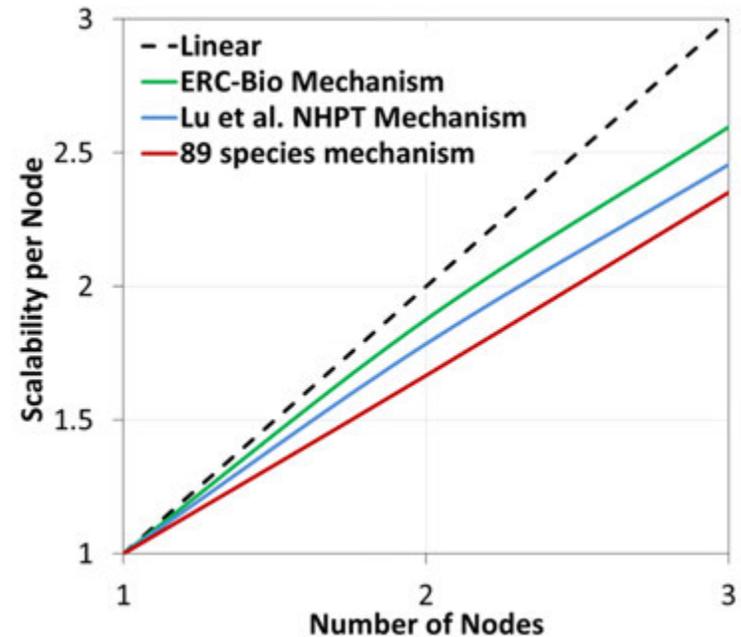
Efficiency per node = $T_1 \times 100 / nT_n$

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





Step 1: Skeletal Reduction with Directed Relation Graph (DRG)

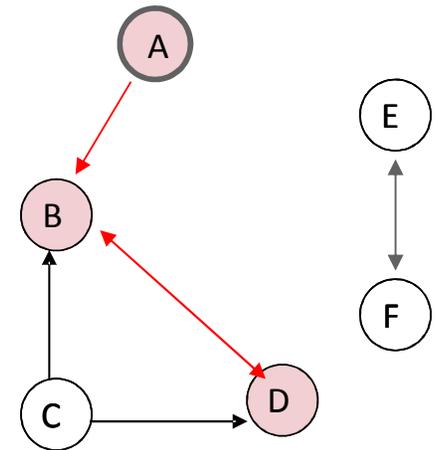
- **DRG**(*Lu & Law, 2005; Luo et al, 2010*): a graph-based algorithm to eliminate unimportant species

- Mapping species relation to a graph:

$$r_{AB} \equiv \frac{\max_i (|\nu_{A,i} \omega_i \delta_{Bi}|)}{\max_i (|\nu_{A,i} \omega_i|)} \quad \delta_{Bi} = \begin{cases} 1, & \text{If reaction } i \text{ involves species B} \\ 0, & \text{otherwise} \end{cases}$$

- $A \rightarrow B$: (if $r_{AB} > \varepsilon$; ε : threshold error)

if A is kept in skeletal mechanism, B should also be kept



- Advantages of DRG:
 - High efficiency(Linear time reduction)
 - Fully automated



Further Reduction



- **Step 2: Isomer lumping**(*Lu & Law; 2008*)
 - Isomers(Identical molecular formula but different structure)
 - >50% isomers in the biodiesel mechanism
 - Governing equations of Isomers can be lumped
 - The variables of the governing equations are reduced

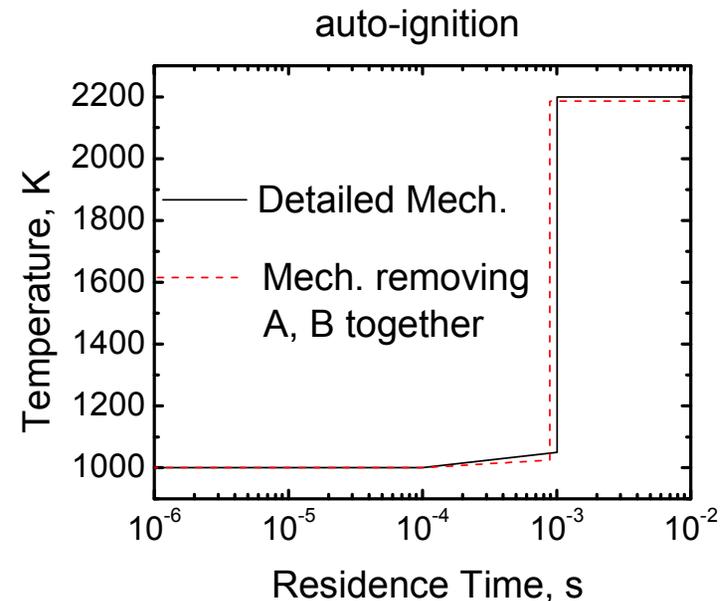
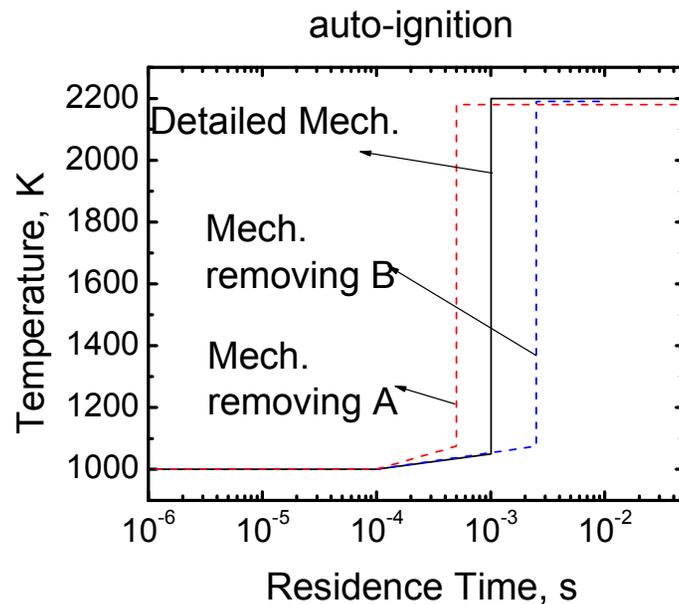
- **Step 3: DRG-aided sensitivity analysis**(*Zheng, et al; 2007 Sankaran, et al; 2007*)
 - Species are not equally important for major parameters
 - Select species for sensitivity analysis based on DRG results(extend to almost every species in the present study)



