Advancement in Fuel Spray and Combustion Modeling for Compression Ignition Engine Applications

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Project ID # ACE075

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Overview

Timeline

Past Funding: FY 09, FY 10
Project start: April 1st 2012

Partners

Project Lead: Sibendu Som
Argonne National Laboratory
Chemical Science and Engineering
Mathematics and Computing Science

Convergent Science Inc.
Lawrence Livermore National Laboratory
Caterpillar Inc.
Sandia National Laboratory (Engine Combustion Network [ECN])
University of Connecticut
Cummins (Pending)

Barriers

- "Inadequate understanding of stochastics of fuel injection"
- "Improving the predictive nature of spray and combustion models"
- "Incorporating more detailed chemical kinetics into fluid dynamics simulations"

Budget

FY 12: 350 K
Starting April 1st 2012

Objectives/Relevance - 1

- Development of dynamically-coupled nozzle flow and spray simulations through improvements in Kelvin Helmholtz – Aerodynamic Cavitation Turbulence (KH-ACT) model
- Extensive validation of the dynamically coupled KH-ACT model:
  - X-ray radiography data from Argonne National Laboratory in the near nozzle region
  - Optical constant volume data from Sandia National Laboratory through the Engine Combustion Network (ECN) under evaporating and combustion conditions

- Fuel spray breakup in the near nozzle region 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, hence, are not predictive in nature with changing fuel types and nozzle orifice geometries

Objectives/Relevance - 2

- "Building a bridge" between fundamental chemical-kinetics (DOE Office of Science) and applied combustion research through computational combustion modeling of more realistic fuel surrogates
- Implementing and validating reduced mechanisms for diesel fuel surrogates against ECN data
  - n-dodecane
  - n-dodecane + m-xylene

- N-heptane is used as a diesel fuel surrogate. Not an ideal choice due to its high-volatility and low carbon content
- N-dodecane + m-xylene is a suitable diesel surrogate since it better mimics diesel Cetane characteristics
- Detailed chemical kinetic models are large, mechanism reduction is necessary

  Computational-time scales with $N^2 \sim N^3$ where 'N' is number of species

Objectives/Relevance - 3

- High Performance Computing (HPC):
  - Demonstrate scalability up to 1000 processors
  - Demonstrate grid-independence of spray and combustion parameters

- Current state-of-the-art for engine simulations in OEMs involve up to 50 processors only
- OEMs prefer quick turn-around times for engine simulations which may not be possible as the resolution, spray, turbulence, and chemical kinetic models become more detailed
- This is possible if scalable simulations are feasible by increasing the number of processors by a factor of 5

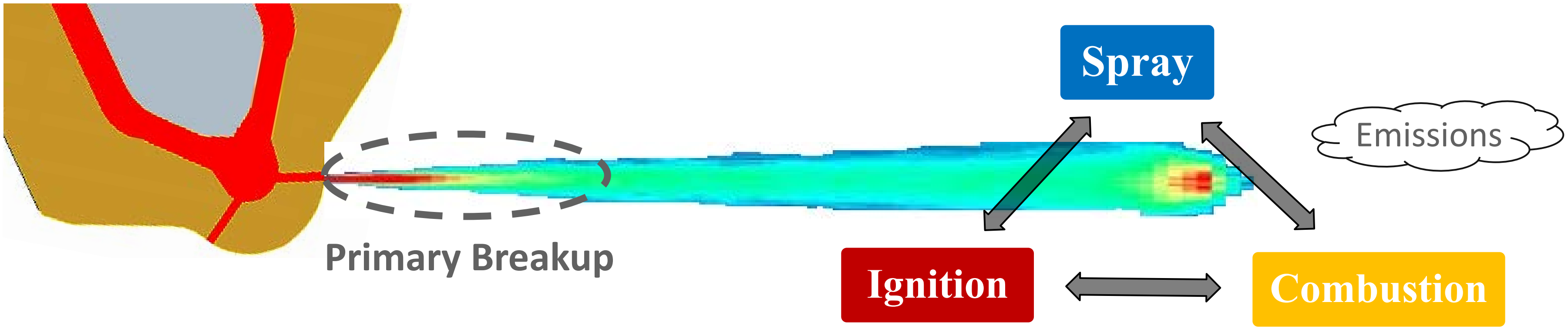
Milestones, FY 12

- Task 1: Dynamic – coupling of injector nozzle and spray processes: Extension of KH-ACT model
  - ❑ Improving the predictive capability of KH-ACT primary breakup model (September 2012)
- Task 2: Develop a surrogate mechanism for diesel fuel for multi-dimensional CFD simulations
  - ❑ Updating the 103-species n-dodecane reduced mechanism (May 2012)
  - ❑ Validation and improvements in combustion modeling based on ECN data (August 2012)
- Task 3: Simulation of Internal combustion engines with HPC tools
  - ❑ Assess grid independence of spray and combustion parameters (June 2012)
  - ❑ Assess scalability of CONVERGE tool on (up to) 100-500 processors (July 2012)

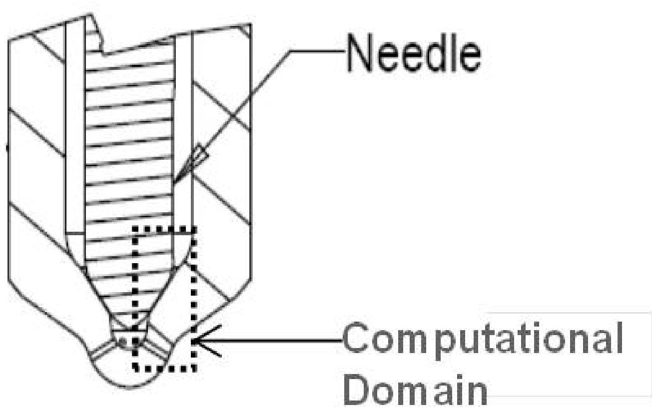
Integrated Modeling Approach

Influence of fuel properties and nozzle orifice geometry on nozzle flow, spray, and combustion characteristics!!

