KH-ACT Primary Breakup Model Enabling Integrated Nozzle flow and Spray-Combustion Simulations

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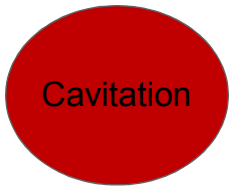
Collaborators

Ms. Anita I. Ramirez, Prof. Suresh K. Aggarwal at **University of Illinois at Chicago**

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

Introduction

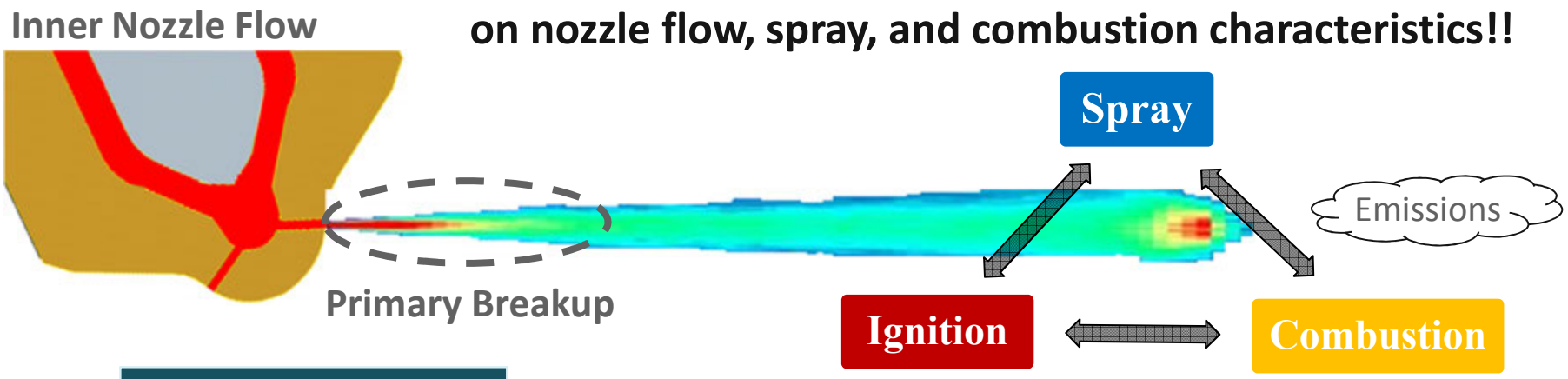
- High-speed fuel injection in Diesel engine combustion chambers represents one of the most challenging and hence most extensively studied multiphase flow phenomena.
- A fundamental understanding of the breakup and atomization of the fuel jet is essential for enhancing the engine combustion efficiency and emission characteristics.
- Fuel breakup in the region near the injector nozzle plays a central role in combustion and emission processes, and is governed by primary breakup mechanism caused by:



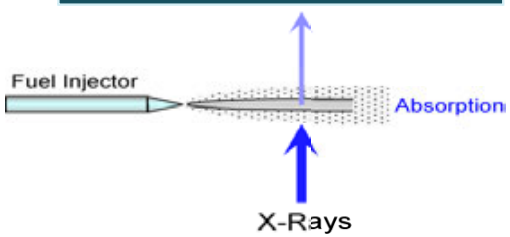
- Current spray models only account for aerodynamic breakup and are developed based on optical data which has inherent limitations in providing quantitative data in the primary breakup region.
- Robust validation of spray breakup models necessary to use it as a predictive tool

Integrated Modeling Approach

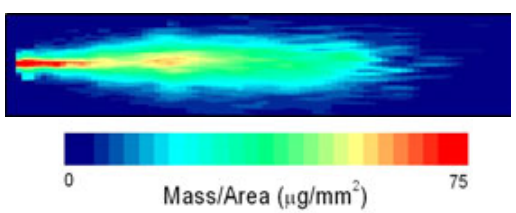
Influence of <u>fuel properties and nozzle orifice geometry</u> on nozzle flow, spray, and combustion characteristics!!



X-Ray Radiography



Number of x-rays absorbed indicates the quantity of fuel.



- Kelvin-Helmholtz Aerodynamic Cavitation Turbulence Induced **(KH-ACT)** primary breakup model: Aerodynamics, Cavitation, Turbulence
  - Detailed inner-nozzle flow modeling with realistic fuel properties
  - Spray Validation

    X-ray radiography data provides information in the near nozzle region
  - Validation against constant volume combustion data from Sandia: Liquid length, vapor penetration, lift-off length etc.

Objectives

- Develop and implement a primary breakup model incorporating:
  - Inner nozzle flow effects like cavitation and turbulence
  - Aerodynamic effects outside the injector
- Perform static-coupling of inner nozzle flow and spray simulations:
  - Provide boundary conditions for turbulence and cavitation levels in addition to discharge coefficient and flow properties etc.
- Extensive validation:
  - X-ray radiography data from Argonne National Laboratory in the near nozzle primary breakup region
  - Validation against data from Sandia National Laboratory http://www.sandia.gov/ecn/workshop/ECN1.php
- Parametric studies:
  - Influence of Nozzle orifice conicity (K_{factor})
  - Influence of Fuel properties (Diesel vs. Biodiesel)

Modeling Set-up

CONVERGE
FLUENT
KH-ACT Primary breakup Model

Spray-Combustion 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	2nd order finite volume
Smallest and largest characteristic grid size(s)	Base grid size: 2mm Finest grid size: 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	550K-650K for 0.25mm – RANS simulations
Parallelizability	Good scalability up to 48 processors

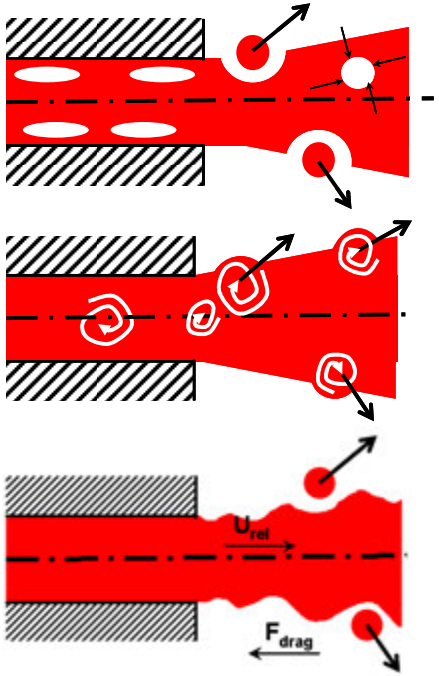
Turbulence and scalar transport model(s)	RNG k-ε
Spray models	Breakup: KH-RT with breakup length concept Collision model: NTC, O'Rourke Coalescence model: Post Collision outcomes Drag-law: Dynamic model
Time step	Variable based on spray, evaporation, combustion processes
Turbulence-chemistry interactions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

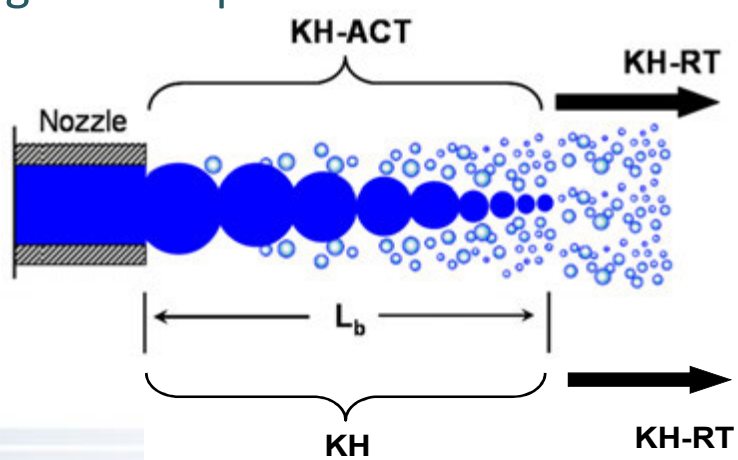
* Senecal et al., SAE 2007-01-0159; Som ,PhD. Thesis 2009

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
- Recent implementation: KH, RT, Cavitation, turbulence induced breakup models compete against each other at the nozzle exit => No ad-hoc breakup length concept





*Som et al., SAE 2009-01-0838
Som and Aggarwal, Combustion and Flame 2010

Primary Breakup Model: KH-ACT Model

Characteristic time scale due to cavitation is assumed to be the smaller of bubble collapse time and bubble burst time:

$$\tau_{CAV} = \min\left(\tau_{Collapse} : \tau_{Burst}\right)$$

Effective radius of an equivalent bubble from the nozzle calculated as: (L_{CAV})

$$R_{CAV} = r_{hole}\sqrt{\left(1 - C_a\right)}$$

Length and time scale for turbulence induced breakup :

$$K(t) = \left\{ \frac{\left(K_0\right)^{C_\varepsilon}}{K_0\left(1 + C_\mu - C_\mu C_\varepsilon\right) + \varepsilon_0 t\left(C_\varepsilon - 1\right)} \right\}^{1/(1-C_\varepsilon)}$$

$$\varepsilon(t) = \varepsilon_0 \left\{ \frac{K(t)}{K_0} \right\}^{C_\varepsilon}$$

Obtained from KH model

$$\frac{L_A}{\tau_A} = \max\left\{ \frac{L_{KH}}{\tau_{KH}} ; \frac{L_{CAV}}{\tau_{CAV}} ; \frac{L_T(t)}{\tau_T(t)} \right\}$$

Due to breakup the radius of the parent droplet 'r' decreases continuously with time according to:

$$\frac{dr}{dt} = -C_{T,CAV} \frac{L_A}{\tau_A}$$

Model constant

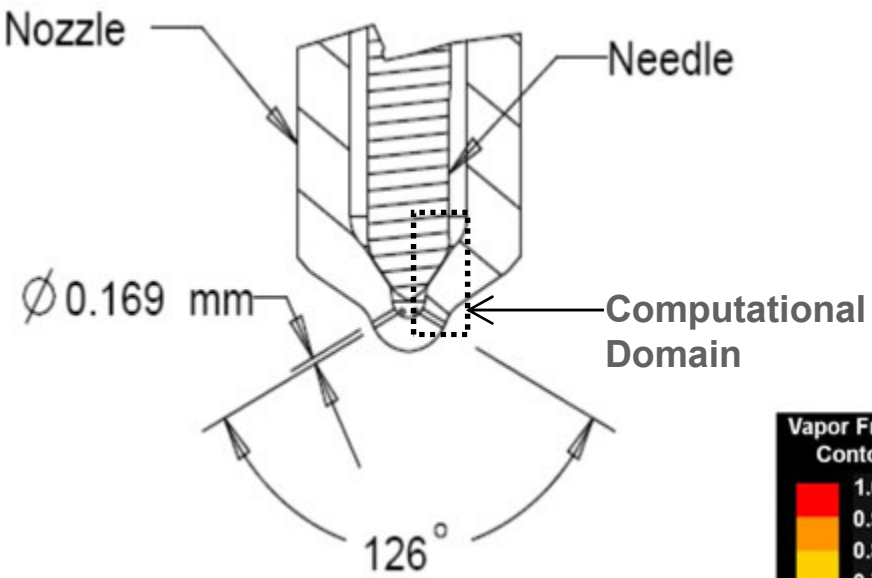
K_0, ε_0, C_a are obtained from nozzle flow modeling