Error Cancellation in DRGASA



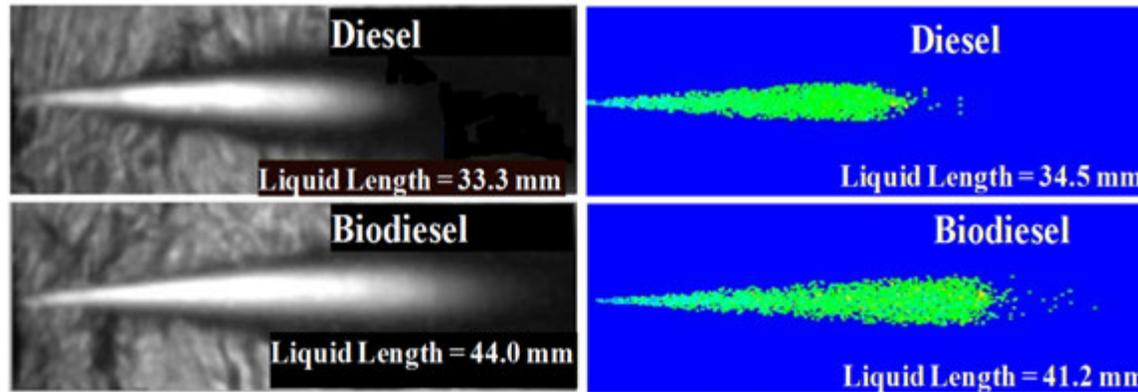
- Example showing error cancellation



- Compromise between practical simulation and mechanism size
- Error cancellation is limited to certain degree
- **Extensive validations** are further performed to guarantee the chemical fidelity of the reduced mechanism



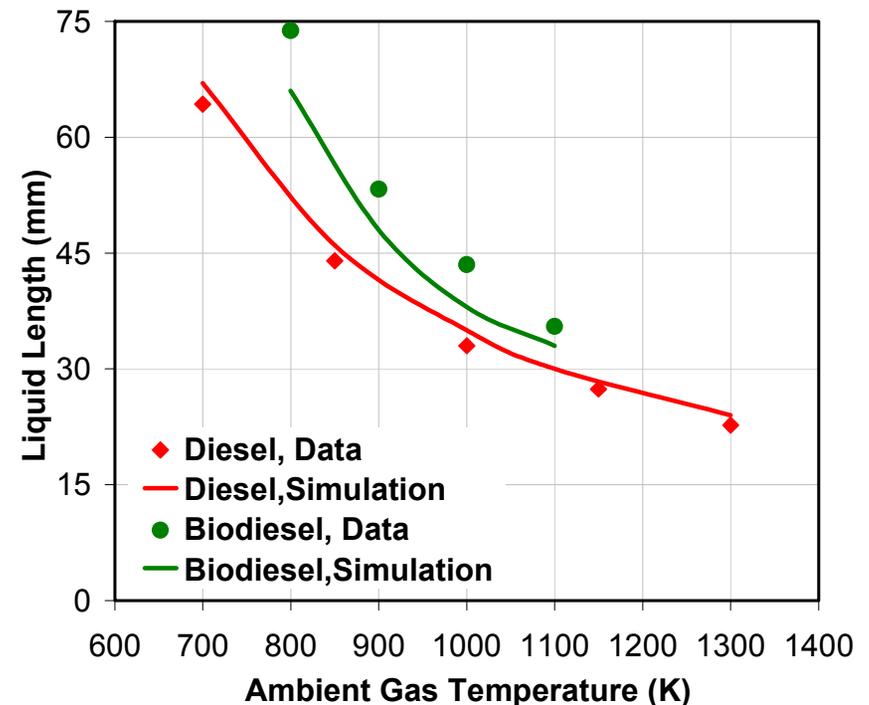
Evaporating Sprays: Liquid



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	$\text{N}_2, \text{H}_2\text{O}, \text{O}_2, \text{CO}_2$
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



Biodiesel Surrogates for Engine Modeling

- ❑ Methyl butanoate: 41 species, 150 reactions (Brakora et al; 2008)
 - Includes low temperature chemistry
 - Cannot well represent the real biodiesel chemical kinetics

