Discussion on IC Engine Spray Applications

Recent Progress in CFD Modeling and Challenges

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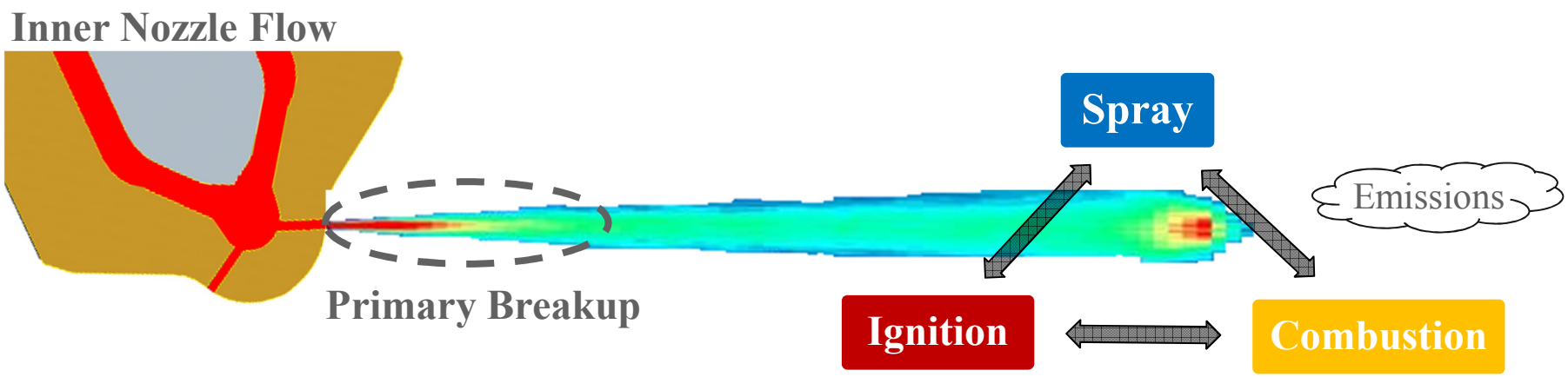
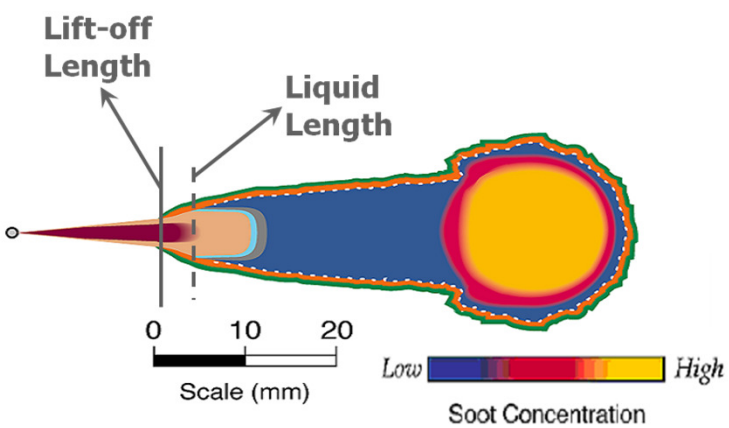
Frontiers of Liquid Atomization: An Indo-US Workshop