Further information available*:

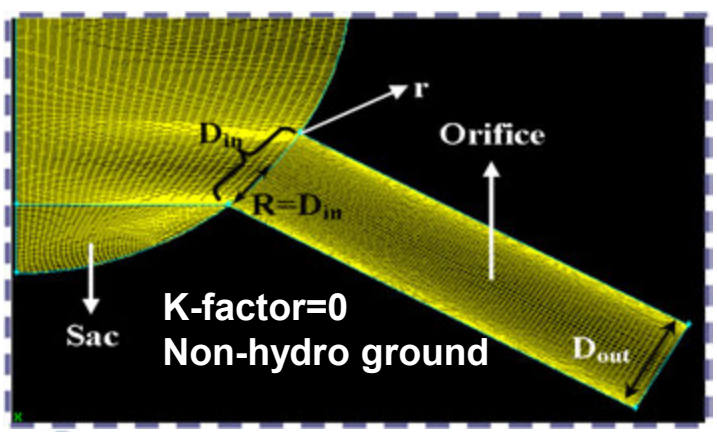
1) **S. Som, Ph.D thesis – University of Illinois at Chicago, 2009**
2) **S. Som, et al. Combustion and Flame (157), 2010**
3) **S. Som, et al. *Fuel (90)*, 2011**

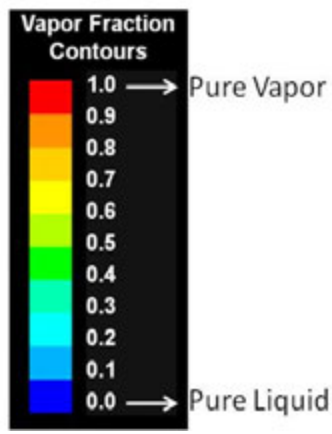
Injector Geometry and 3D Grid Generated: FLUENT

6-hole production Injector

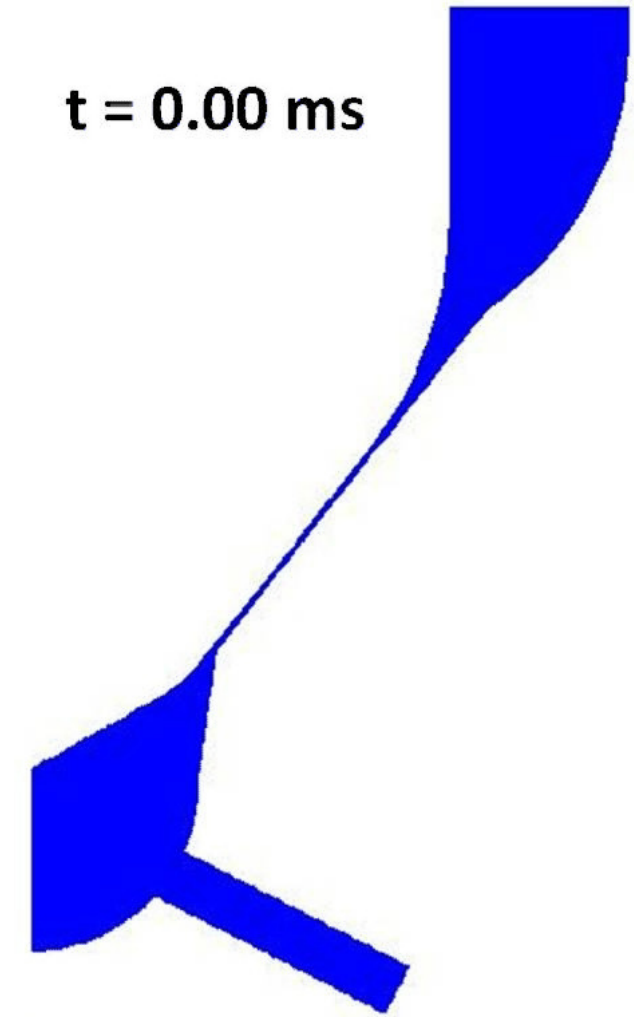


Nozzle Orifice





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

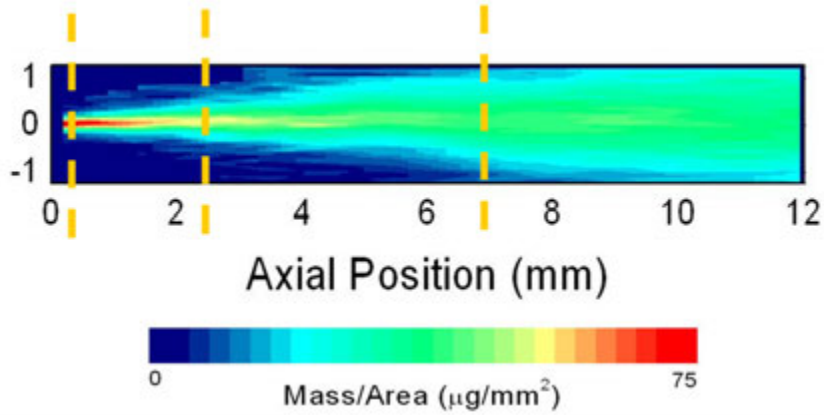


*Som et al., *FUEL* (2010)
Som et al., *JEGTP* (2010)

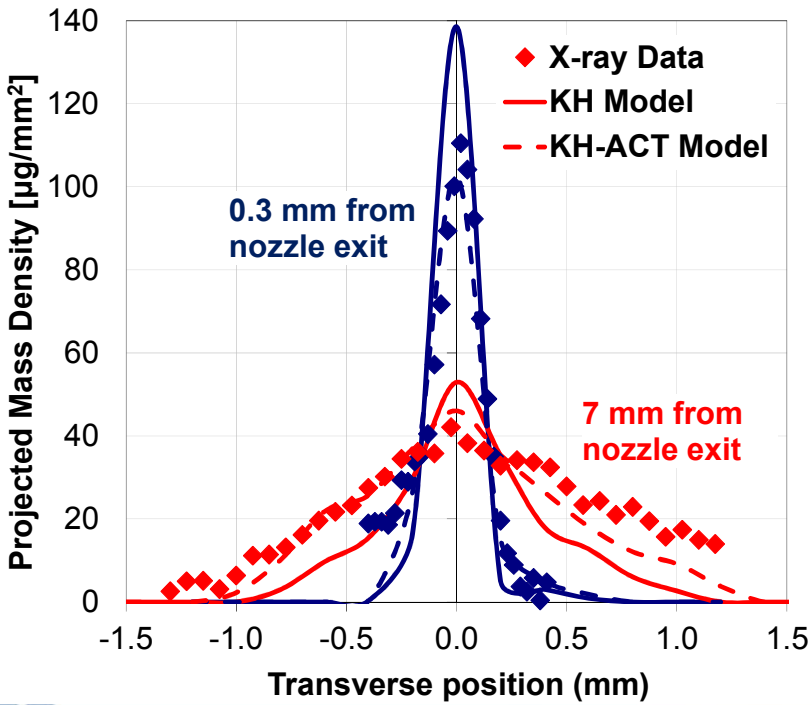
Extensive Validation

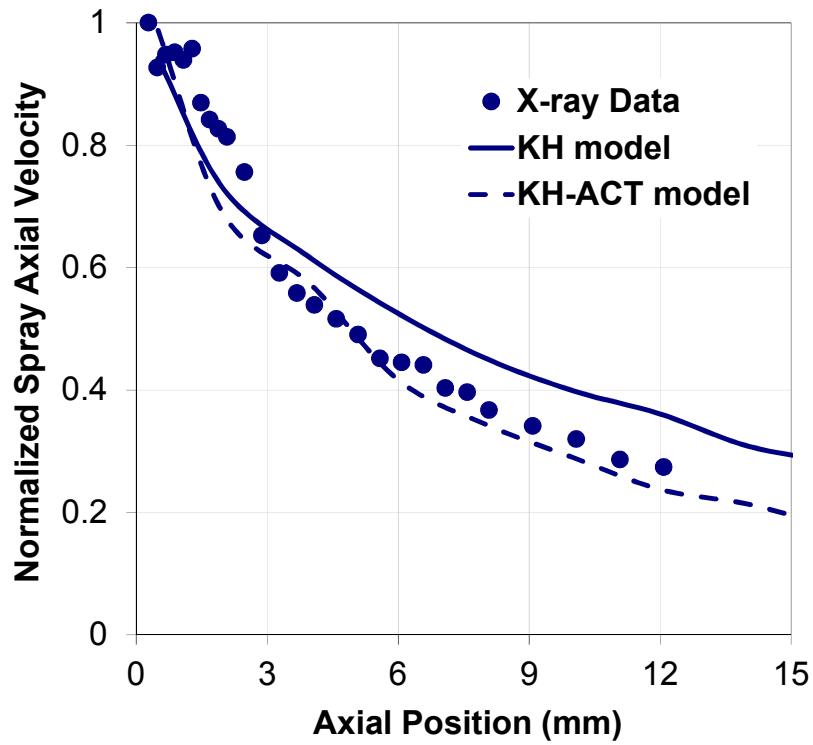
X-ray radiography data: Argonne
Optical Data: Sandia

Spray Validation against X-ray Data - 1



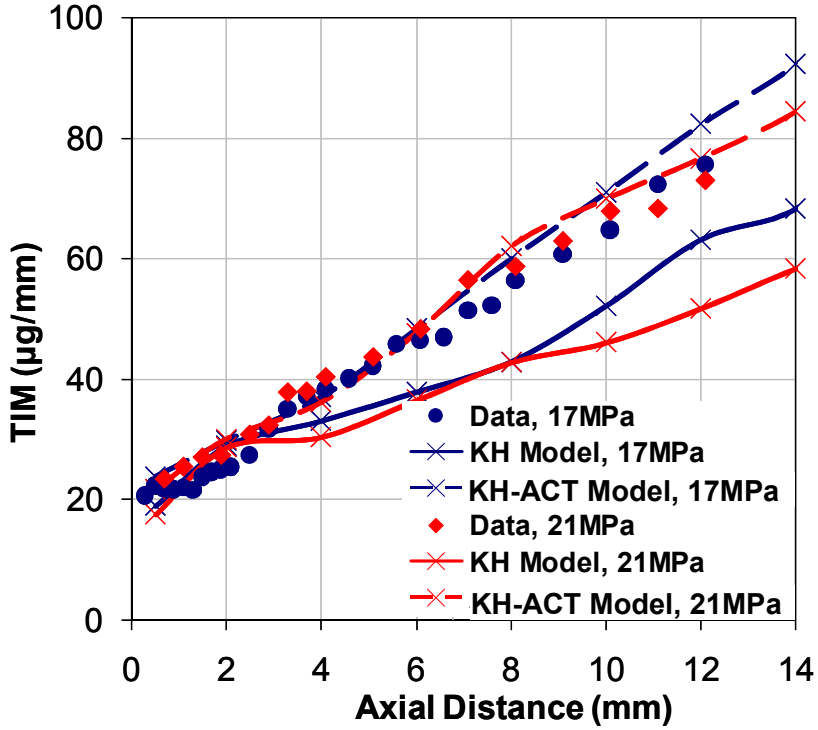
X-ray radiography Data: Ramirez et al., JEF 2009