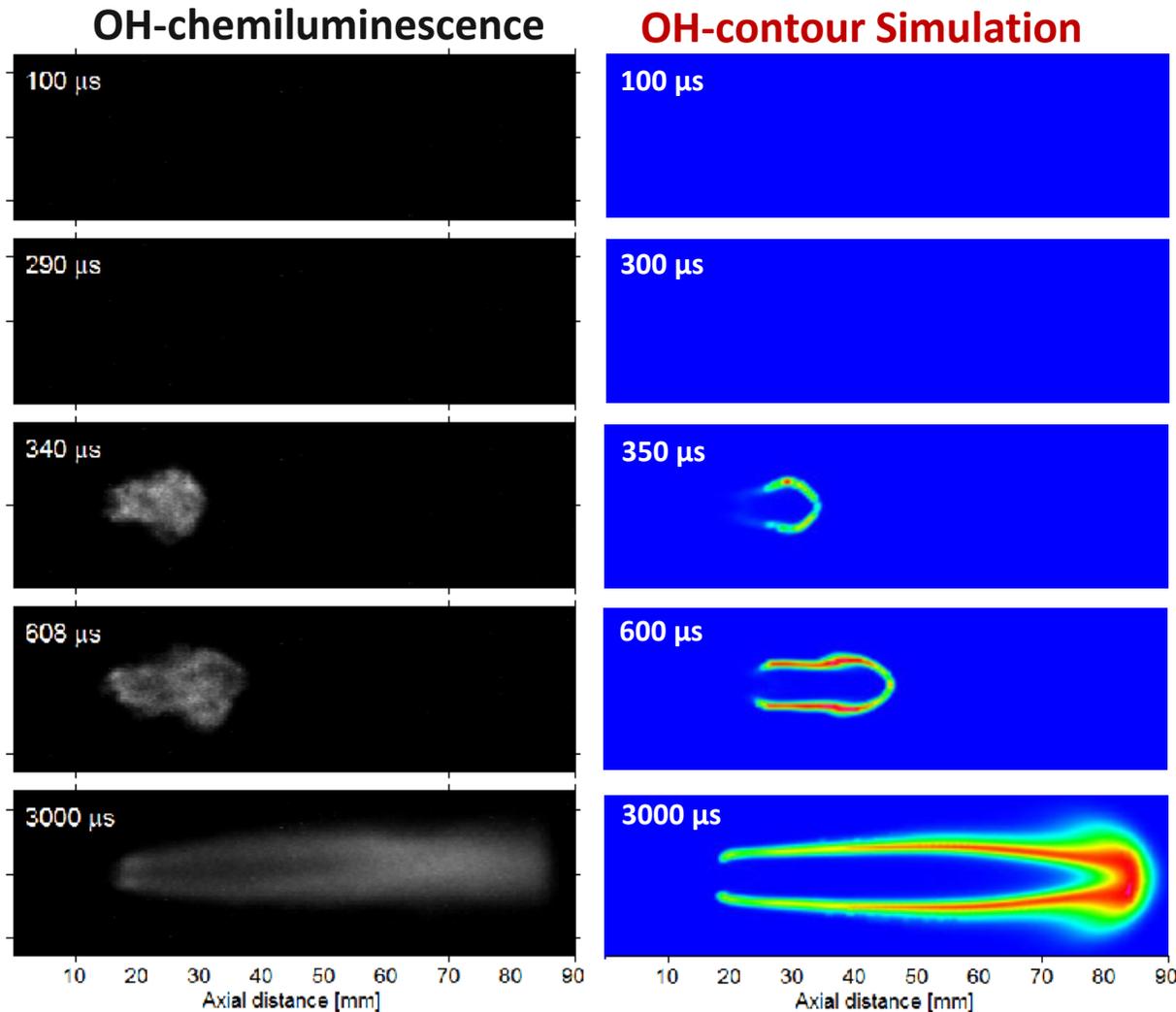
- ❑ Methyl decanoate (MD):648 species and 2998 reactions (Sarathy et al; 2011)
 - Includes low temperature chemistry
 - Too large to be applied in practical engine simulations

- ❑ 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

Further Validation: 89 species mechanism



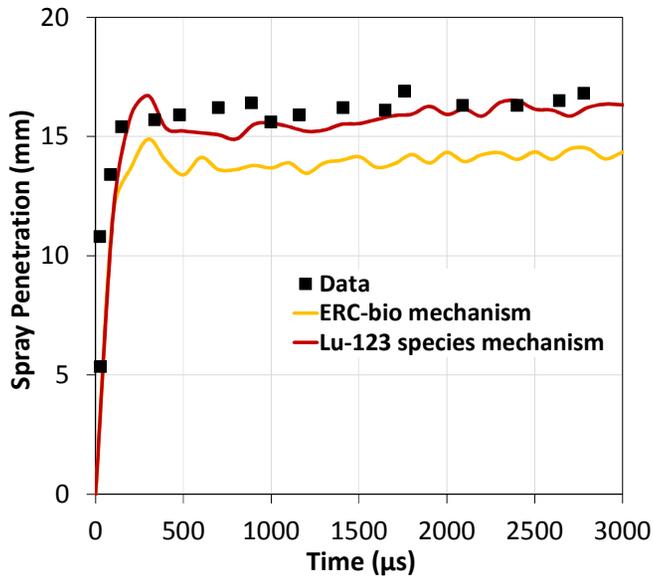
@ T= 1000 K

- ❑ Chemiluminescence data from Sandia National Laboratory
- ❑ Simulation plots OH contour and is able to predict OH* distribution very well!