3-D Integrated Modeling Approach



Conceptual Combustion Model from Sandia National Laboratory



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

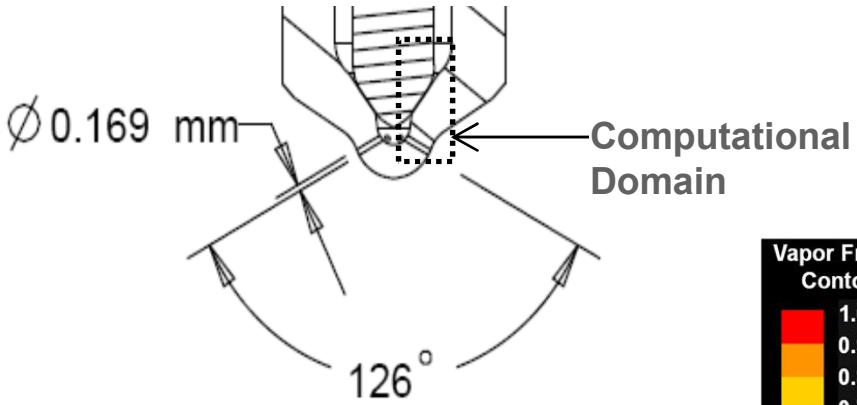
Validation: **X-ray radiography** data

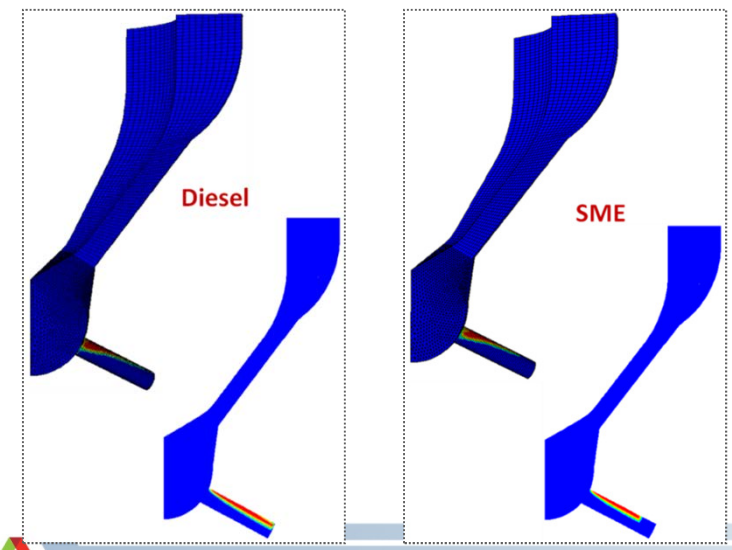
- ❑ **Detailed Chemistry**:
  n-heptane – Diesel surrogate
  n-dodecane – Diesel surrogate
  Methyl Decanoate – Biodiesel surrogate

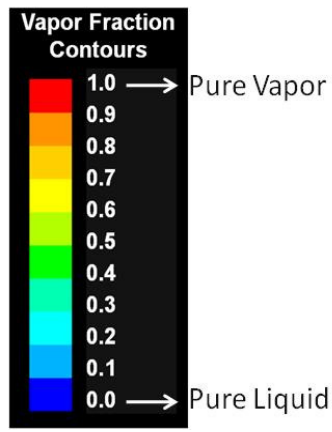
Validation:
Constant-volume vessel (Sandia National Laboratory)
Engine data (Argonne National Laboratory)

Inner Nozzle Flow Modeling

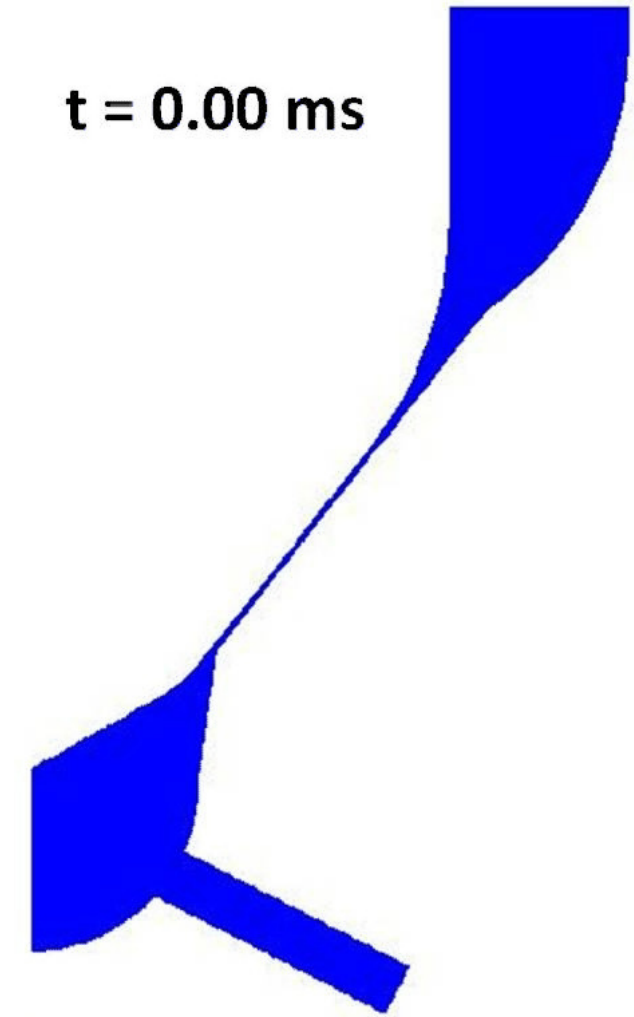
- Lack of quantitative data for validation of nozzle flow models
- Current nozzle flow models only consider cavitation due to geometry changes







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

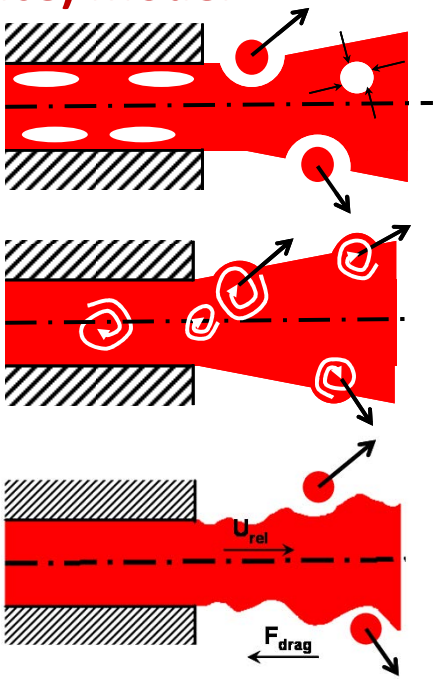


*Som et al., *FUEL* (2010)
Som et al., *JEGTP* (2010)