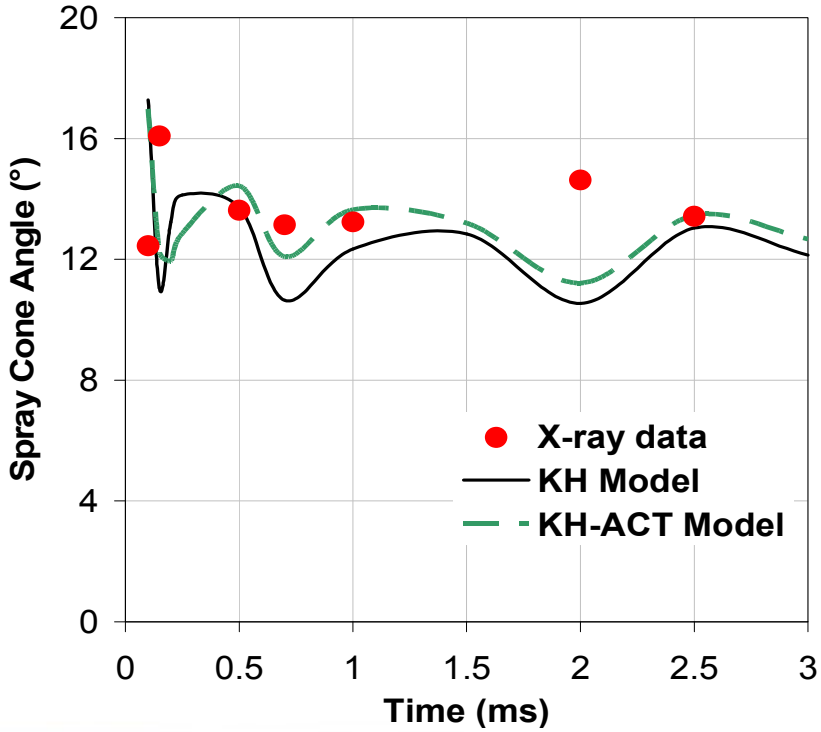


- The spray loses half of its initial velocity within the first 6 mm
- Simulation capture the Gaussian mass distributions from x-ray data well
- Spray Dispersion accurately captured by only the KH-ACT model. KH model under-predicts spray spreading

Spray Validation against X-ray Data - 2

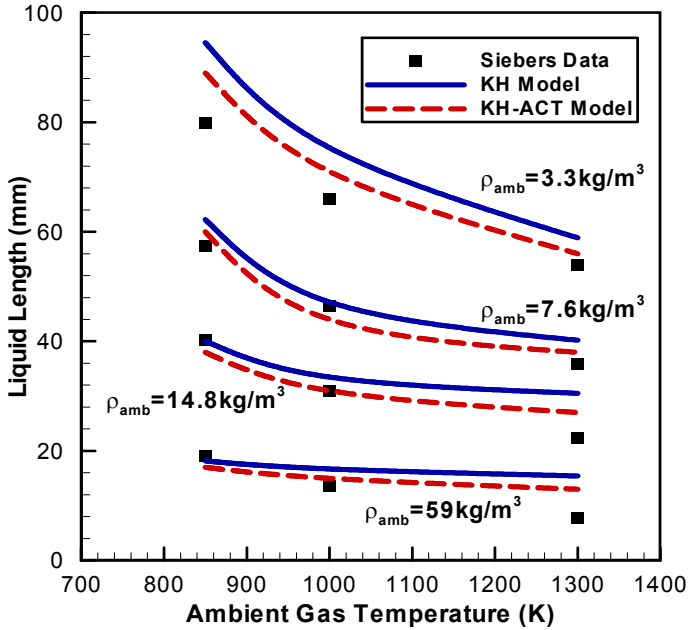


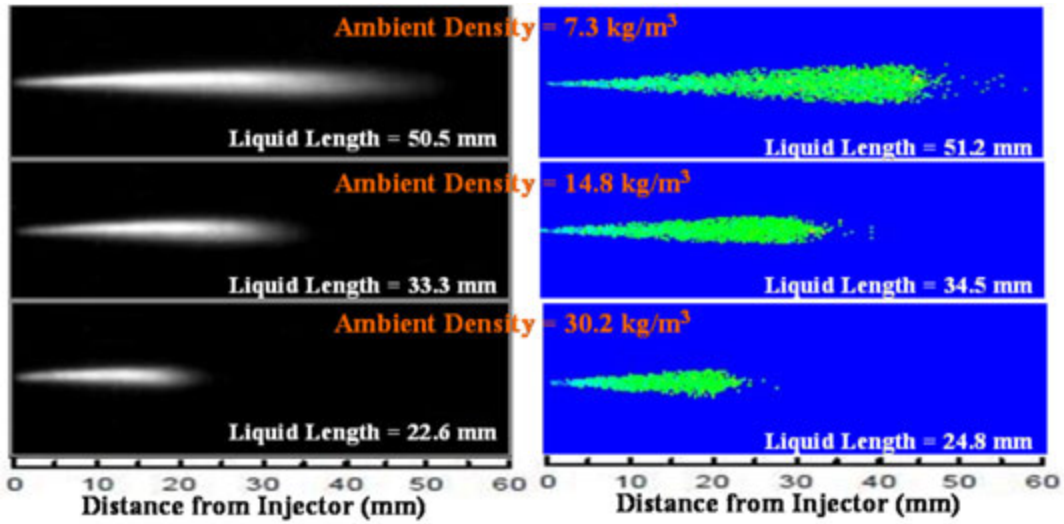
- Transverse Integrated Mass (TIM) is calculated by integrating the area under the spray transverse mass distribution plots
- TIM gives mass per unit length at any axial location

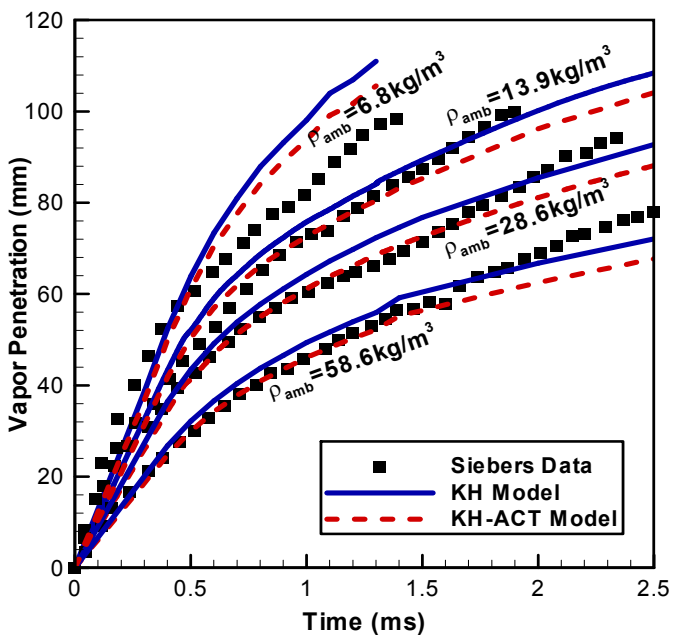


- Spray cone angle calculated at 4mm based on the extent of spreading of droplets
- KH-ACT model predicts higher spray cone angle which is consistent with earlier results where spreading was higher

Validation against Evaporating Spray Data





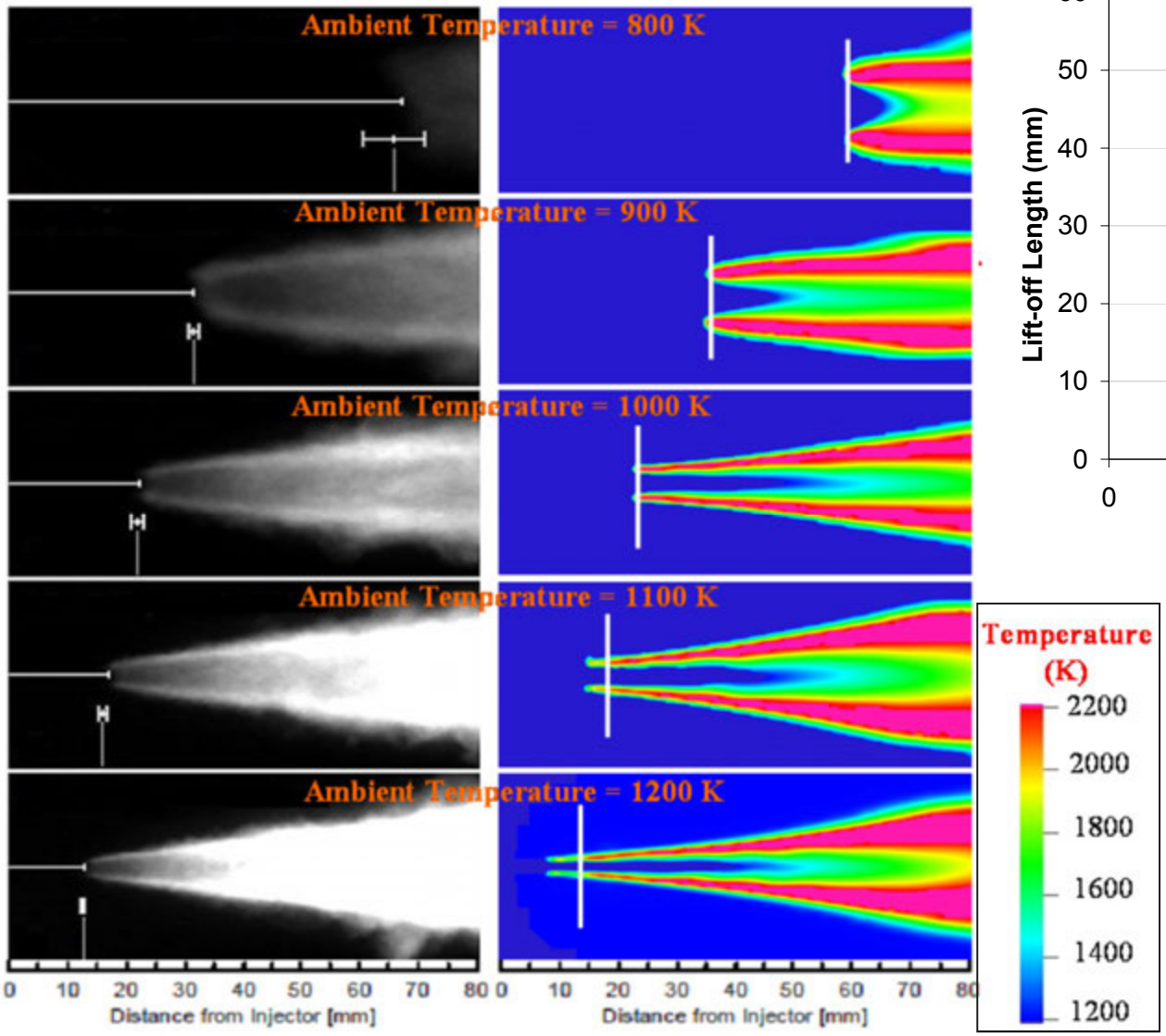


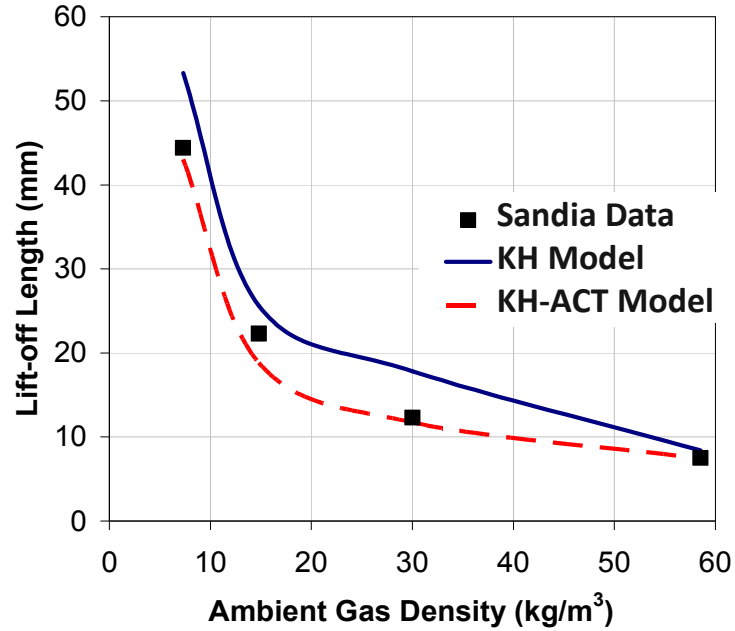
- KH-ACT model performs better than the KH model in predicting constant-volume combustion data
- Lower liquid length with KH-ACT model is due to enhanced breakup predicted by the model
- Vapor penetration marginally better predicted by the KH-ACT model