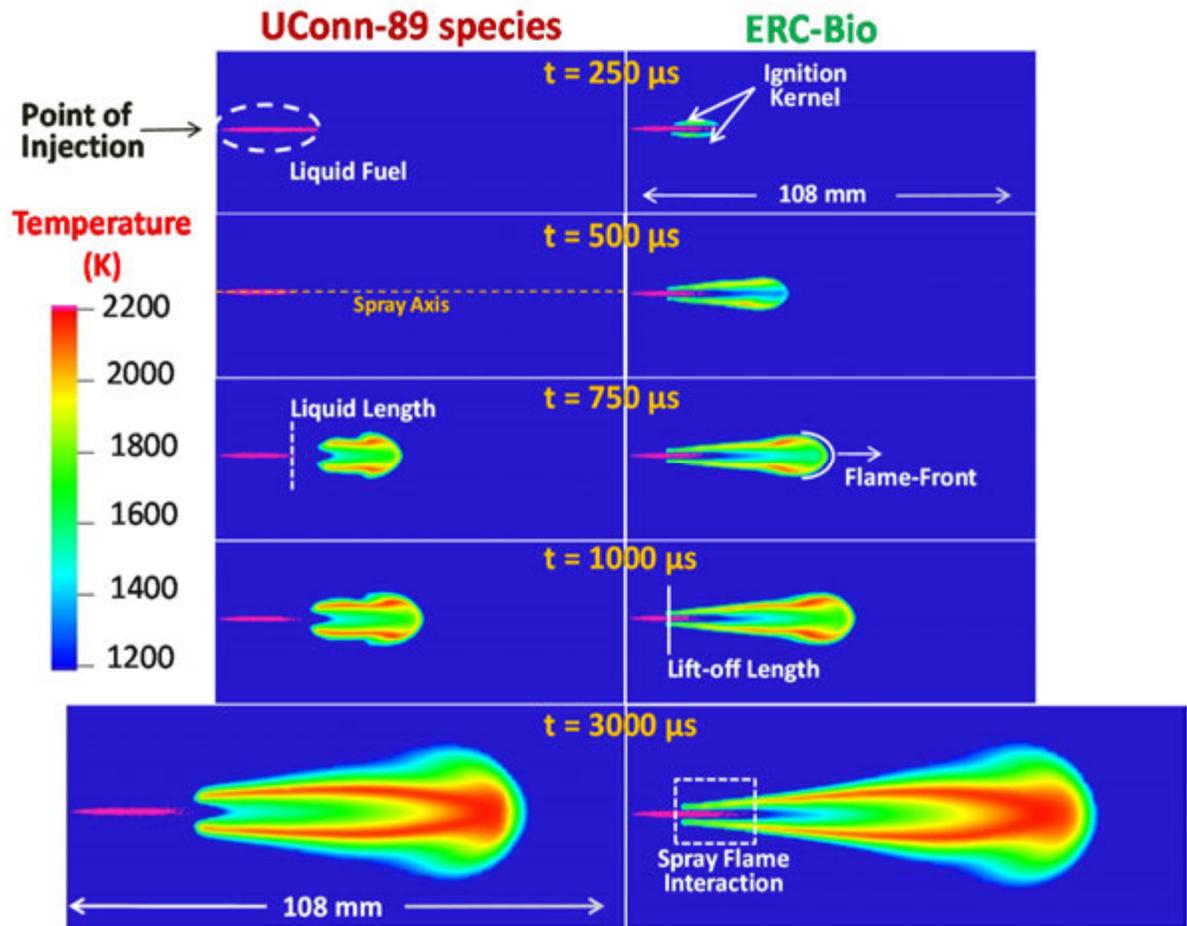
Som et al. ASME ICE2011-60051



Flame Structure with Different Mechanisms



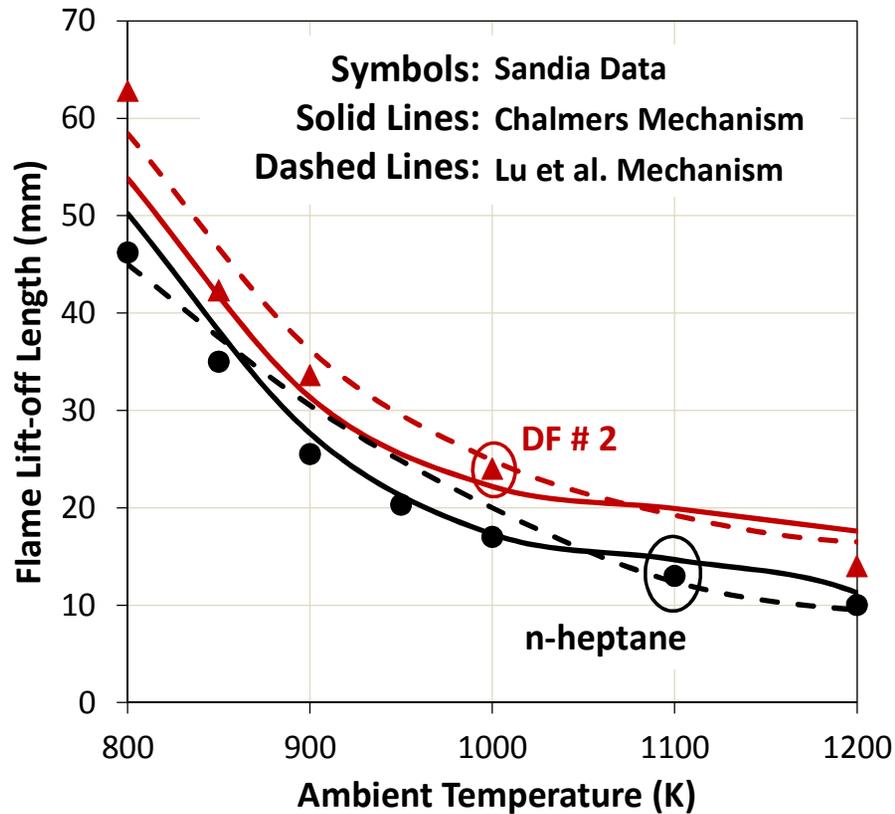
* Som et al. SAE World Congress 2011



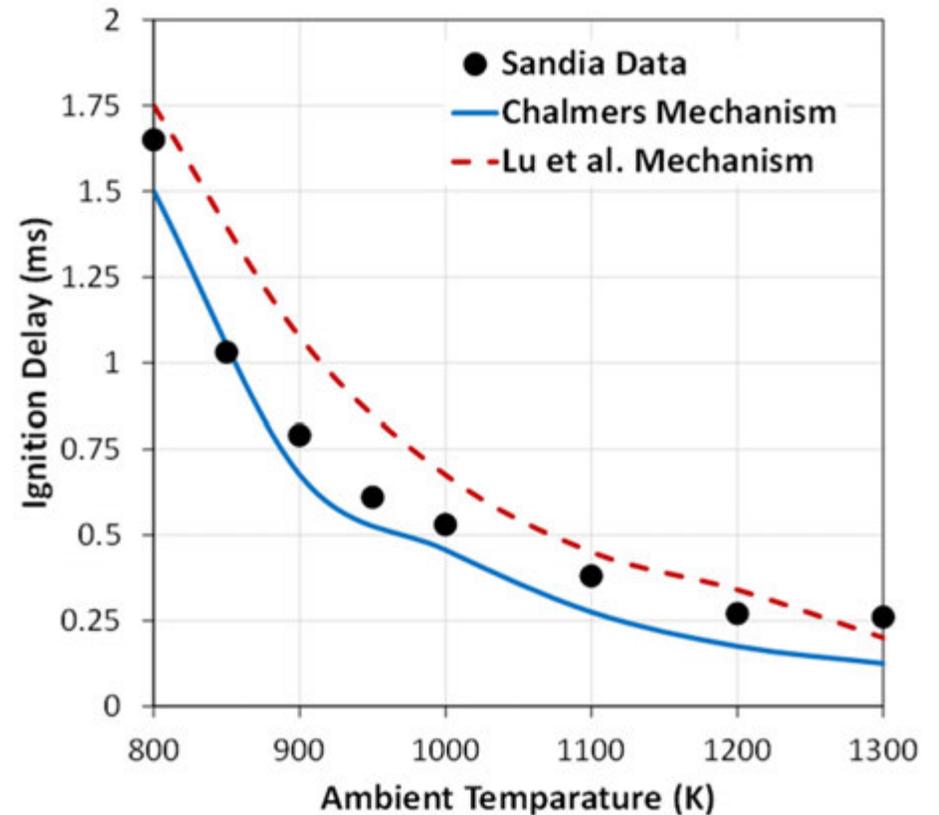
Due to enhanced spray-flame interaction, liquid