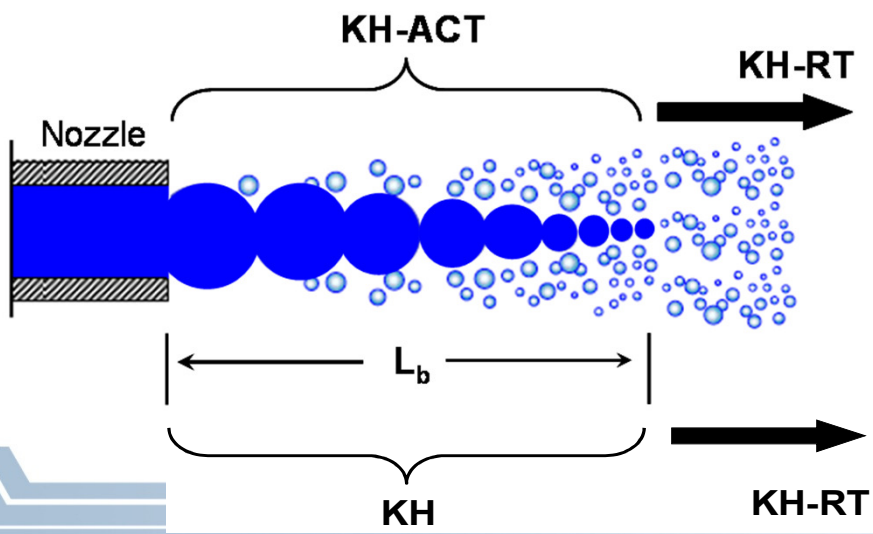
Primary Breakup Model*

Underlying physic itself is not well-understood, developing models is challenging

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



- **Spray models are phenomenological**
  - **Tuning is necessary with KH-RT models to account for changes in nozzle geometry, fuel variability, etc.**
- **The breakup length is *ad-hoc***

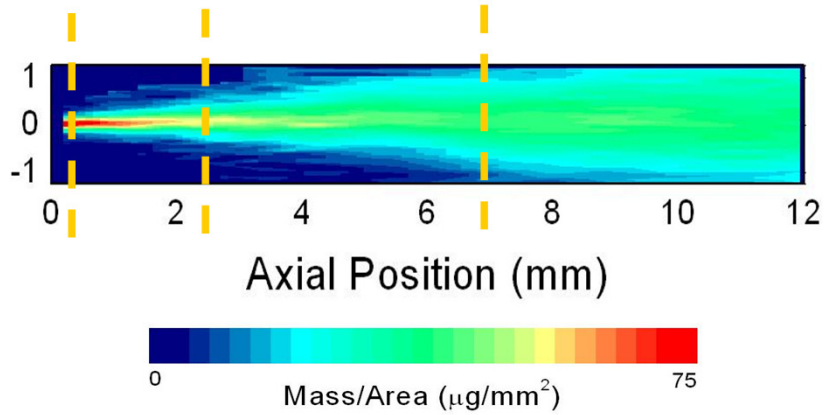
***Som et al., *Combustion and Flame* 2010**

3-D Modeling Set-up

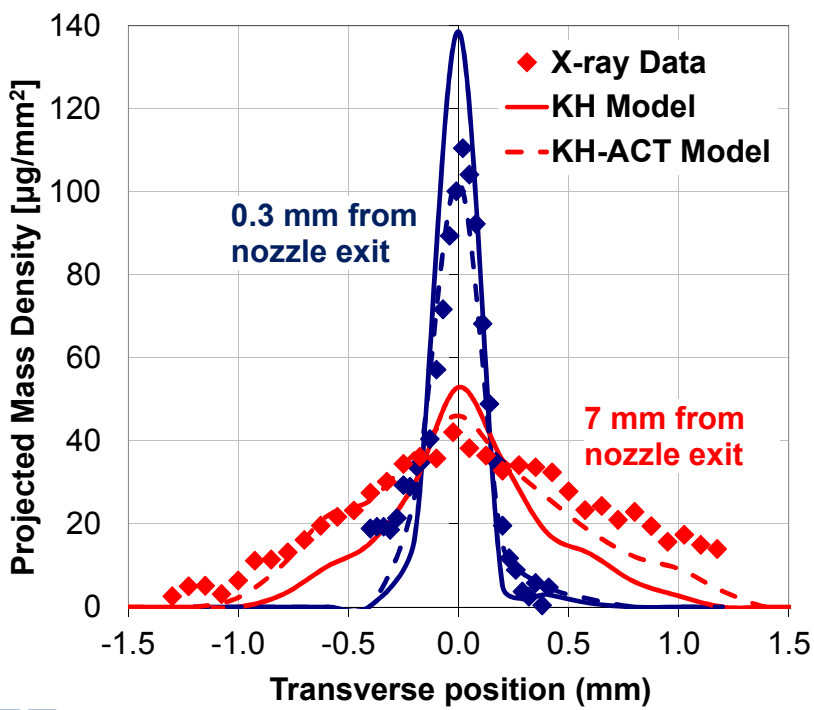
Modeling Tools	CONVERGE, FLUENT, OpenFOAM Source code access for spray and combustion modeling
Dimensionality and type of grid	3D, structured with Adaptive Mesh Resolution
Spatial discretization approach	2nd order finite volume
Smallest and largest characteristic grid size(s)	Base grid size: 2mm or 4mm Finest grid size: 0.125mm, 0.25mm Gradient based AMR on the velocity and temperature fields. Fixed embedding 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)