Inner Nozzle Flow



6-hole production Injector



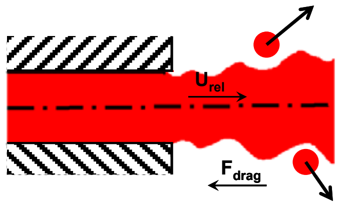
- **KH-ACT** primary breakup model: Aerodynamics, Cavitation, Turbulence
- Detailed inner-nozzle flow modeling with realistic fuel properties
- **Dynamic – coupling** of inner nozzle flow and spray simulations
- Spray Validation: **X-ray radiography** data provides information in the near nozzle region

Approach

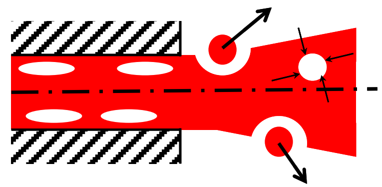
Primary Breakup Model

KH-ACT (Kelvin-Helmholtz-Aerodynamics Cavitation Turbulence) Model*

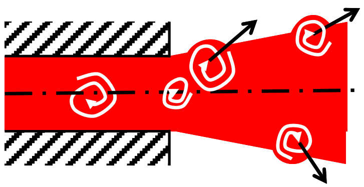
- ❑ Length and time scales are calculated



Aerodynamically induced breakup: Based on Kelvin-Helmholtz (KH) and Rayleigh Taylor (RT) instability



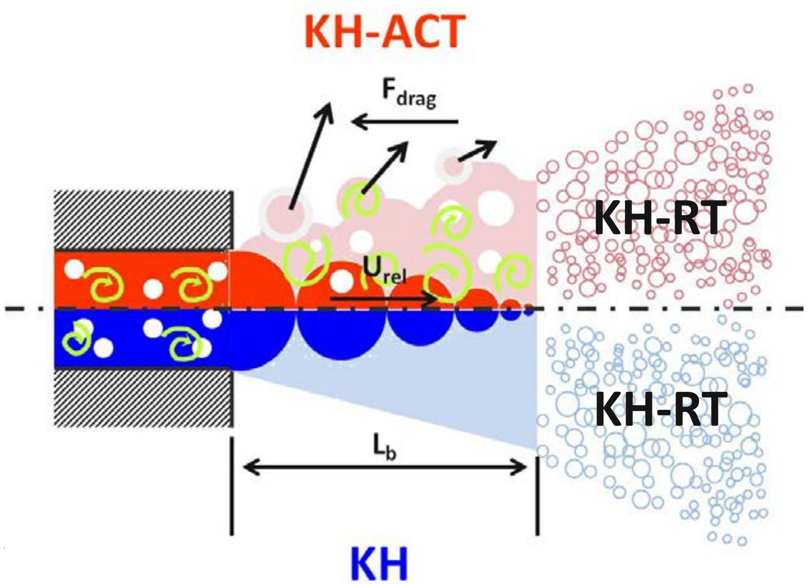
Cavitation induced breakup: Based on bubble collapse and burst times



Turbulence induced breakup: Based on k-ε model

- ❑ Dominant ratio of length/time scale causes breakup
- ❑ Different combinations of length and time scales for ACT model will be tested (more information in back-up slides)

*Som et al., SAE 2009-01-0838, Combustion and Flame 2010, Fuel 2010, Fuel 2011



Approach

Detailed Chemical Mechanisms in Engine Simulations

Typical LLNL mechanism
~1000 species, ~10000 reactions
Ideal for 0D, 1D simulations

Mechanism Reduction* →

Reduced mechanism
~150 species, ~1000 reactions
Ideal for 3D-CFD simulations

Research on mechanism reduction techniques is funded by DOE office of Science at Chemistry group at Argonne, and University of Connecticut

Our Approach:

- Provide the mechanism reductionists with fuel surrogates of interest for the transportation sector
- Extensive validation against ECN spray-combustion and engine data
- Provide feedback on the performance of the reduced mechanism to the mechanism developers, based on 3D-CFD simulations

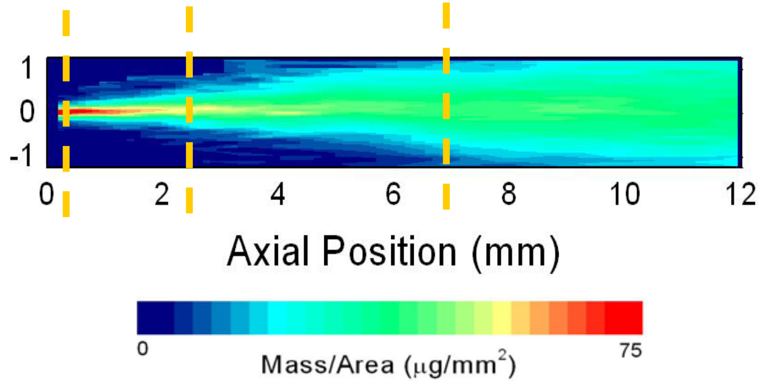
n-Dodecane Mechanism (from LLNL)
2115 species, 8157 reactions