length is lower with the ERC-MB mechanism!



n-heptane mechanisms vs. Diesel # 2 data



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

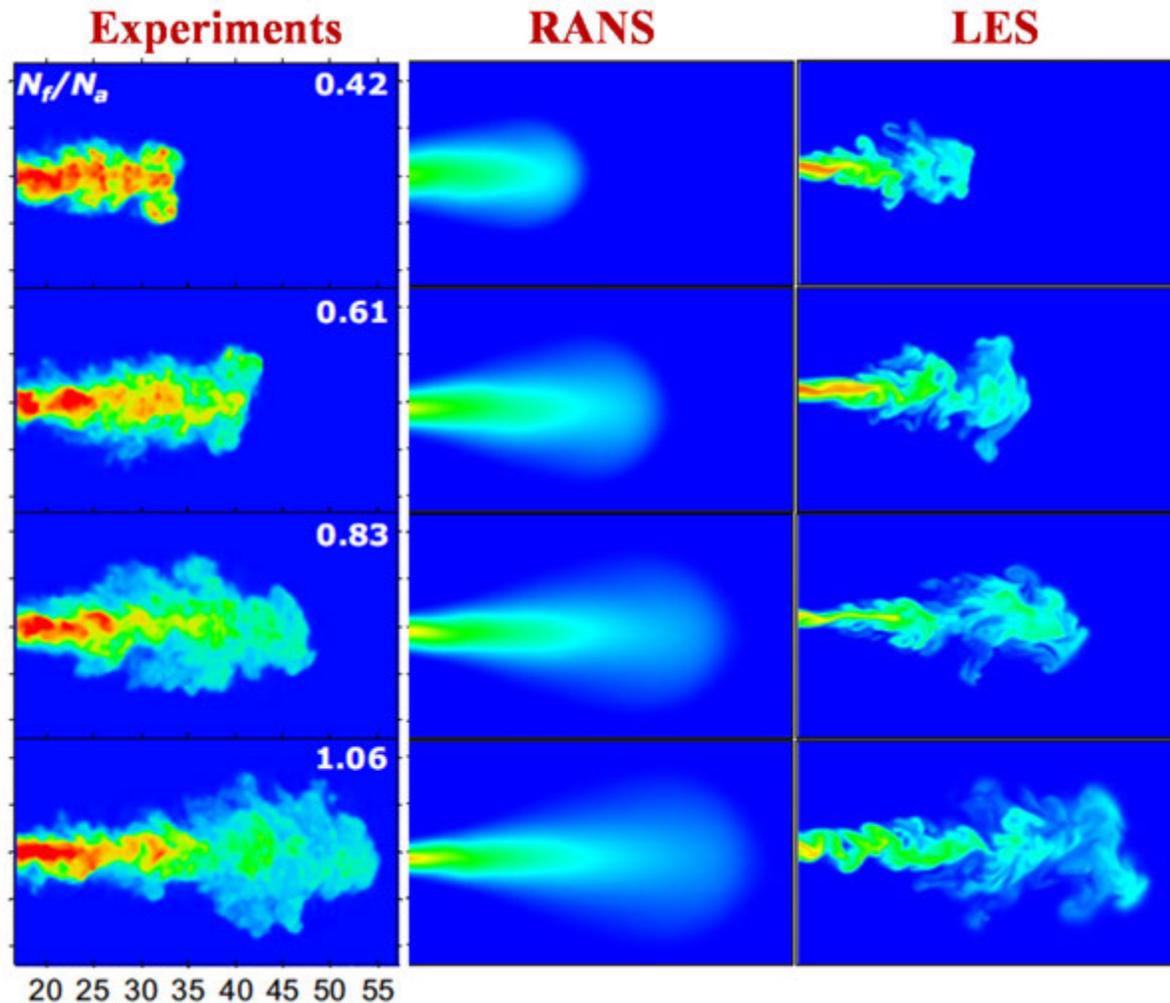


Lu et al. (larger) mechanism does a marginally better job in predicting diesel # 2 characteristics!!