Spray Model Validation against X-ray Data



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

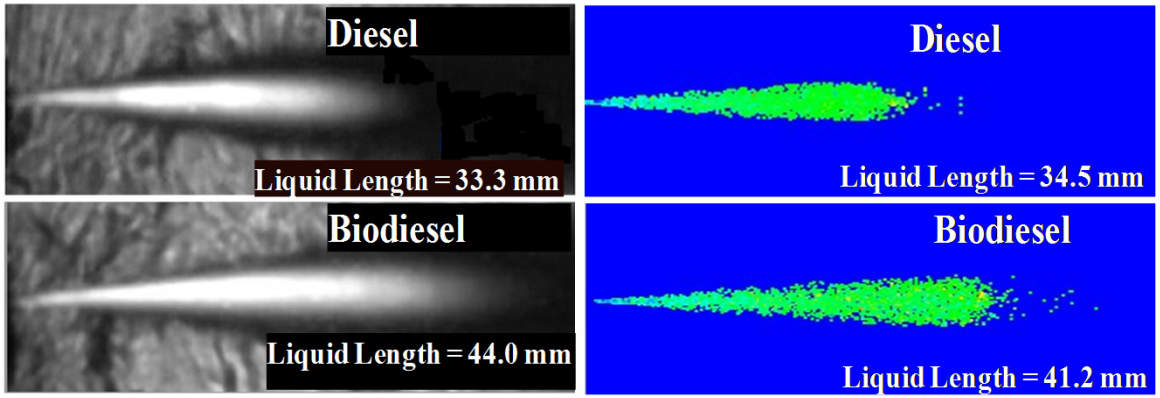


Accurate fuel distribution (equivalence ratio) is critical for reliable combustion predictions!

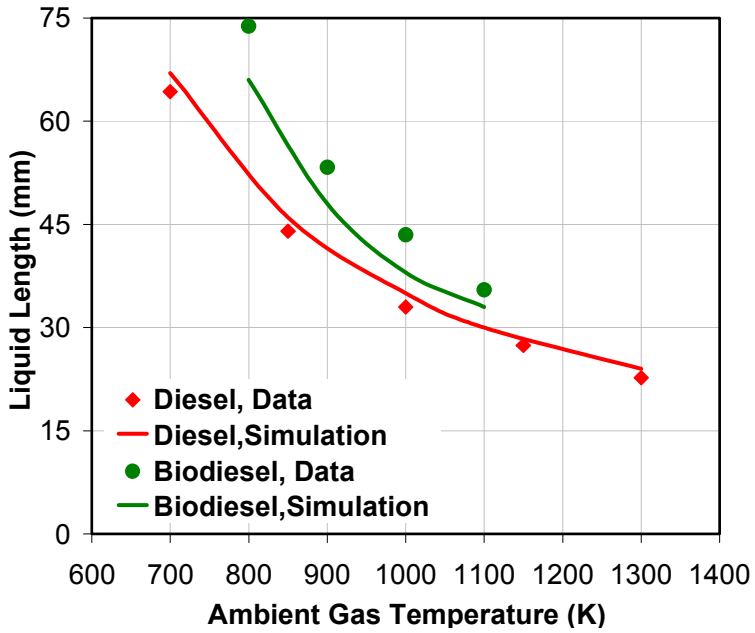
- **Optical techniques do not provide quantitative information in the near nozzle region**
- **X-ray techniques do not provide droplet size distributions in the near nozzle region**
- **All necessary boundary conditions for modeling are not available from experiments**