Data from:

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

Validation against Combusting Spray Data





Data from:
Siebers and co-workers
2001-01-0918, 2001-01-0530

N-heptane mechanism: 42 species, 168 reactions (**Lu et al.**): Combustion and Flame 2009.

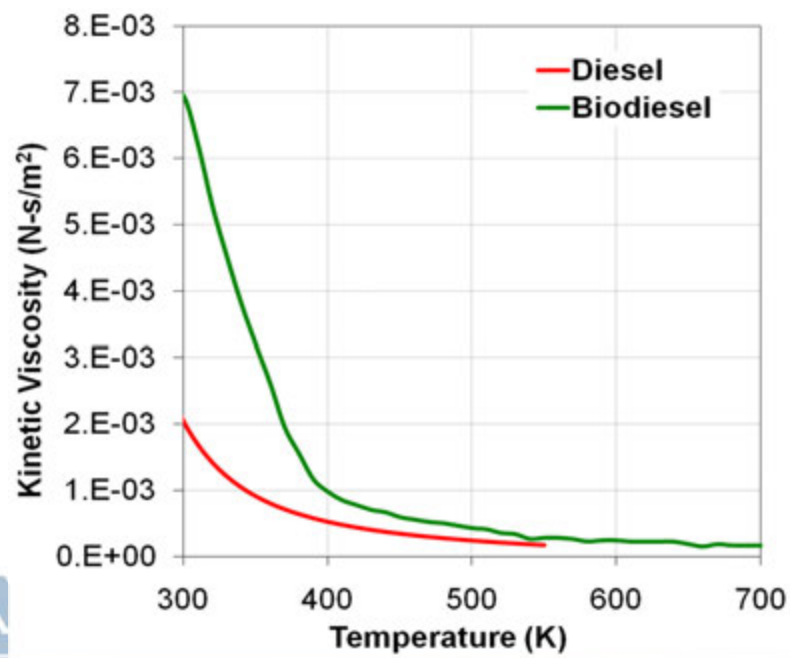
Parametric Study

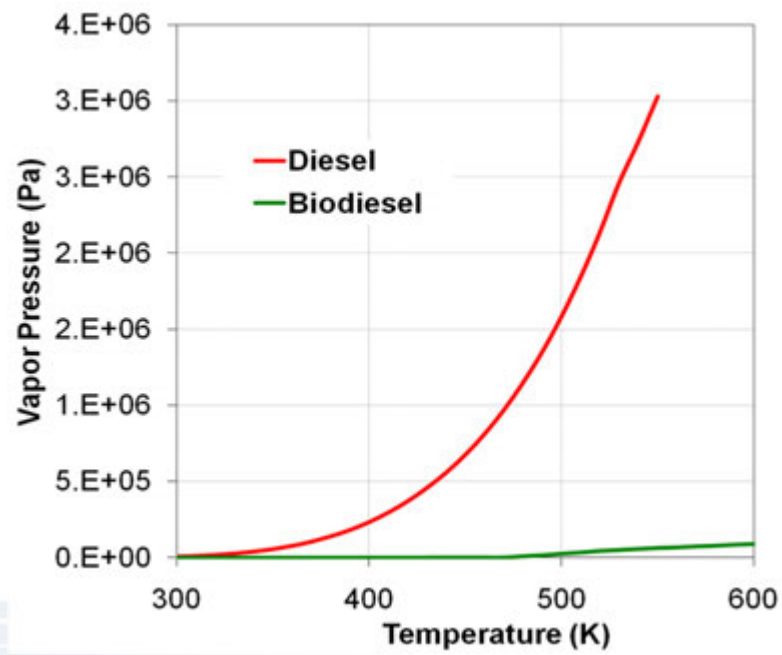
Effect of Fuel Properties
Effect of nozzle orifice Geometry

Differences in Fuel Properties*

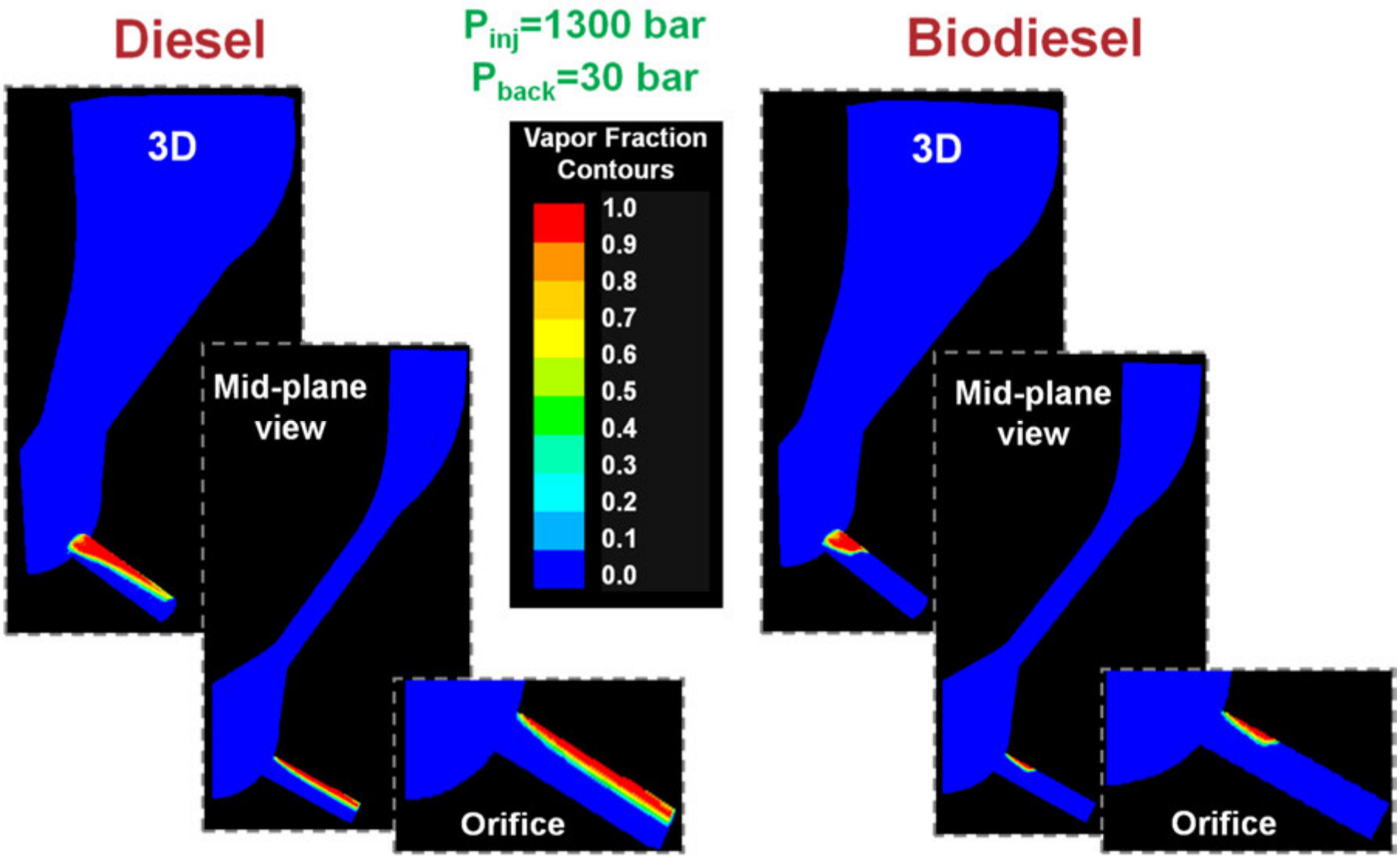
Fuel Property	Diesel	Biodiesel (SME)
Carbon Content [wt %]	87	76.74
Hydrogen Content [wt %]	13	12.01
Oxygen Content [wt %]	0	11.25
Density @ 15°C (kg/m3)	**820**	**877.2**
Surface Tension @ 25°C (N/m)	**0.020**	**0.0296**
Heat of Combustion (MJ/Kg)	**42.0**	**37.4**
Heat of Vaporization (KJ/Kg)	**361.0**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