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



Instantaneous Equivalence Ratio Distribution

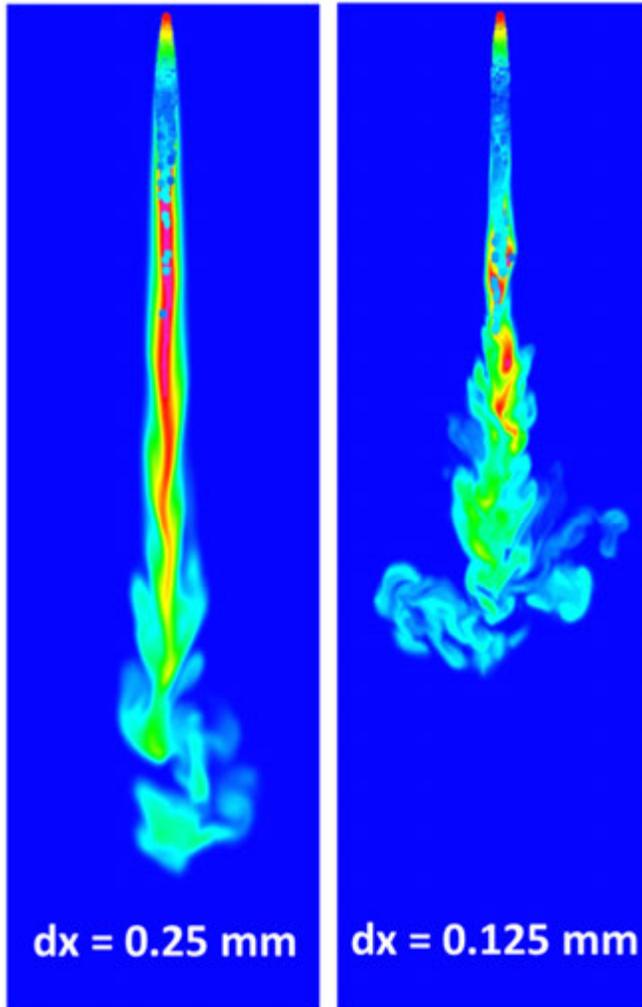


n-heptane: $T_{amb}=1000K$, $\rho_{amb}=14.8Kg/m^3$, O_2 Concentration = 0%,

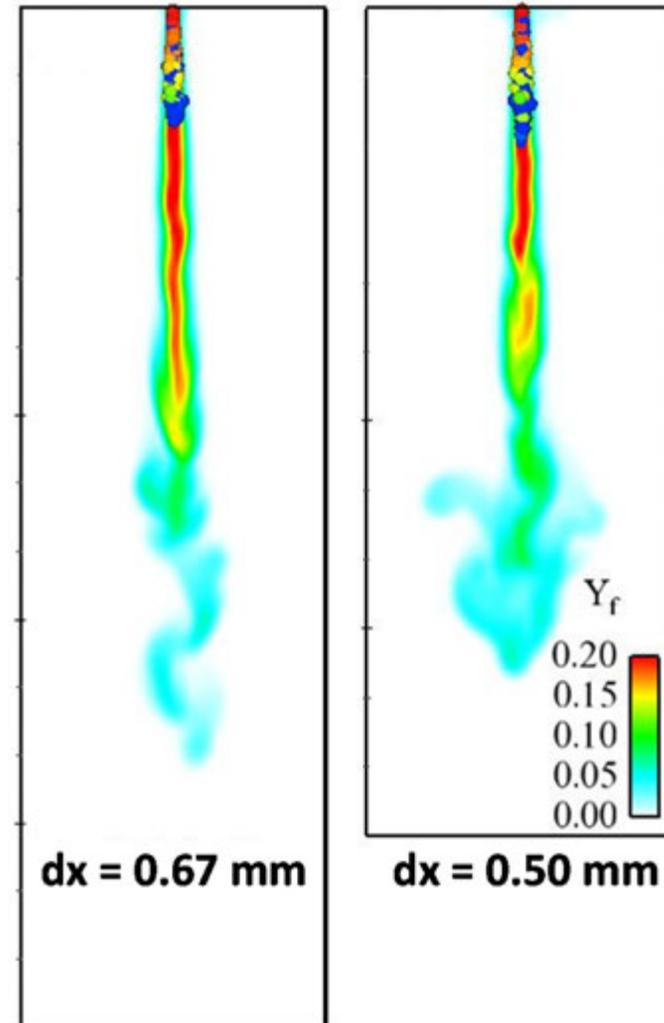
Orifice diameter = 100 μ m, $P_{inj}=1500bar$, $T_{fuel}=373K$