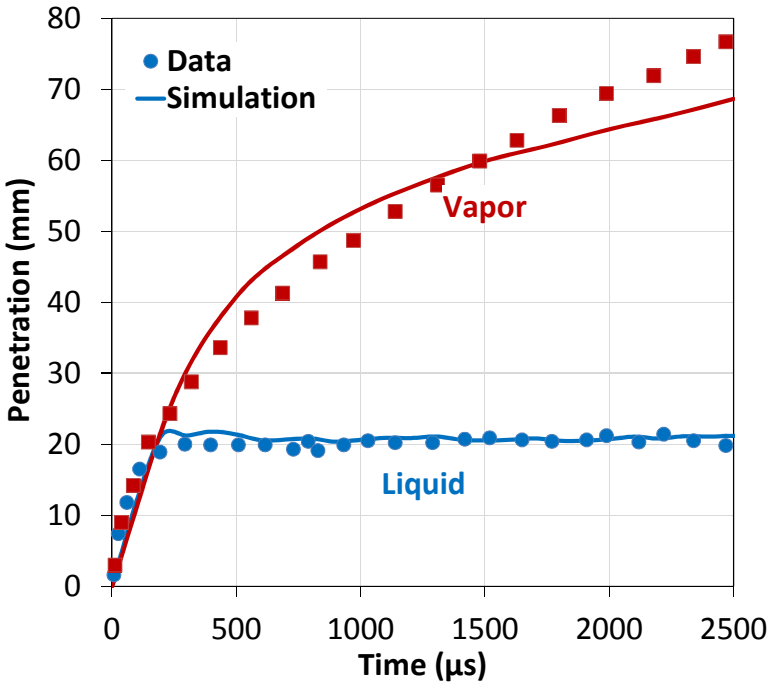
- Spray Dispersion accurately captured by only the KH-ACT model. KH model under-predicts spray spreading

Diesel vs. Biodiesel Sprays



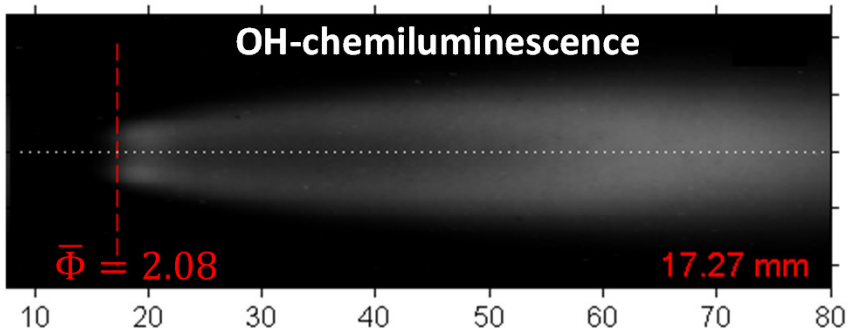
Data from Sandia Labs:
1) DL Siebers: SAE 980809
2) BS Higgins, CJ Mueller, DL Siebers: SAE 1999-01-0519

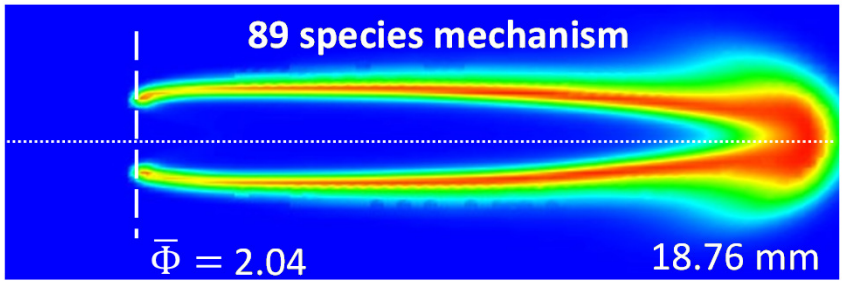




Accurate prediction of liquid length with biodiesel is challenging especially at low ambient densities