*S. Som et al., FUEL 2010



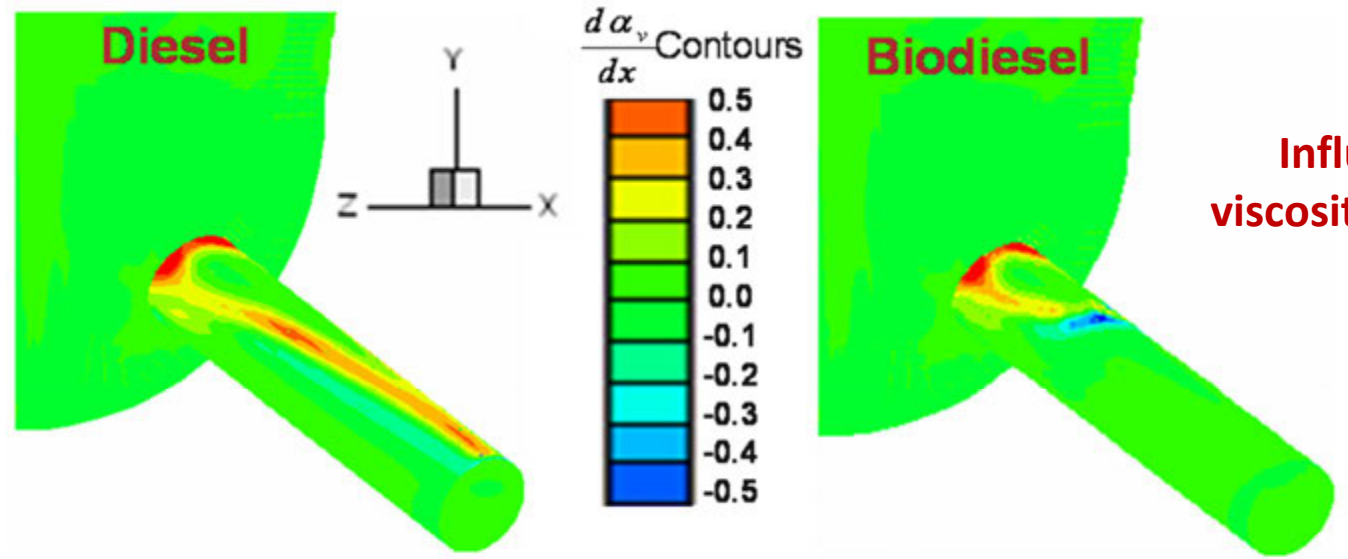


Vapor Distribution

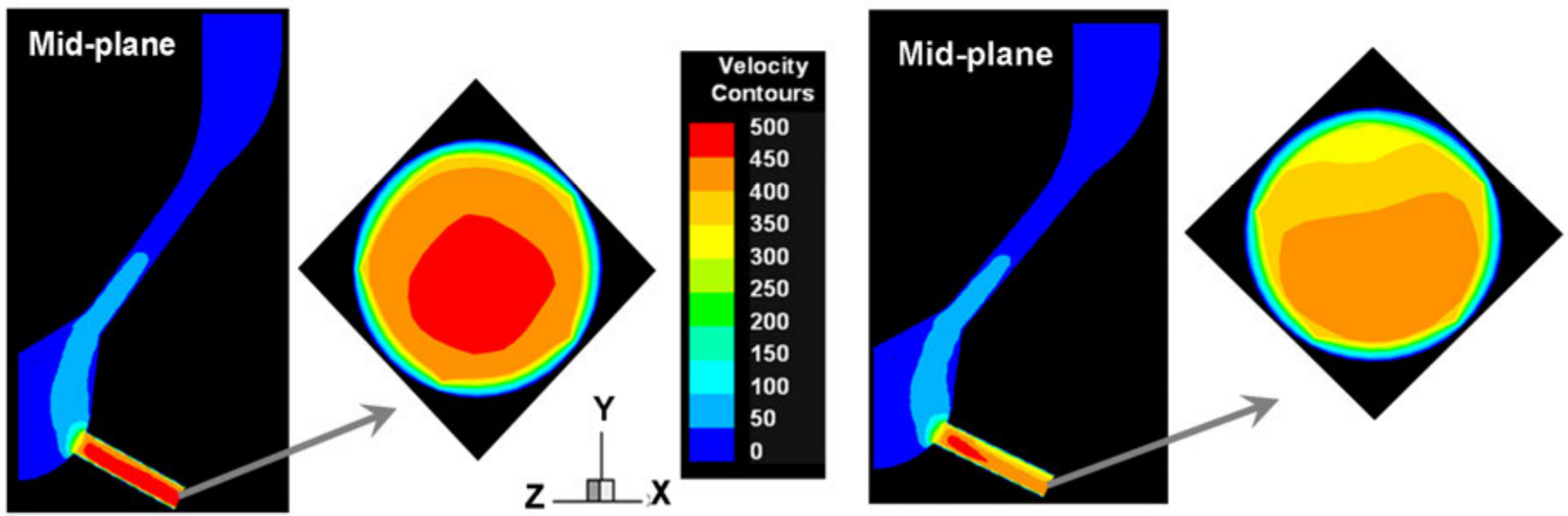


Results at full needle open position

Vapor Volume Fraction & Velocity Distribution

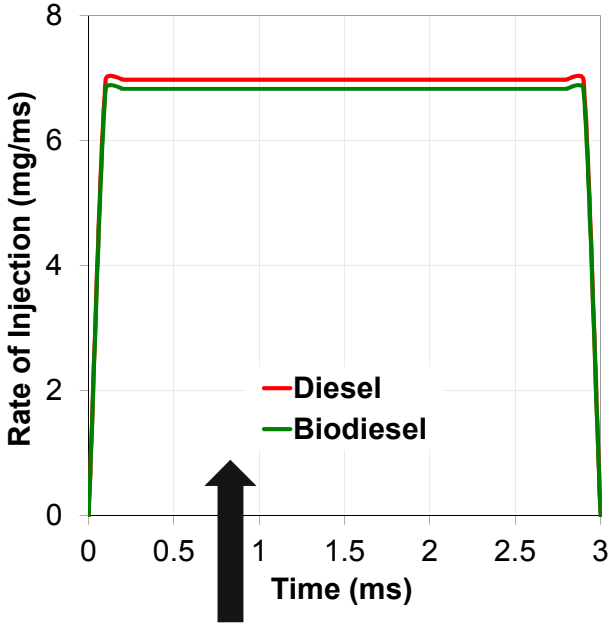


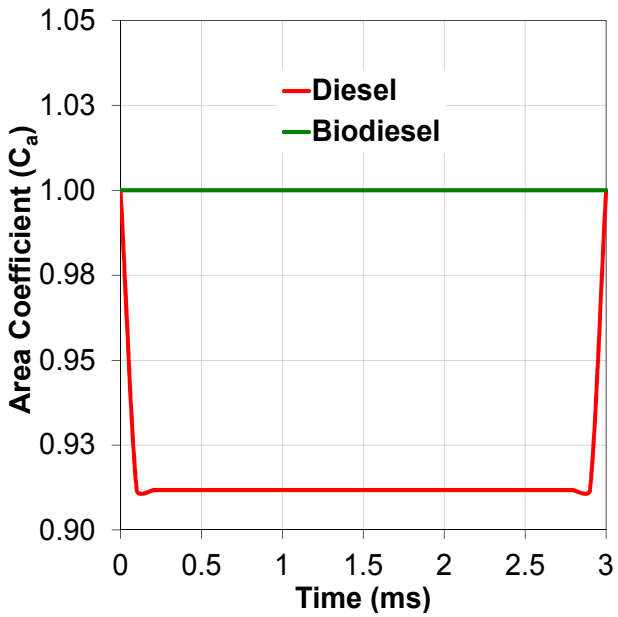
Influenced by density, viscosity, and vapor pressure

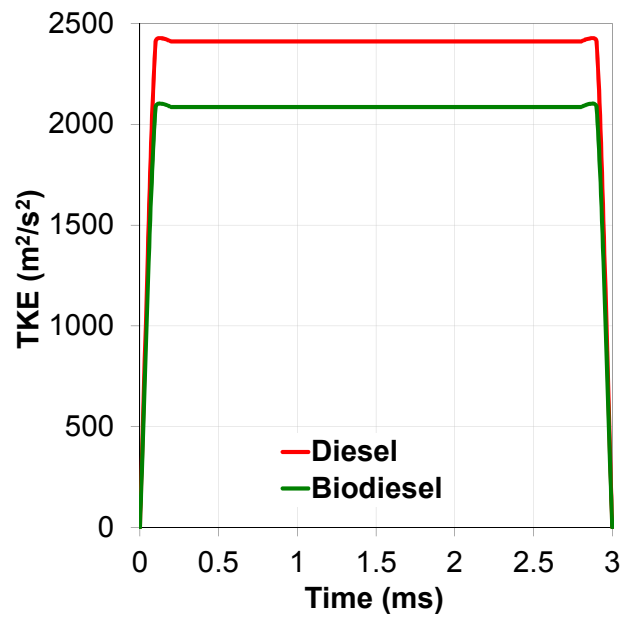


Static Coupling Strategy

Boundary condition for KH-ACT model





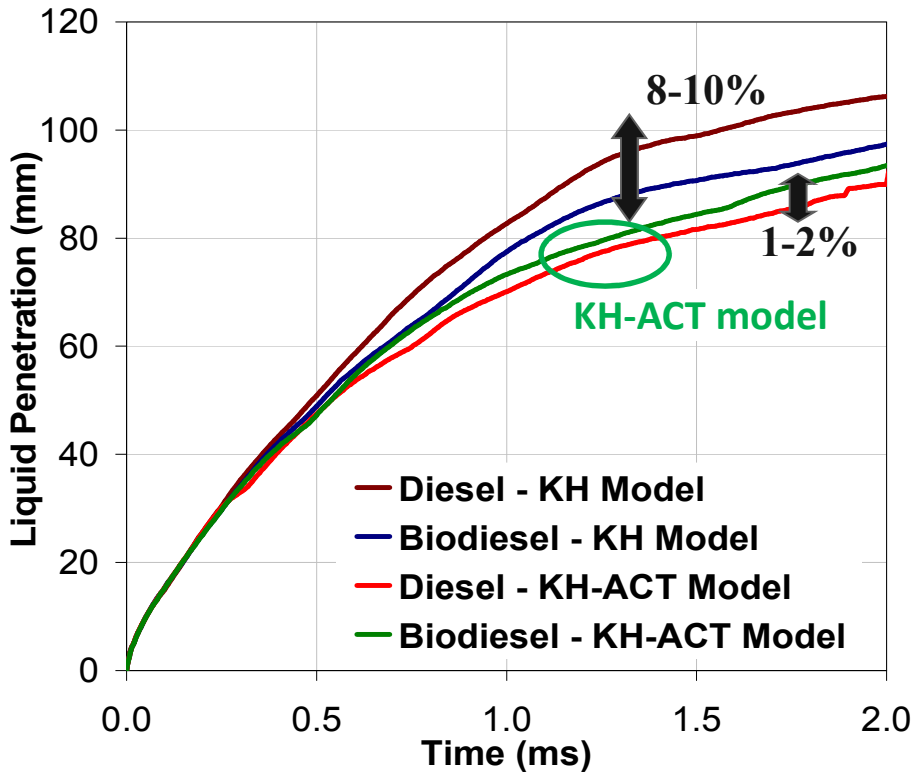


Boundary condition for KH model

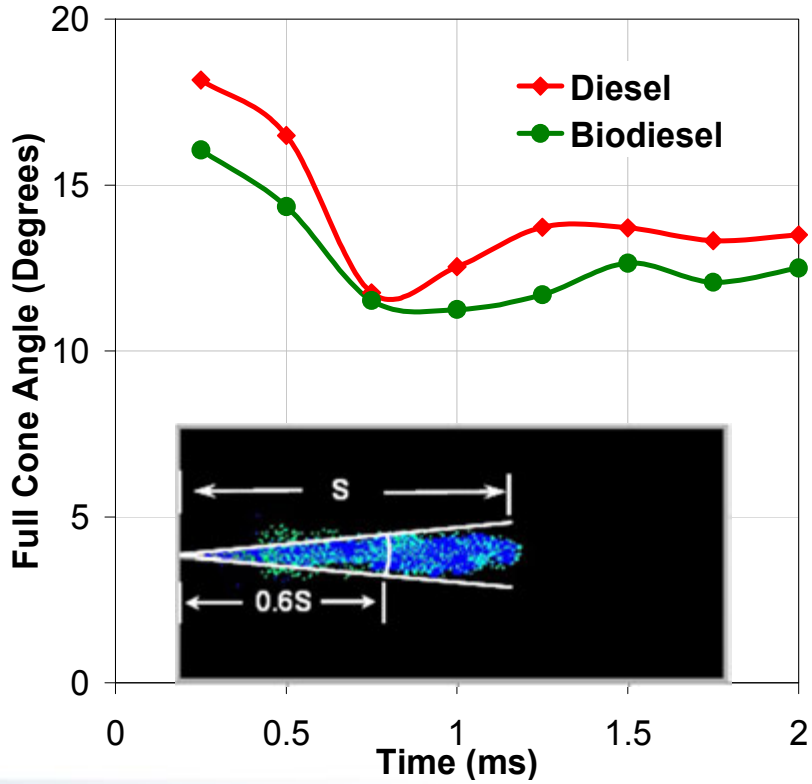
1) S Som et al. SAE 2009-01-0838
2) Ramirez et al. JEF 2009
3) Som and Aggarwal, Combustion and Flame 2010