Fuel Mass fraction distribution

ANL



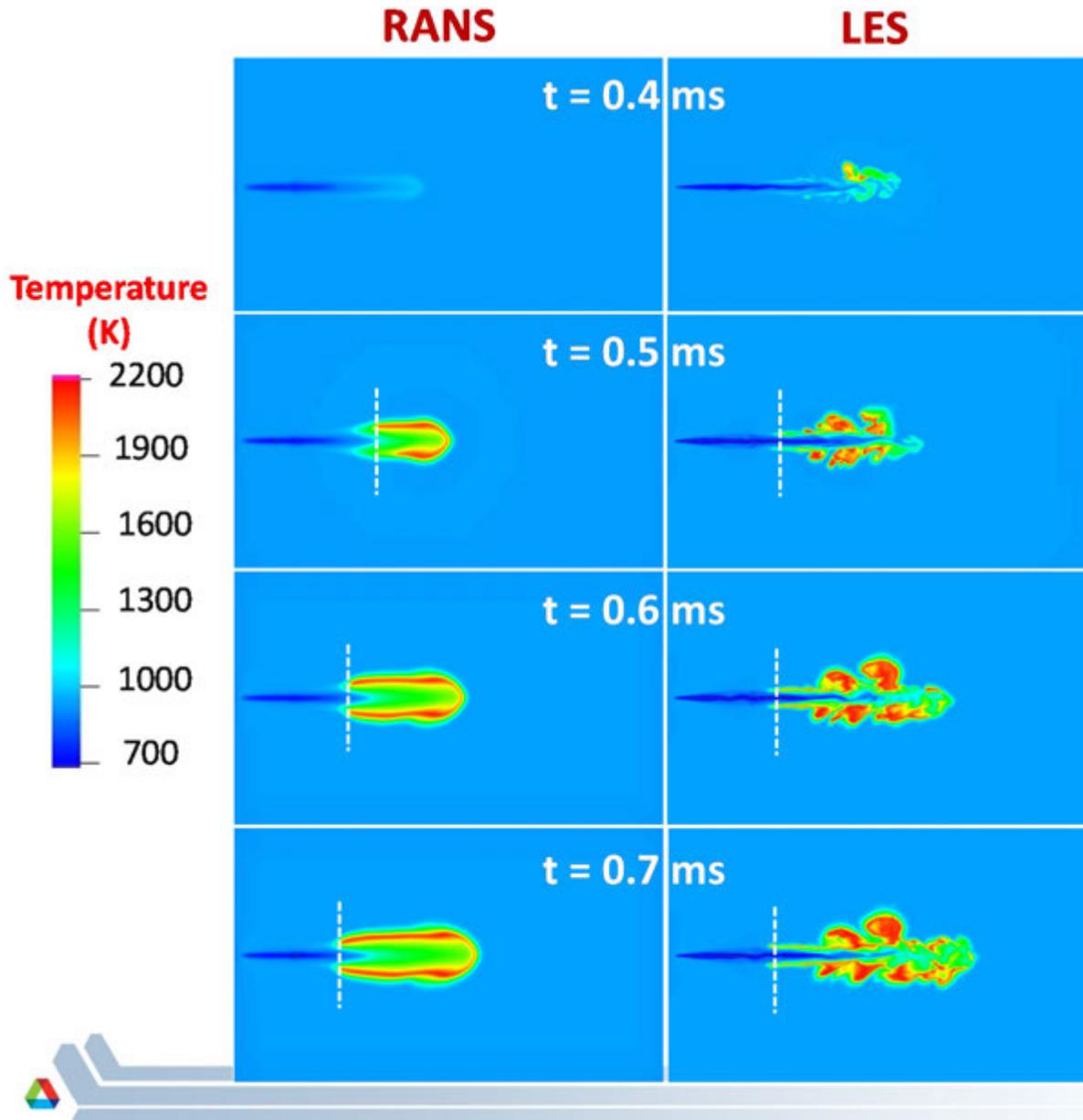
UW-ERC



Smaller grid sizes results in earlier initiation of instabilities at the vapor-air interphase which results in faster breakup and reduction in vapor penetration!

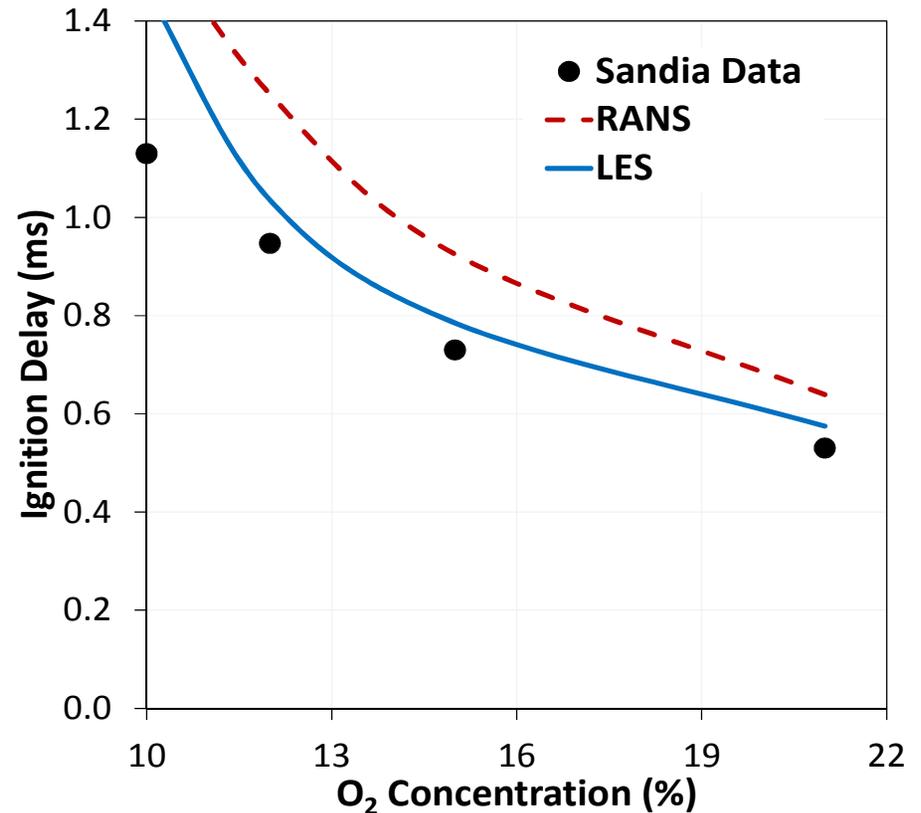
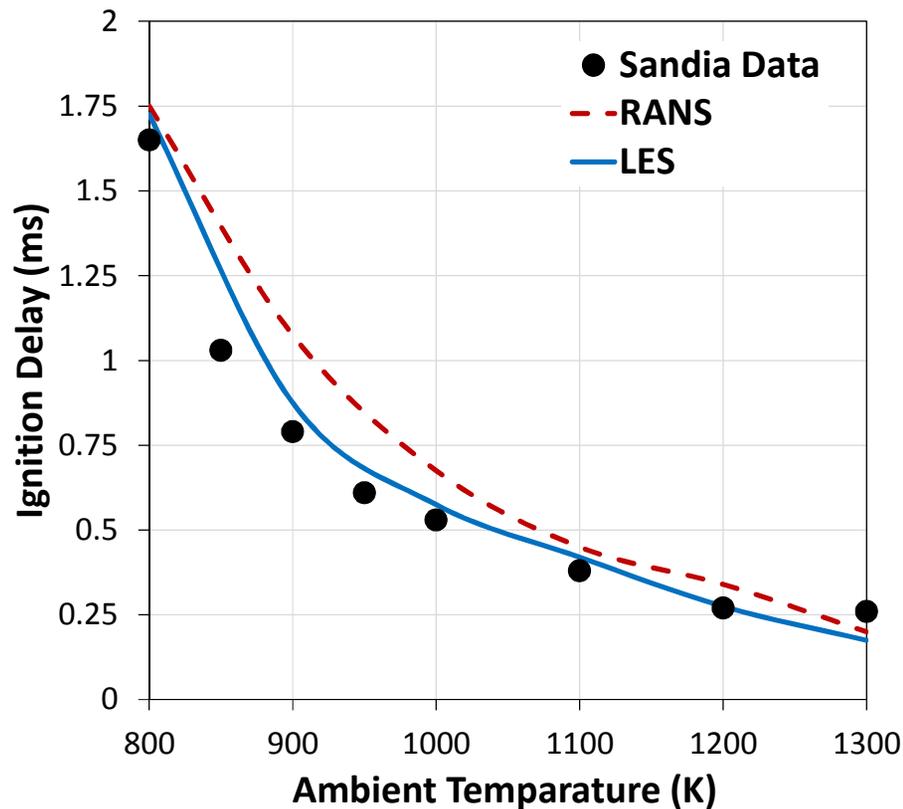