Mechanism Reduction* →

Reduced Mechanism
103 species, 370 reactions

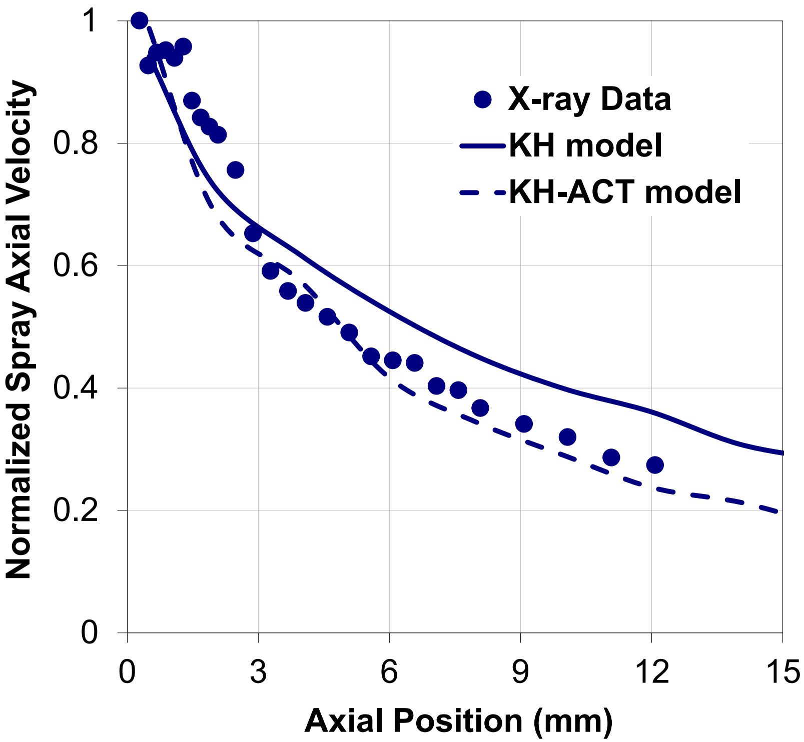
* Z Luo, M Plomer, T Lu, M Maciaszek, S Som, DE Longman. *Energy and Fuels* (24) 2010
* T. Lu, M. Plomer, Z. Luo, S.M. Sarathy, W.J. Pitz, S. Som, D.E. Longman,. *US Combustion meeting, 2011*

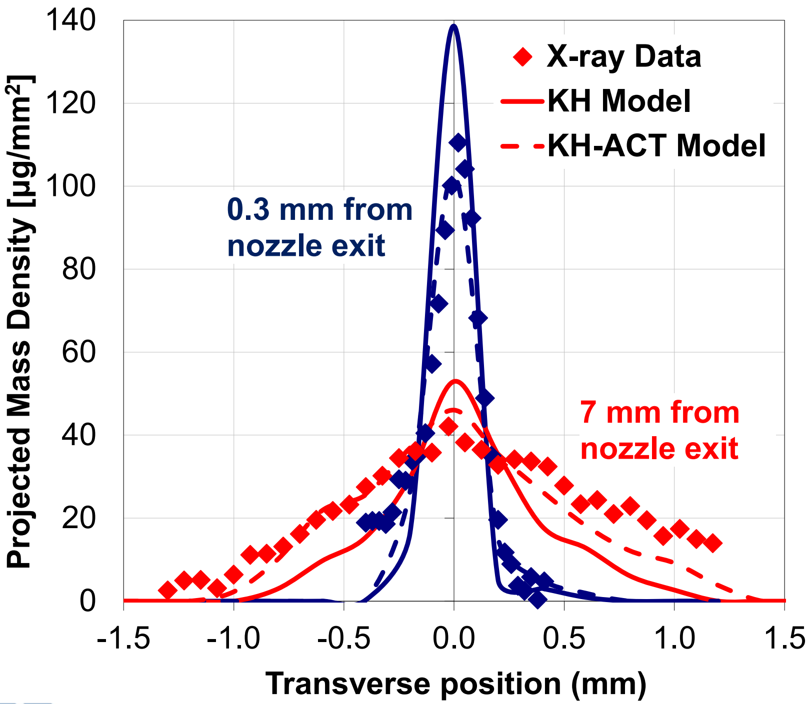
KH-ACT Model Validation against X-ray Data*



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

(Experimental conditions available in back-up slides)





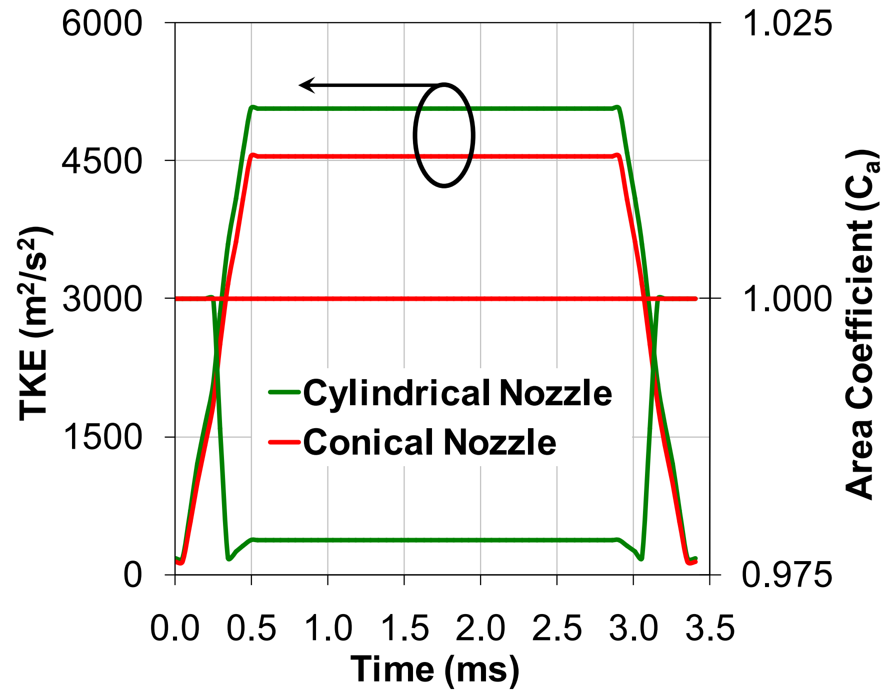
- The spray loses half of its initial velocity within the first 6 mm
- Simulation capture the Gaussian mass distributions from x-ray data well
- Spray Dispersion accurately captured by only the KH-ACT model. KH model under-predicts spray spreading