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

Spray Penetration & Cone-angle

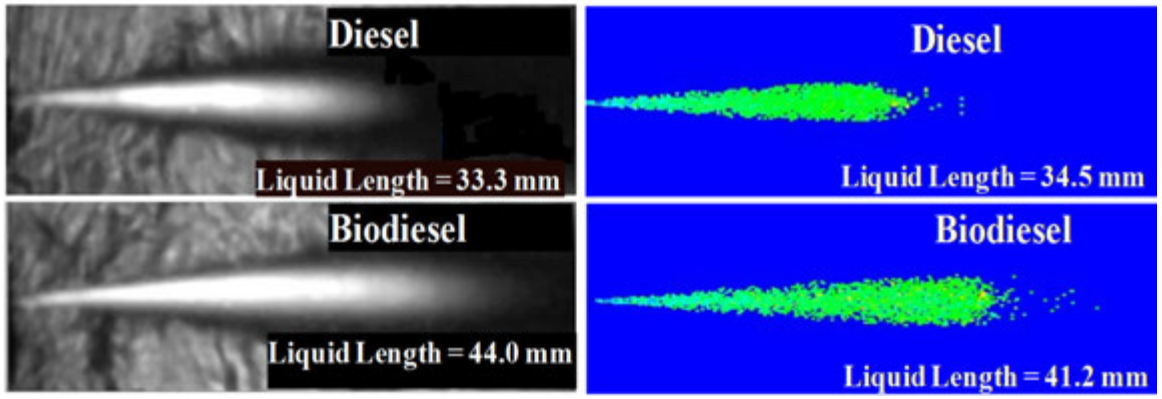


- Experimental trend: Biodiesel penetrates more than diesel
- KH-ACT model accurately captures the experimental trend i.e., biodiesel penetrates marginally more than Diesel



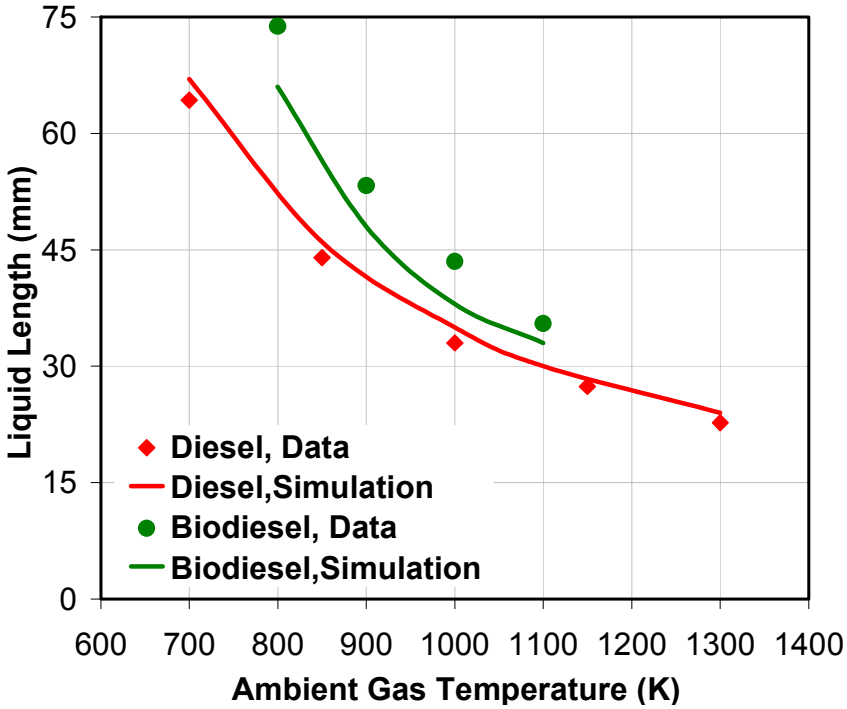
- Spray dispersion is lower for biodiesel in the far field region
- Poorer atomization characteristics for biodiesel due to its higher viscosity, surface tension, lower cavitation and turbulence

Evaporating Sprays: Liquid Length

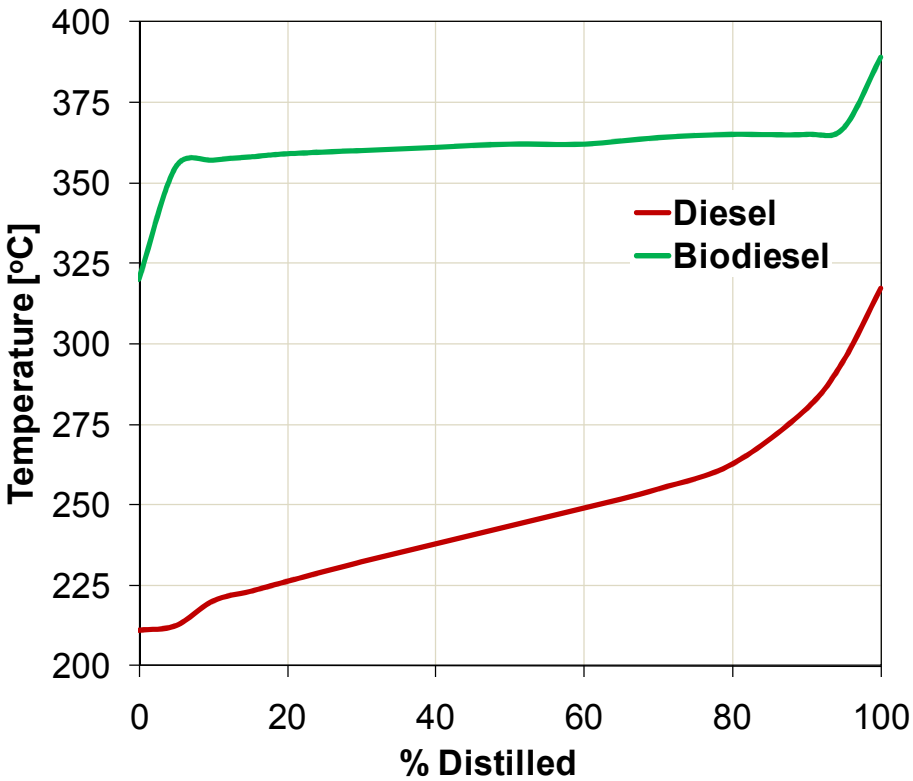


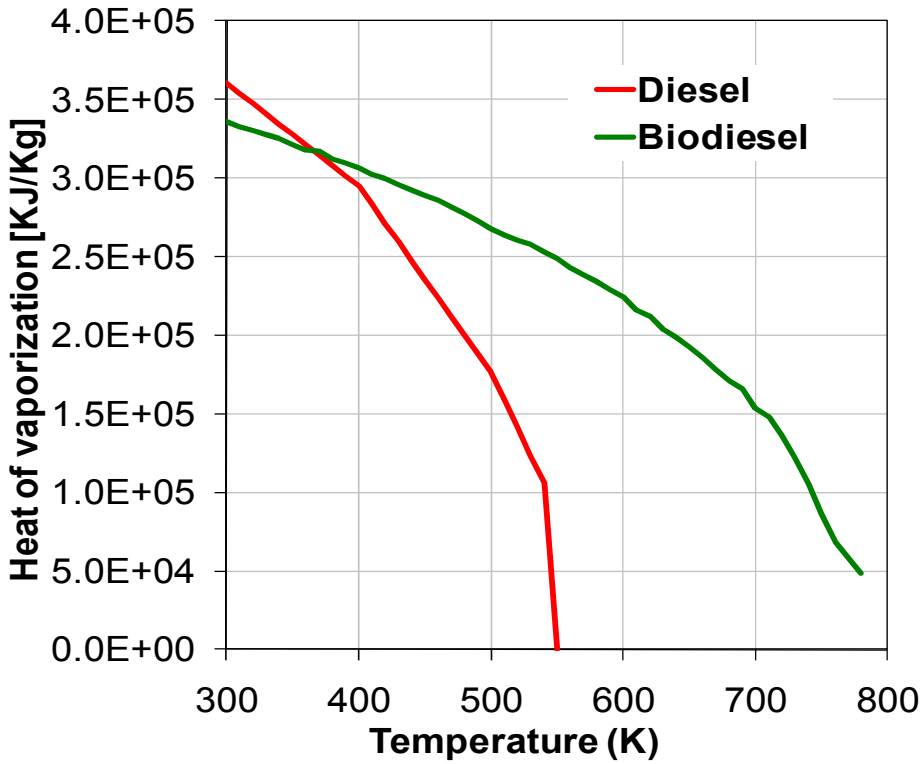
Data from:
1) DL Siebers: SAE 980809
2) BS Higgins, CJ Mueller, DL Siebers: SAE 1999-01-0519

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?





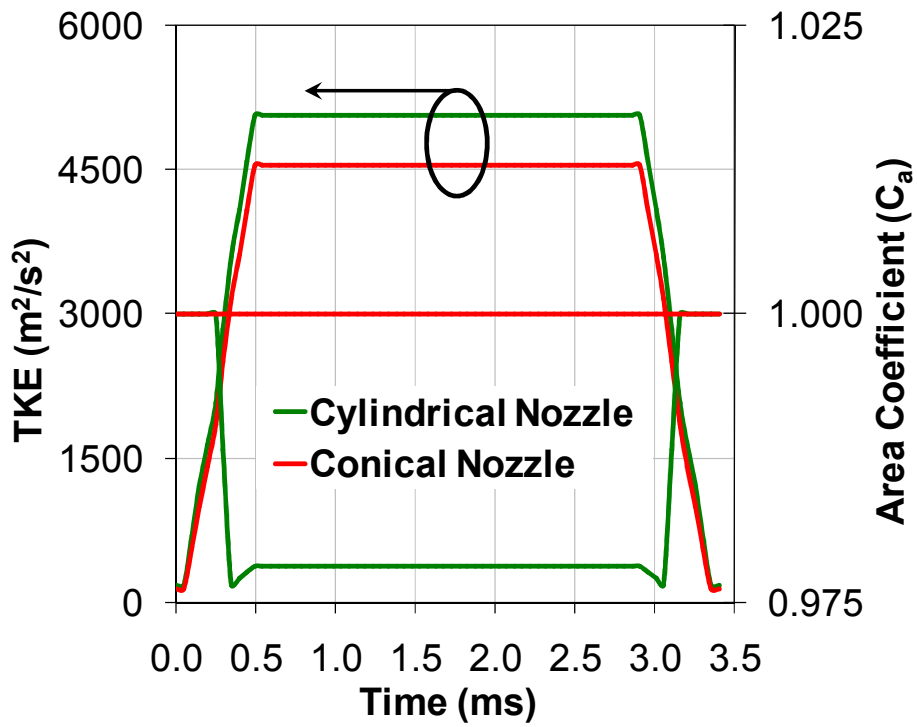
Slower breakup for biodiesel* is due to lesser amount of inner nozzle turbulence and cavitation. This results is increased spray penetration and reduction in spray cone-angle!