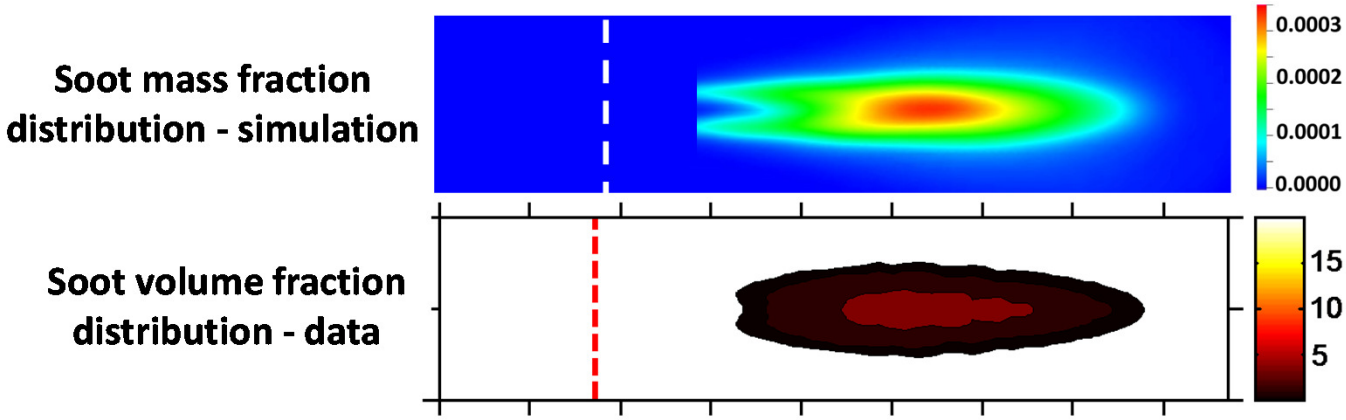
Combustion Modeling with Biodiesel





- Data from Sandia National Laboratory
- Simulations plot OH contours at a cut-plane
- 89 species mechanism (using Methyl Decanoate + Methyl Decenoate + n-heptane as a surrogate)

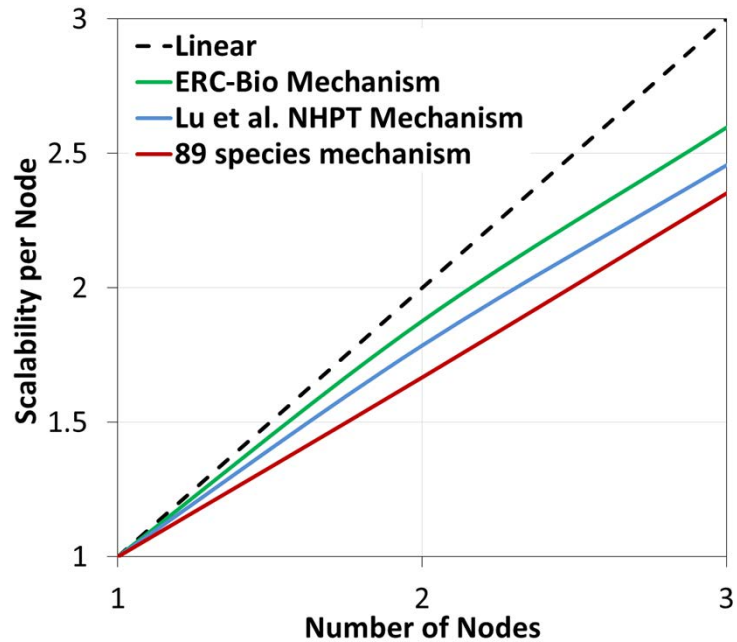
@ T = 1000 K	Ignition Delay (µs)
Sandia Data	396
89 species	391



- Need for multi-component evaporation models
- Computational cost increases massively by the use of such detailed kinetic models together with fine resolutions and LES based turbulence models employed

Computational Cost & Scalability

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

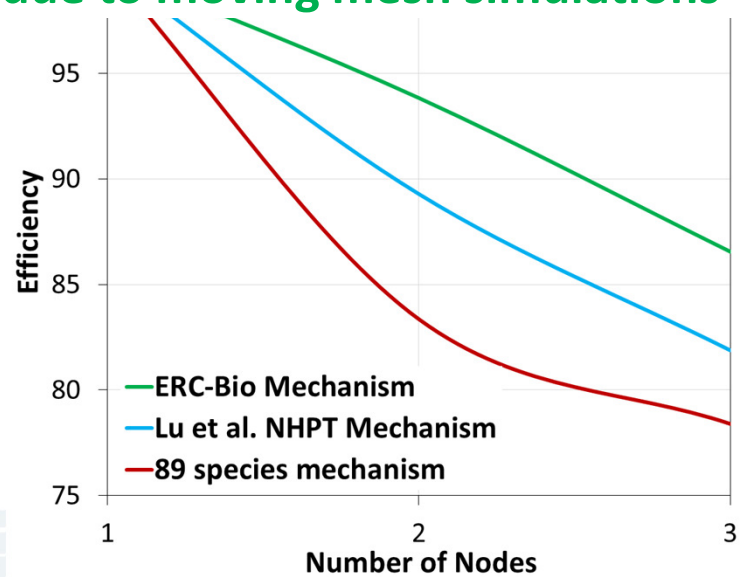


Scalability per node = T_1/T_n
Efficiency per node = $T_1 x100/nT_n$
n = Number of compute nodes