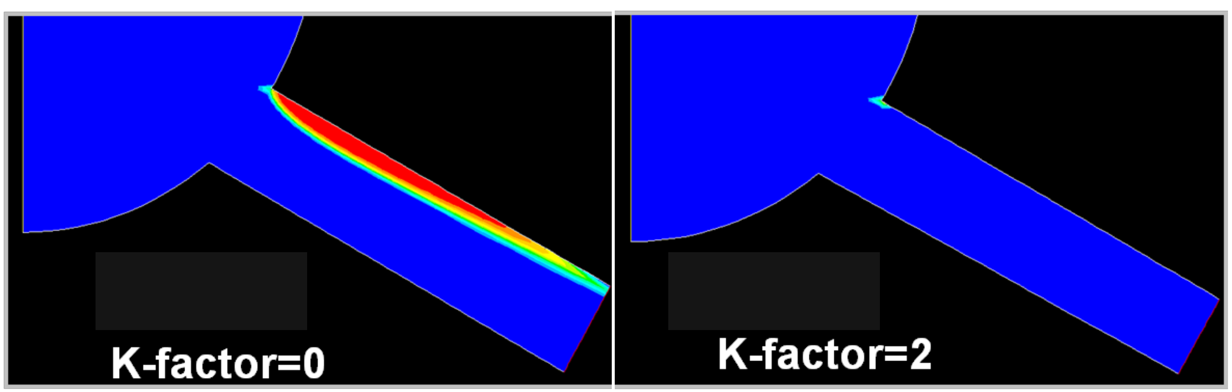
Technical Accomplishment and Progress

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

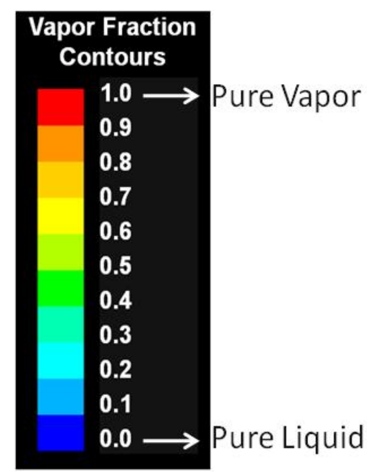
$$K_{factor} = \left(\frac{D_{in} - D_{out}}{10} \right) \mu m$$



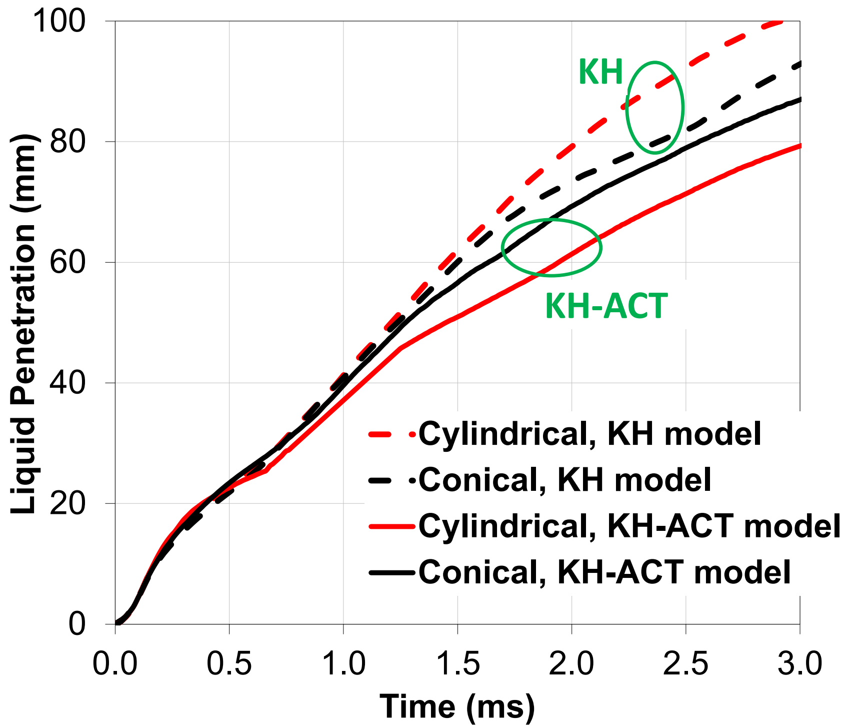


Cylindrical Nozzle

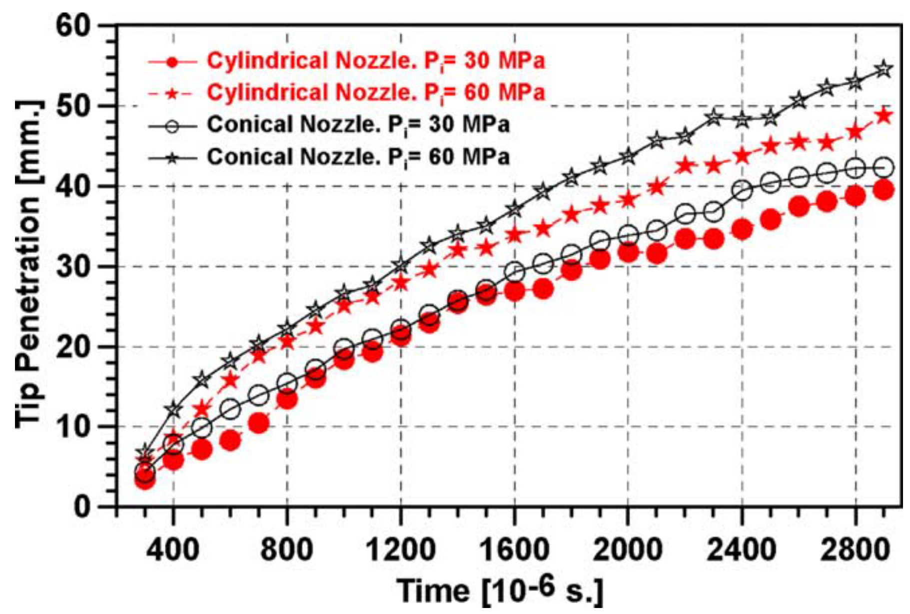
Conical Nozzle



KH-ACT model Accurately Predicting the Influence of Nozzle Geometry



F Payri, V Bermudez, R Payri, FJ Salvador: FUEL (2004)