RANS vs. LES: Temperature Contours



- Earlier ignition with LES
- LES predicts enhances flow structures
- RANS produces smooth distributions
- Volumetric auto-ignition observed with LES
- Flame stabilization more realistic with LES. Similar to experimental data
- Quasi-steady L_f values with RANS and LES are similar

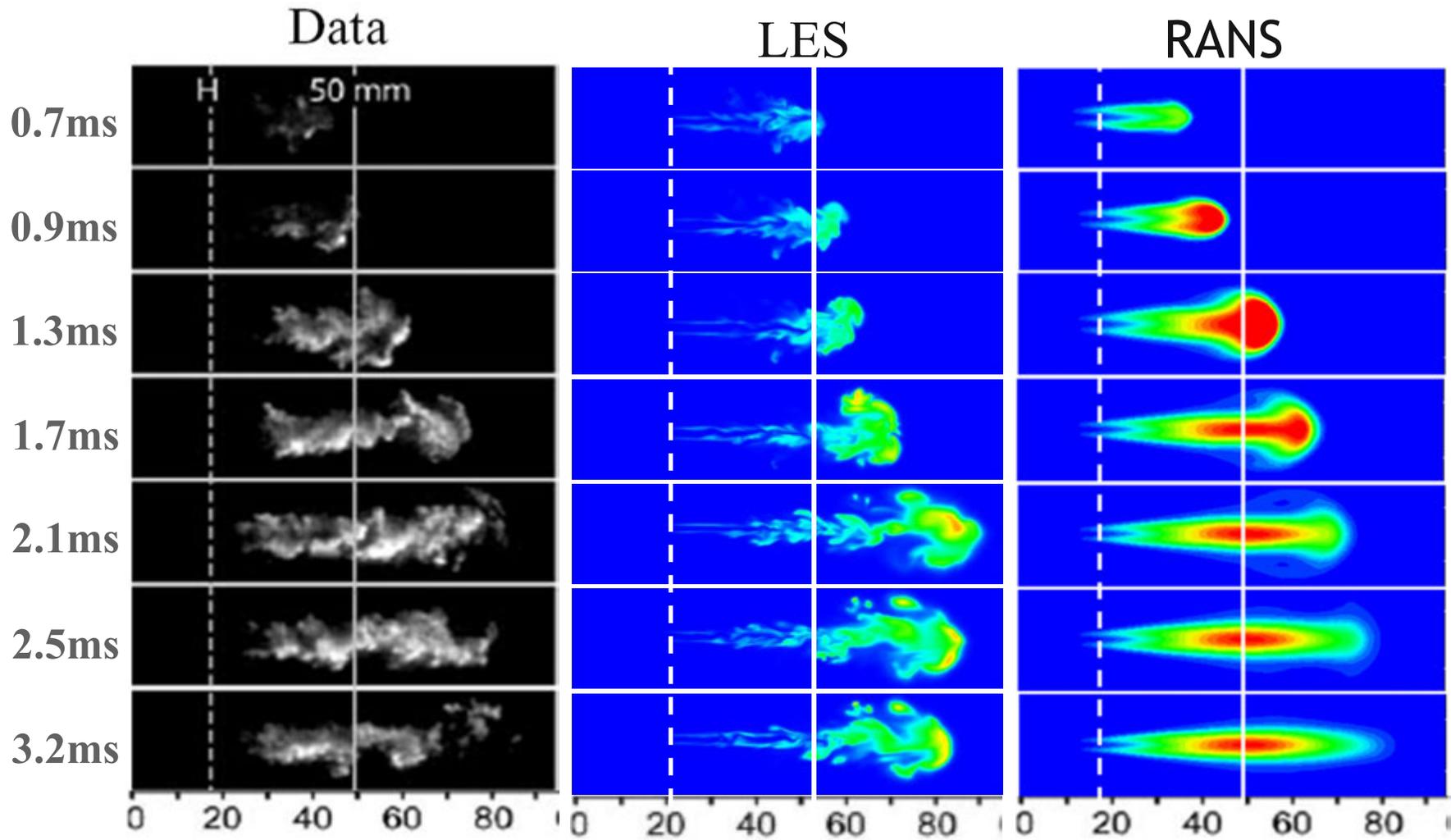
RANS vs. LES: Ignition Delay



- Earlier ignition with LES under all conditions investigated
- Quasi-steady Lift-off length values with RANS and LES are similar



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!