Poor scalability due to load balancing issues due to moving mesh simulations

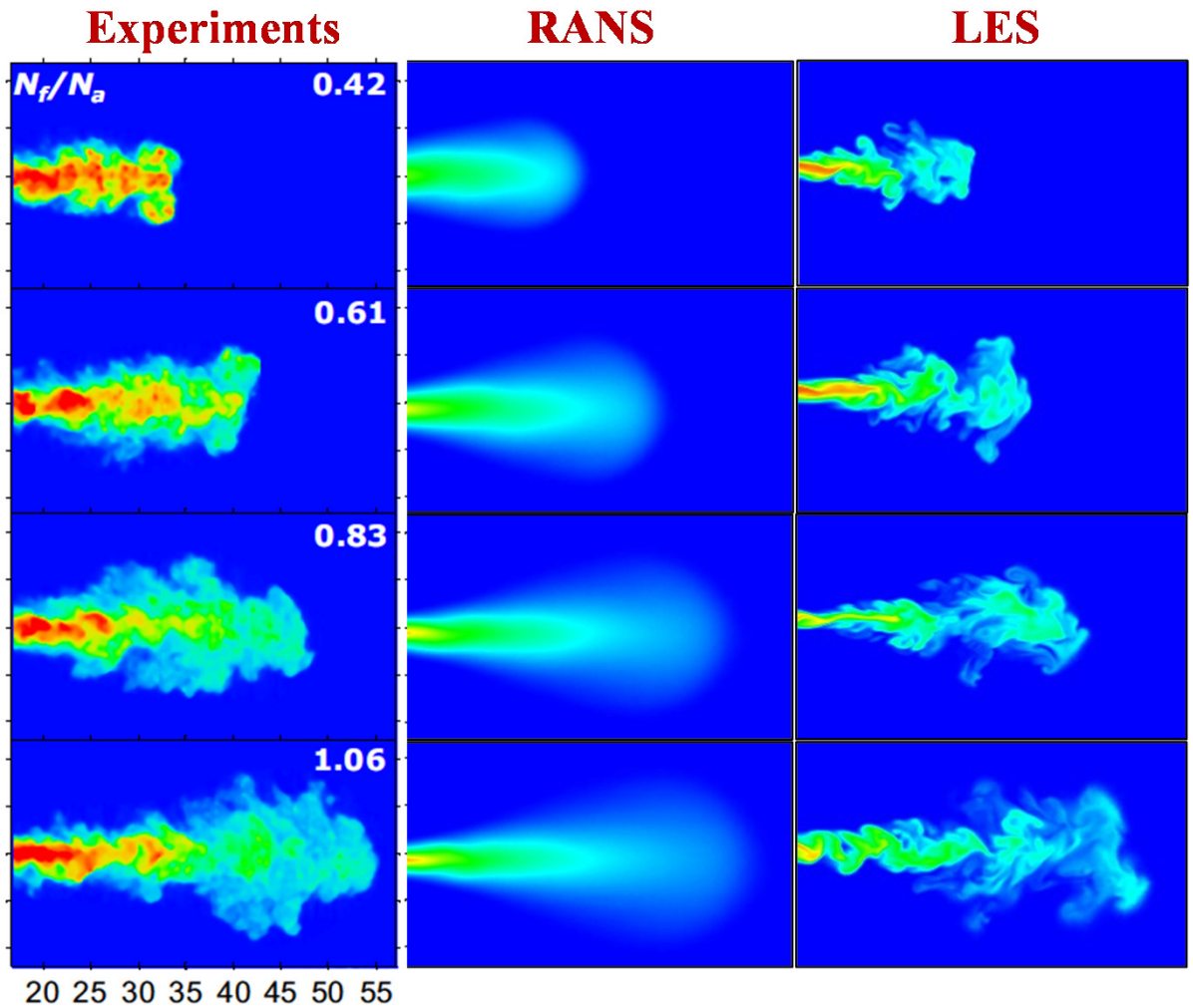
Fusion Cluster @ Argonne:

- ✓ 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



RANS vs. LES

n-heptane: T_{amb}=1000K, ρ_{amb}=14.8Kg/m^3, O_2 Concentration = 0%,
Orifice diameter = 100μm, P_{inj}=1500bar, T_{fuel}=373K