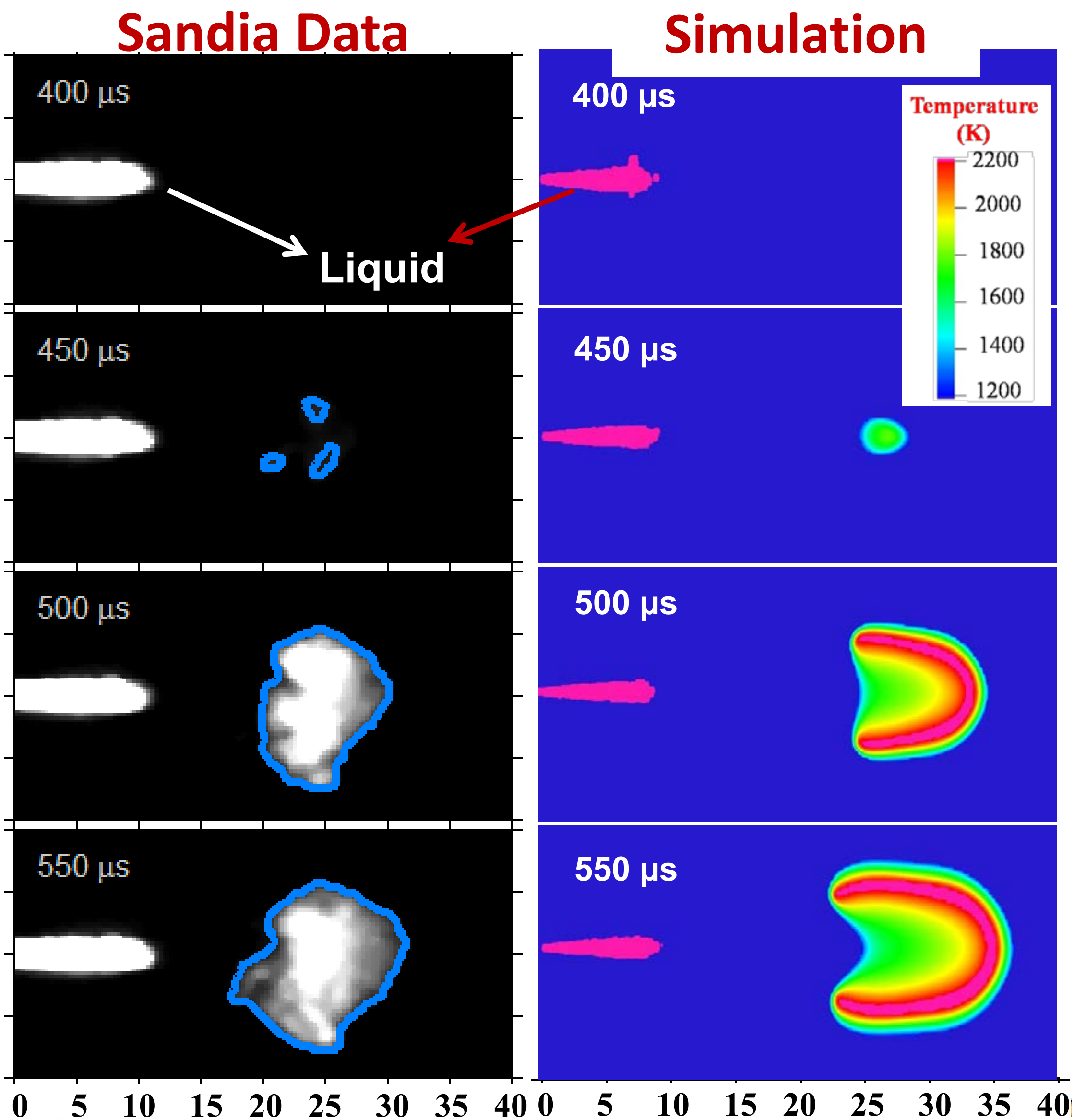


- Penetration characteristics of cylindrical and conical nozzles predicted by KH-ACT model (only) are consistent with experimental trends observed by Payri et al.
- Cylindrical nozzle predicts fastest breakup. This is due to enhanced cavitation and turbulence thus: 1) SMD, 2) Spray penetration are lower

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

Technical Accomplishment and Progress

Combustion modeling with n-dodecane



Experiments:
(Conditions available in back-up slides)

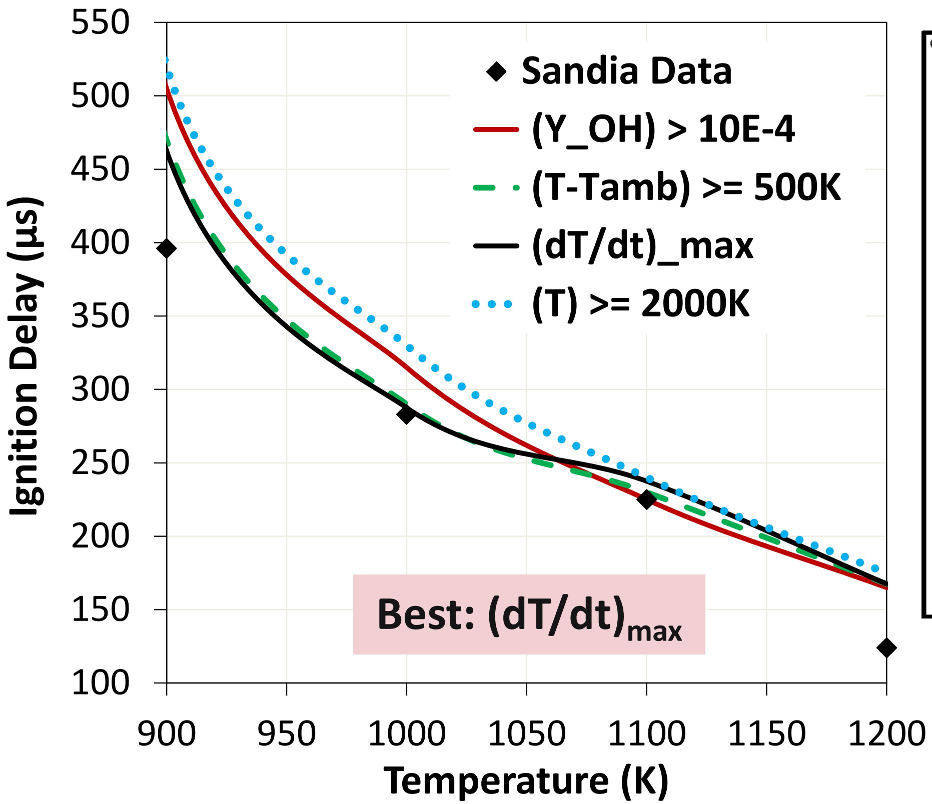
Simulation:
Temperature contours plotted to capture ignition location and delay simulated using the 103 species n-dodecane reduced mechanism (cf. Slide 9)