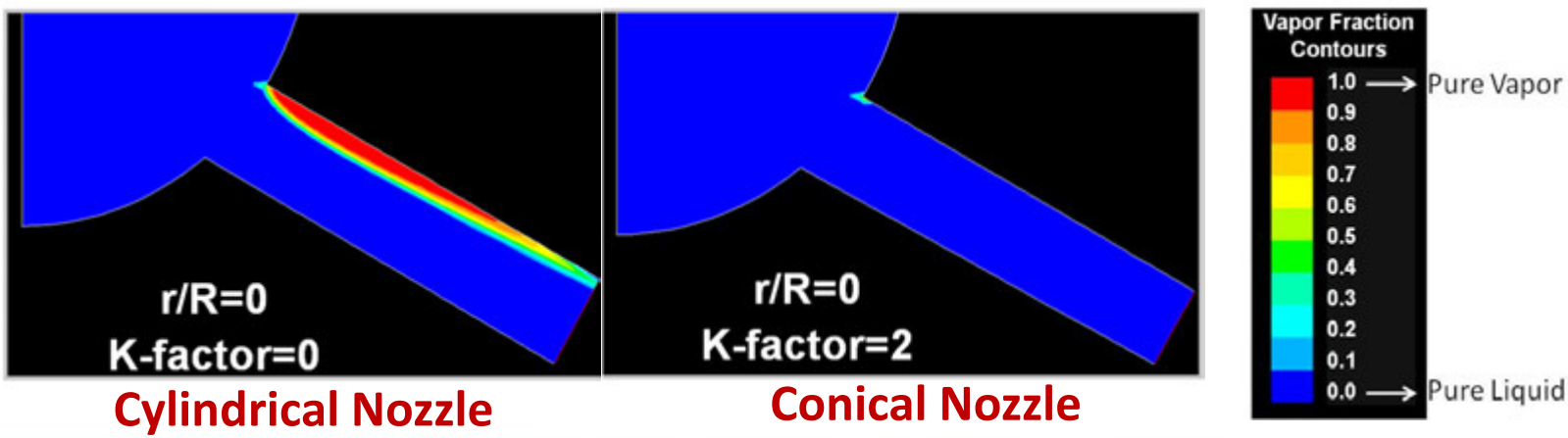
*S Som, DE Longman, AI Ramirez, SK Aggarwal. *FUEL* 2011

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

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

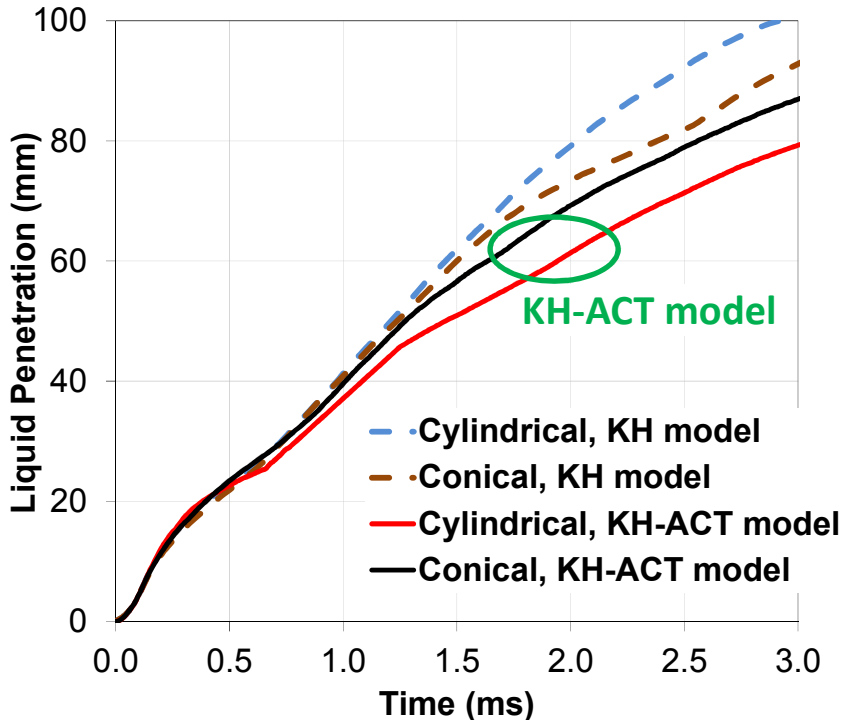




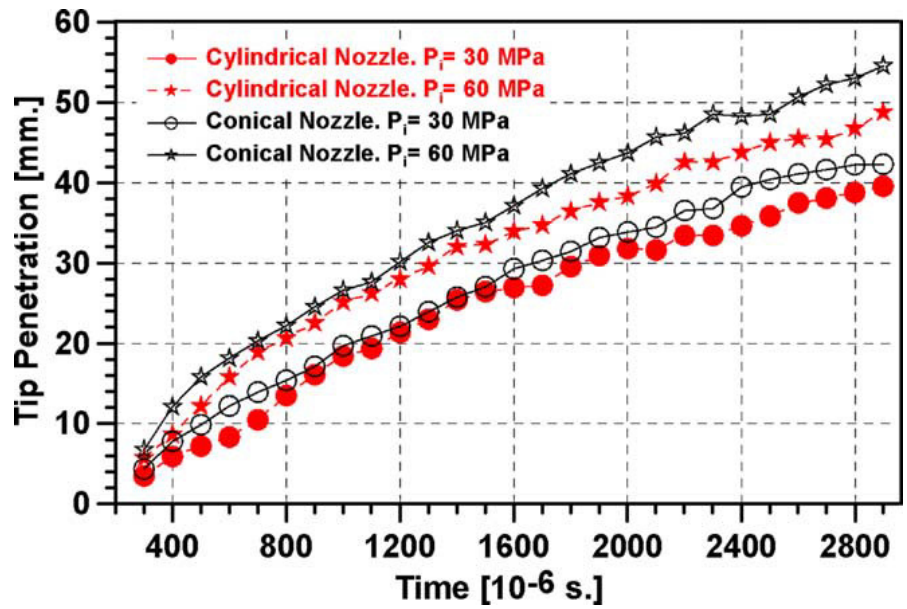
Cylindrical Nozzle

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

Summary

- Developed **KH-ACT primary breakup** model:
  - ✓ Accounts for nozzle flow effects on spray and combustion processes
  - ✓ Captures biodiesel spray characteristics accurately
  - ✓ Predicts influence of nozzle orifice geometry
- **Integrated Modeling** Approach:
  - ✓ Coupled nozzle-flow, spray, and combustion modeling
  - ✓ Robust validation against x-ray radiography data
  - ✓ Validation against constant volume data from Sandia

KH-ACT model implemented

- ✓ CONVERGE software, will be available in the next version release
- ✓ Implemented in Caterpillar Inc., software
- ✓ Currently in discussion with Ford Motor Company on inner-nozzle flow modeling implementation
- ✓ UW-Madison testing the model implementation in KIVA

Future Work

Dynamic-Coupling !!

- ✓ **Nozzle flow simulation dynamically coupled in the same spray and combustion model**
- ✓ **Capability to run with Large Eddy Simulation based turbulence models**
- ✓ **Full-cycle engine simulations**

Thank You!

???

Contact: ssom@anl.gov

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

Back-up Slides

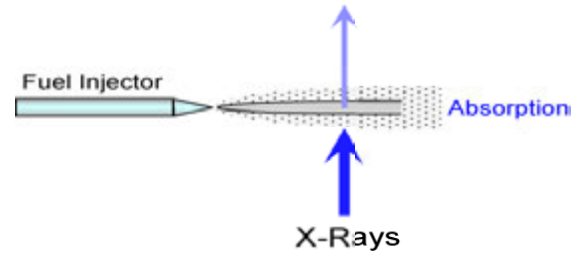
Experimental Conditions: X-ray radiography data*

Parameter	Quantity
Injection System	Caterpillar HEUI 315B
Number of Orifices	6
Orifice Diameter	169 µm with L/D = 4.412
Oil Rail Pressure	Case 1: 17 MPa
Pressure Intensification ratio	6.6
Fill Gas	Nitrogen (N_2)
Chamber Density	34.13 kg/m^3
Fuel Density	865.4 kg/m^3
Fuel Temperature	40 °C
Fuel Injection Quantity	100 [mm^3/stroke]

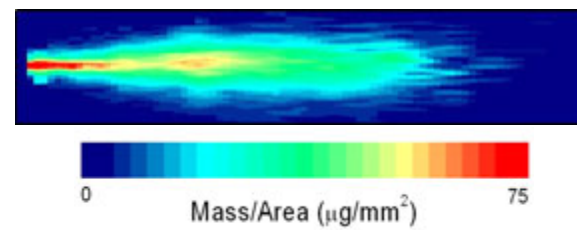
Further information available*:

1) **A.I. Ramirez, S. Som, et al. *Experiments in Fluids* 47: 119-134, 2009.**
2) **A.I. Ramirez, S. Som, et al. *SAE Paper No*. 2009-01-0846,, 2009.**

X-Ray Radiography

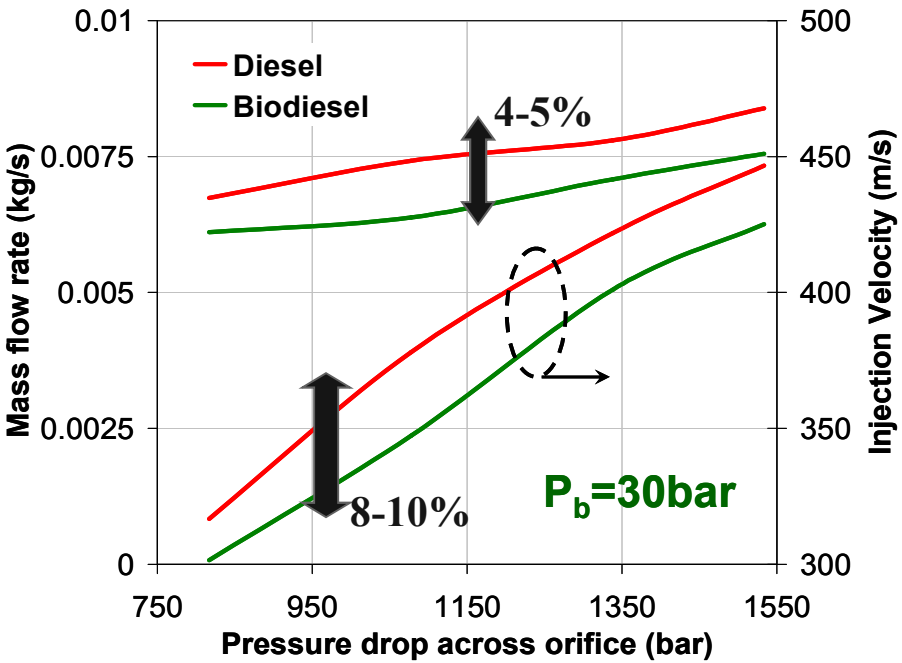


Number of x-rays absorbed indicates the quantity of fuel.