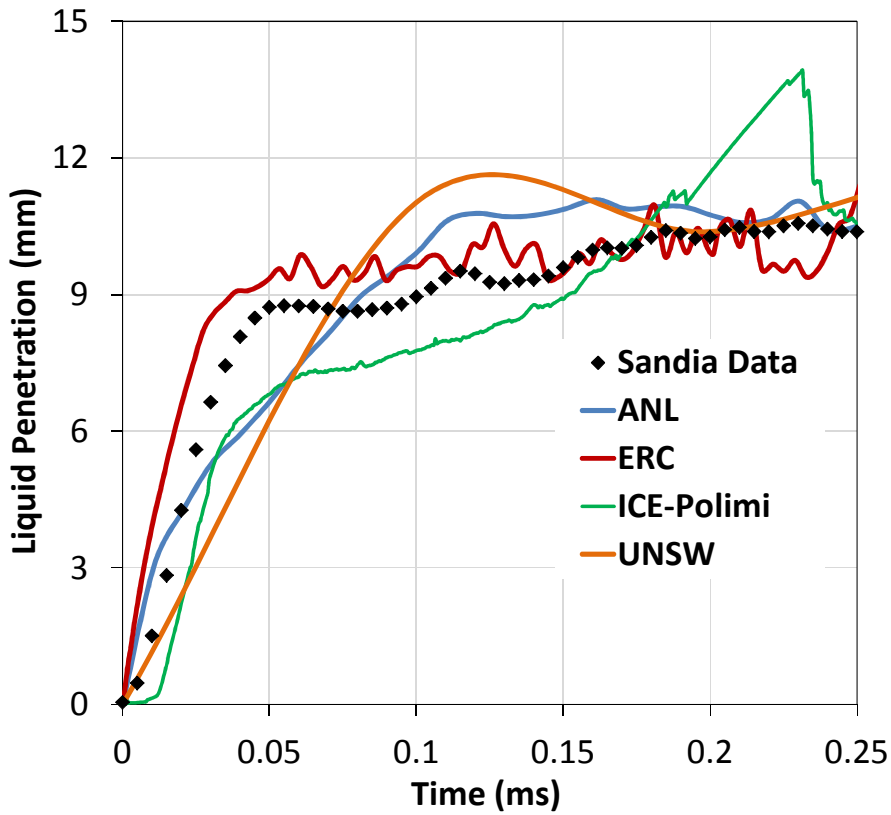


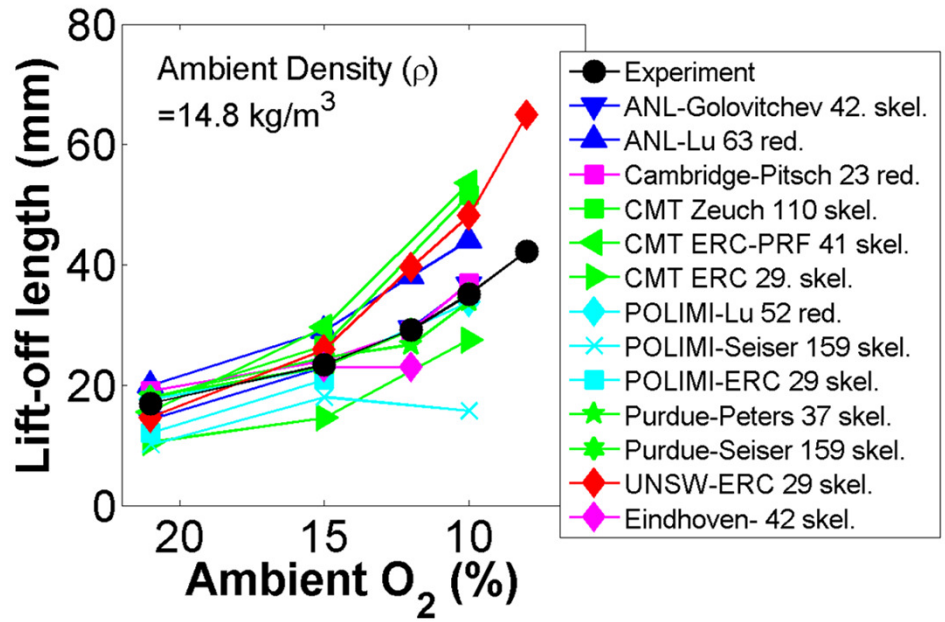
- Need for instantaneous data rather than time-averaged information. Such data is recently available from Sandia National Labs.

Engine Combustion Network Modeling Effort

	CODE	Turbulence model(s)	Grid type
ANL	CONVERGE	RNG k-ε, LES Smagorinsky	3D, structured with AMR
Cambridge	StarCD 4.1	RNG k-ε	2D, uniform
CMT	OpenFOAM	k-ε with C_{s1} round jet adjustment	2D, uniform
Eindhoven	AVBP (LES)	LES	3D, unstructured tetrahedral
ERC-UW	KIVA-3V	RNG k-ε	2D, structured
Penn. State	OpenFOAM	RNG k-ε	2D, unstructured
POLIMI	OpenFOAM	Realizable k-ε	3D, structured, with AMR
Purdue	In-house (REC)	k-ε	2D, structured
UNSW	Fluent 13.0	Realizable k-ε	2D, structured

Comparison of different CFD codes @ ECN-1





- In ECN-1, all groups could not converge upon a specific set of models. However, several parameters were quite similar between modeling approaches of different groups
- Future research will focus on ensuring same models, constants, and definitions for simulations
- In general, simulations capture global characteristics very well, however, details are often not well predicted
- Models are not able to capture the influence of parametric variations. They can capture characteristics at one ambient temperature or oxygen concentration

Thank You

Contact: ssom@anl.gov

http://www.transportation.anl.gov/engines/multi_dim_model_home.html