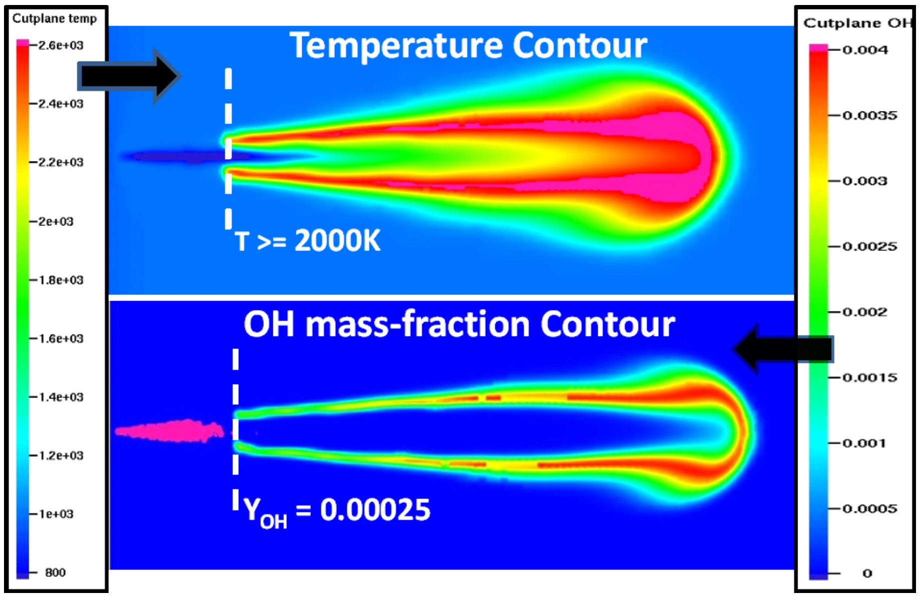
Spray and Combustion modeling able to predict the liquid fuel distribution, ignition location, ignition time, flame shape, etc.

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

Technical Accomplishment and Progress

Identify Appropriate Definitions for Ignition Delay and Flame Lift-off Length



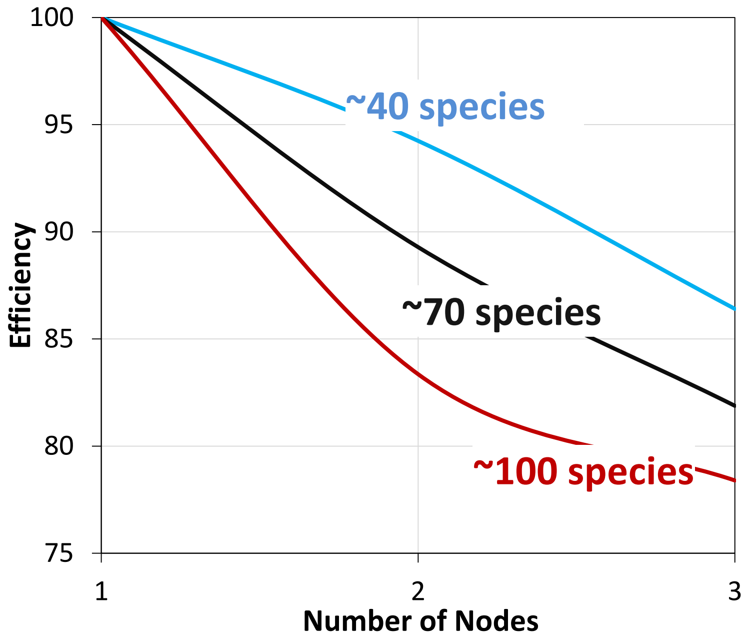


Best: $(Y)_{OH} = 0.00025$

- Differences are observed in predicted ignition delays and flame lift-off lengths based on definitions chosen
- Most relevant definitions for ignition delay and flame lift-off lengths identified. This will be proposed to the Engine Combustion Network

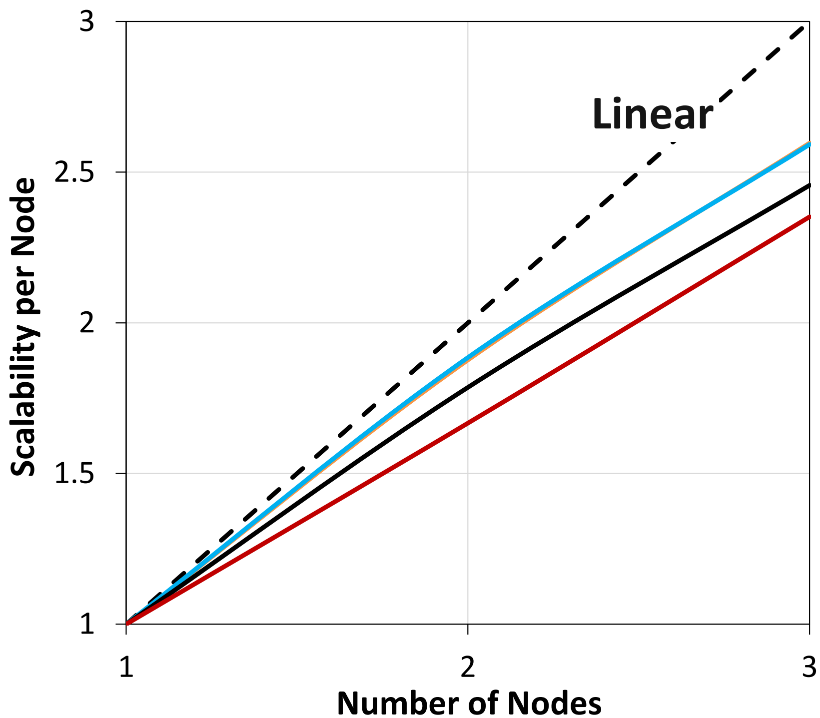
Computational Cost & Scalability

Increasing the number of species results in rapid decrease in scalability and efficiency.
Our focus is on improving the load-balancing schemes to obtain better scalability.