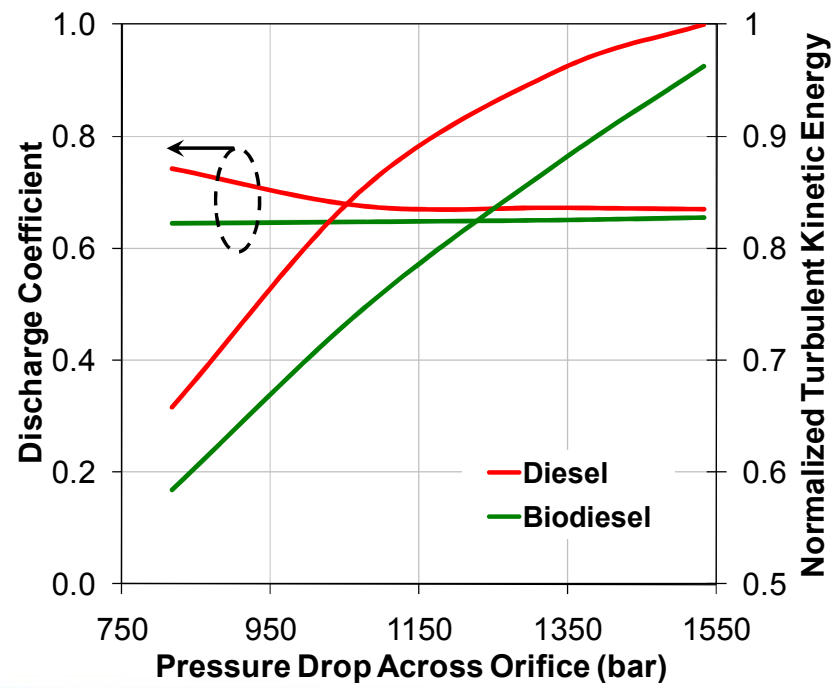
- Experiments performed under non-evaporating conditions at engine relevant densities
- Data available for : Spray penetration, cone-angle, fuel mass distribution near nozzle, normalized spray axial velocity, transverse integrated mass

Nozzle Exit Characteristics



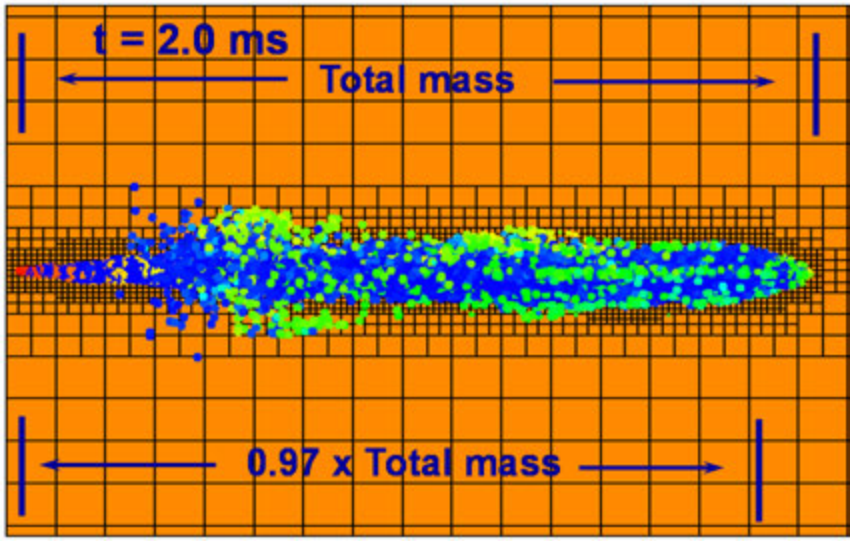
- Lower levels of turbulence and cavitation for biodiesel
- Breakup process with biodiesel may be slower!

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



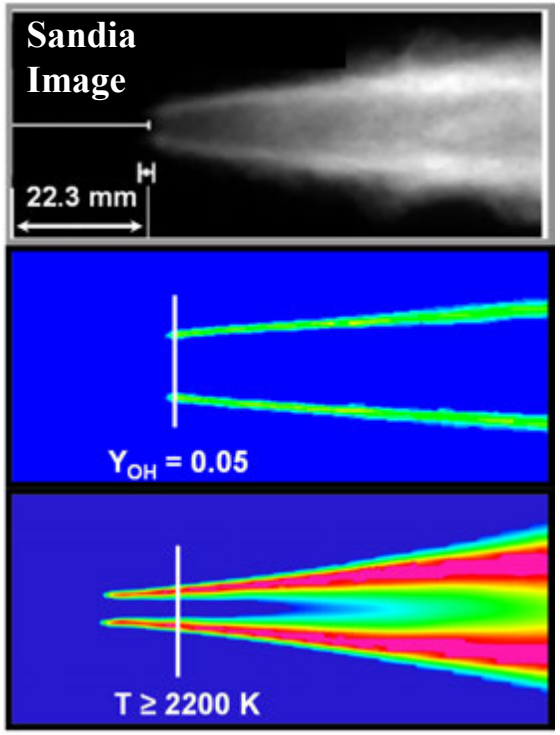
- Lower injection velocity, mass flow rate, and discharge coefficient for biodiesel
- This is due to biodiesel's significantly <u>higher molecular and turbulent viscosity</u>
- Significant differences in inner nozzle flow characteristics

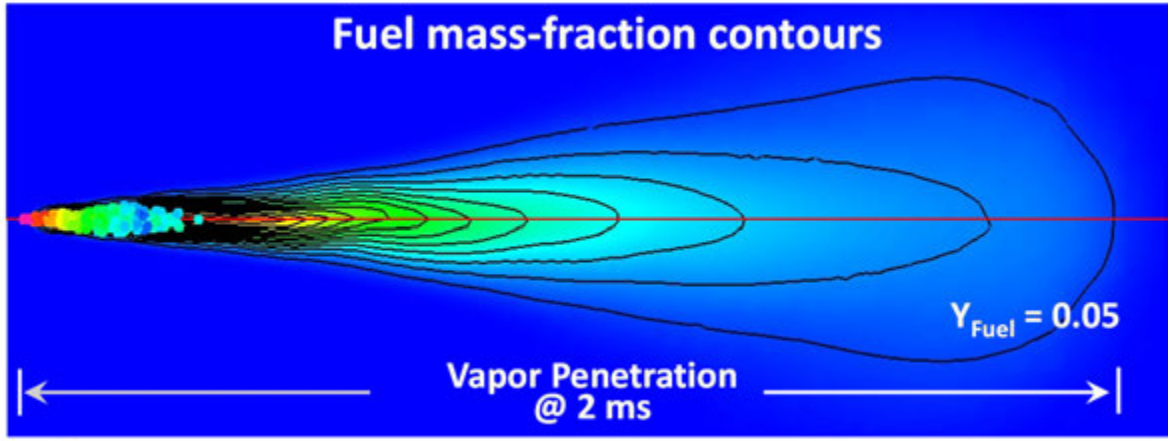
3D Simulations: Some Definitions



Spray penetration @ 2 ms

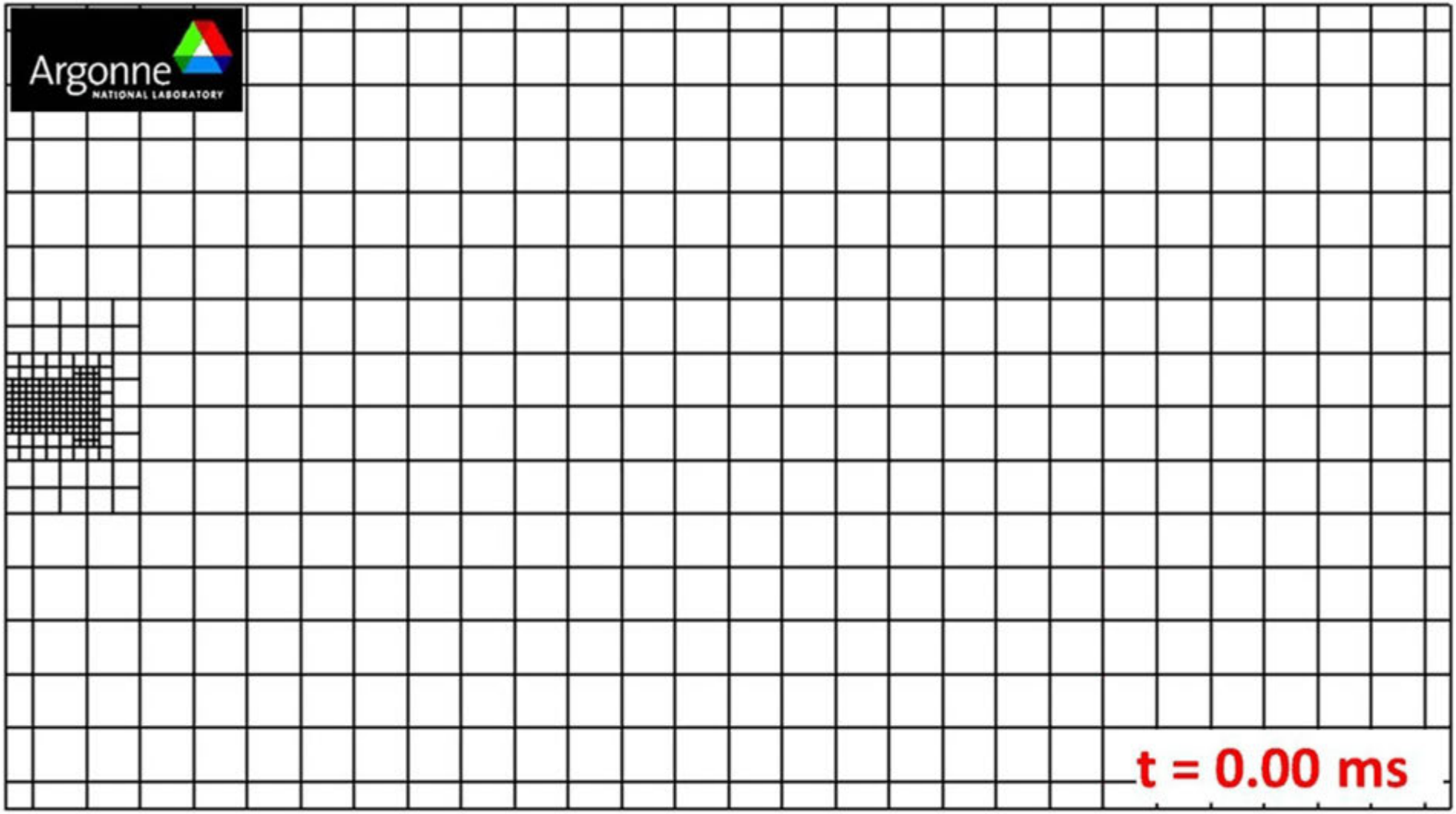
Lift-off length





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

Adaptive Mesh Generation



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