Mechanisms	Wall-clock Time (for node)
~40 species: n-heptane	~ 42 hours
~100 species: n-dodecane	~ 120 hours

Scalability per node = T_1/T_n
Efficiency per node = $T_1 x100/nT_n$
n = Number of compute nodes
T_1 = Wall-clock time on 1 node
T_n = Wall-clock time on n nodes
Each node has 8 processors



Technical Accomplishment and Progress

Collaborations

Argonne National Laboratory

Engine and Emissions Group: (Provide data for model validation)
Chemical Science and Engineering Group: (Mechanism development and reduction)
Mathematics and Computing Science: (HPC resources)

Convergent Science Inc. (Algorithm and code development in CONVERGE)

Sandia National Laboratory (Provide experimental data through the ECN)

Lawrence Livermore National Laboratory (Mechanism development)

University of Connecticut (Mechanism Reduction)

Cummins (Provide experimental data, alpha testing) {Pending}

Caterpillar Inc. (Testing and implementation of HPC tools)

Collaborations and Coordination

ECN Modeling Coordination

University of Wisconsin (USA)

Sandia National Laboratory (USA)

Argonne National Laboratory (USA)

Cambridge University (UK)

CMT (Spain)

Objectives

1) Standardization of spray and combustion parameter definitions
2) Development of engine models
3) Assessing capabilities of different open source and commercial engine modeling codes

Politecnico di Milano (Italy)

TU – Eindhoven (Netherland)

KAIST (Korea)

IFP (France)

UNSW (Australia)

Penn. State (USA)

Purdue University (USA)

- Coordinated Spray A modeling session in ECN 1 (Ventura, May 2011): 9 groups
- Coordinating modeling sessions in ECN 2 (Heidelberg, September 2012): 12-15 groups expected

Collaborations and Coordination

Proposed Future Work in FY13

- **Task 1: Dynamic – coupling of injector nozzle and spray processes: Extension of KH-ACT model**
  - Implement an improved nozzle flow model with moving needle capability
  - Implement and test a dynamic-coupling approach
  - Validation against x-ray radiography data
- **Task 2: Develop a surrogate mechanism for diesel fuel for multi-dimensional CFD simulations - Validation against ECN data**
  - Further reduction and testing of the 103 species n-dodecane mechanism
  - Implement and test n-dodecane + m-xylene reduced mechanism for 3D combustion simulations
  - Capture the influence of ambient temperature and density variations on combustion characteristics such as ignition delay, flame lift-off length etc.
- **Task 3: Simulation of Internal combustion engines with high-performance computing tools**
  - Demonstrate grid independence for multi-cylinder simulations involving intake and exhaust ports
  - Assess scalability of CONVERGE tool on (up to) 1000 - 1500 processors

Future Work

Summary

- **Objective**
  - Development of predictive spray and combustion models aided by high-performance computing tools and robust validation
- **Approach**
  - Coupling expertise from DOE Office of Science on fundamental chemical kinetics and HPC resources for development of robust engine models
- **Technical Accomplishment**
  - KH-ACT model performs static coupling of nozzle flow and spray simulations
  - n-dodecane reduced mechanism captures combustion characteristics well
- **Collaborations and coordination**
  - with industry, academia, and national laboratories in US
  - through ECN with researchers world-wide
- **Future Work - FY13**
  - Dynamic coupling of nozzle flow and spray
  - Development of realistic diesel surrogate model
  - Demonstrate scalability of engine models on 1000-1500 processors

Technical Back-Up Slides

(Note: please include this "separator" slide if you are including back-up technical slides (maximum of five). These back-up technical slides will be available for your presentation and will be included in the DVD and Web PDF files released to the public.)

3D Spray-Combustion Modeling Set-up

Modeling Tool	CONVERGE
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 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**

Back-up

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 :

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

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

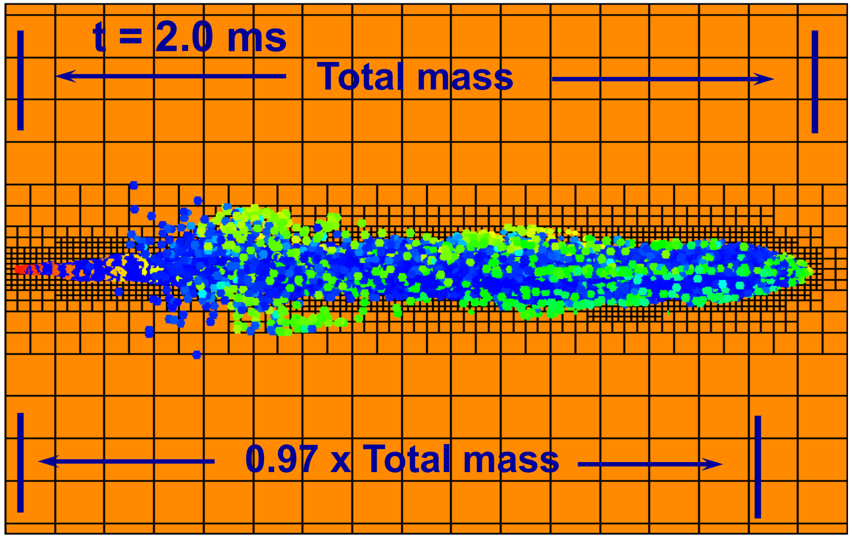
K_0, ε_0, C_a are obtained from nozzle flow modeling

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**

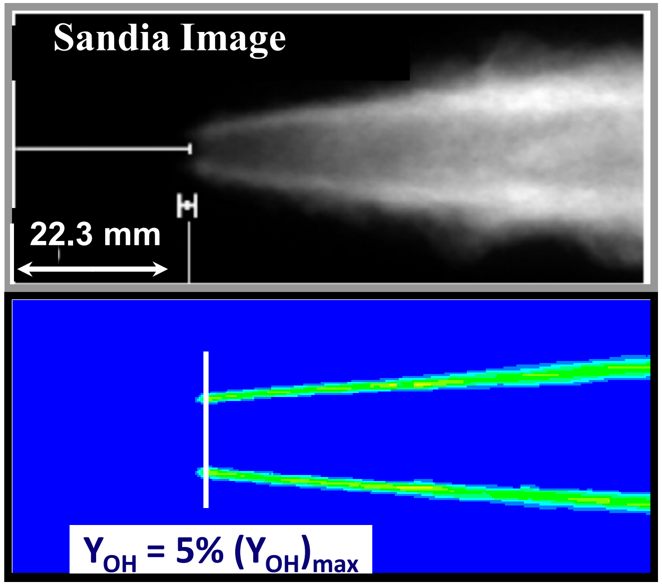
Back-up

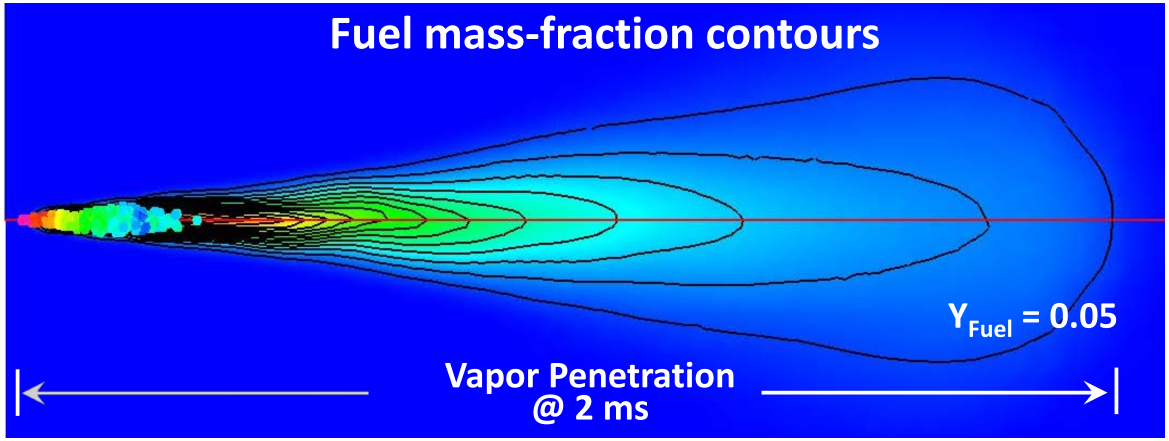
3D Simulations: Standard Definitions Used



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.

Back-up

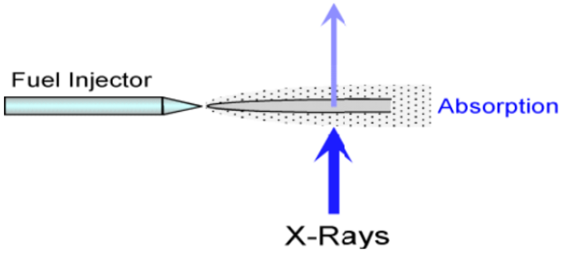
Experimental Conditions: X-ray radiography data*

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]

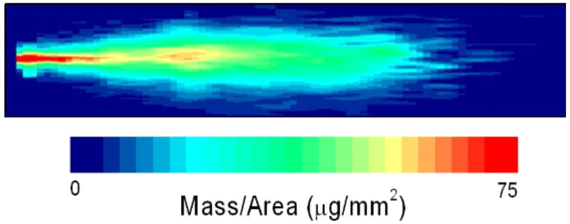
Further information available*:

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

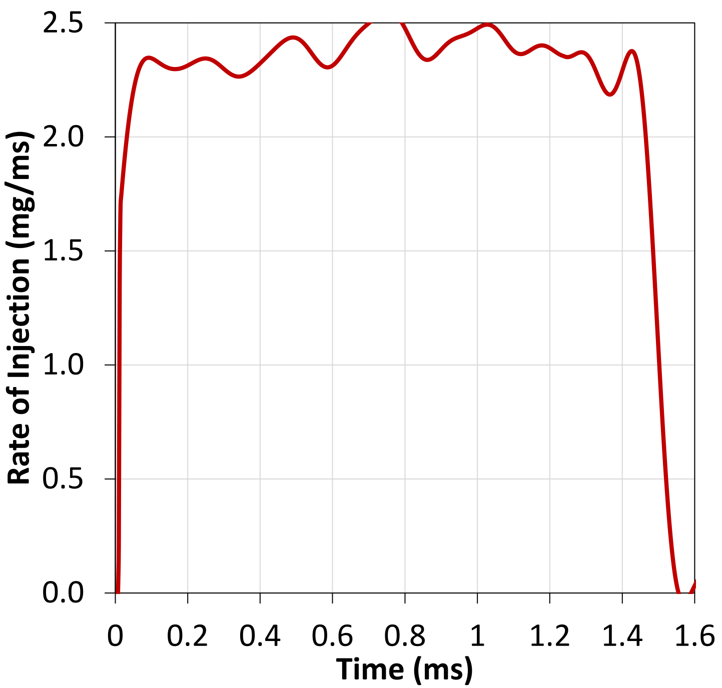
Back-up

Experimental Conditions from ECN

Parameter	Quantity
Fuel	n-dodecane
Nozzle outlet diameter	90 µm
Nozzle K-factor	1.5
Nozzle shaping	Hydro-eroded
Discharge coefficient	0.86
Fuel injection pressure	150 MPa
Fuel temperature	363 K
Injection duration	1.5 ms
Injected fuel mass	3.5 mg
Injection rate shape	Square
Ambient temperature	800 - 1200 K
Ambient gas density	22.8 Kg/m^3
Ambient O_2 Concentration	15 %

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

- Experiments performed under both evaporating and combusting conditions.
- Data available for : Spray penetration, liquid length, vapor penetration, mixture fraction, ignition delay, flame lift-off length, soot distribution , high-speed movies



Back-up