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

Sibendu Som

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Leo Breton

Project ID # ACE075

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U.S. DEPARTMENT OF **ENERGY**

Overview

Timeline

Project start: April 1st 2012

Partners

Argonne National Laboratory
Chemical Science and Engineering
Mathematics and Computing Science
Leadership Computing Facility
Transportation Hutch at x-ray beamline

Convergent Science Inc. {CRADA}
Caterpillar Inc. {CRADA}
Cummins Engine Company {CRADA}

Lawrence Livermore National Laboratory
Sandia National Laboratory (Engine Combustion Network [ECN])
Advanced Engine Combustion (AEC) Working group

University of Connecticut
Politecnico di Milano, University of Perugia (Italy)

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"
- ❑ "Development of High-Performance Computing (HPC) tools to provide unique insights into the spray and combustion processes"

Budget

FY 12: 350 K
FY 13: 500 K
FY 14: 500 K

Objectives & Approach

In general Engine simulations involve:

- Unresolved Nozzle flow
- Simplified combustion models
- Coarse mesh => grid-dependence
- Poor load-balancing algorithms
- Simplified turbulence models

Extensive tuning to match experimental data

High-Fidelity Approach:

- Detailed chemistry based combustion models
- Fine mesh => grid-convergence
- High-fidelity turbulence models: LES based
- Two-phase physics based fuel spray and nozzle-flow models

✚

- High-Performance Computing

Towards Predictive Simulation of the Internal Combustion Engine

Long Term Objective:

- ❖ Develop reliable engine modeling capability with fewer tuning constants
- ❖ Sub-models published in open-literature and available to the industry through software packages of interest

Relevance

- **Nozzle flow and Spray research**
  - ❑ Fuel spray breakup in the near nozzle region plays a central role in combustion and emission processes
  - ❑ Improving in-nozzle flow and turbulence predictions is key towards the development of predictive engine models
- **Combustion modeling using detailed chemistry**
  - ❑ Accurate chemical kinetics for fuel surrogates are key towards developing predictive combustion modeling capability
    - • Mixture of n-dodecane + m-xylene is a more suitable diesel surrogate
- **High-Performance Computing**
  - ❑ Current state-of-the-art for engine simulations in OEMs involve up to 50 processors (approx.) only
  - ❑ Will be needed in order for OEMs to retain quick turn-around times for engine simulations

Cluster   **Super-Computer**

Milestones, FY 14

- **Nozzle flow and Spray Research (CRADA with Cummins and CSI)**

  - ✓ Eulerian-Eulerian near nozzle spray model development and validation under non-evaporating conditions {Completed: January 2013}

  - ✓ Contribute nozzle flow, spray, and combustion results for Engine Combustion Network (ECN) and co-ordinate ECN efforts {Completed: April 2014}

  - ❏ Improved understanding of injection transients {90% complete: May 2014}

  - ❏ In-nozzle flow simulations of Cummins Fuel Injectors {25% Complete: August 2014}

  - ❏ Coupling Eulerian-Eulerian near nozzle model with Eulerian-Lagrangian model to simulate reacting sprays and engine cases {20% complete: September 2014}

- **Combustion Modeling with Detailed Chemistry**

  - ❏ Validating n-dodecane + m-xylene mixture reduced model (updated rate parameters from Pitz et al., LLNL) against experimental data available from Sandia {20% complete: July 2014}

- **High-Performance Computing (Funds-in CRADA with Caterpillar and CSI, signed in February 2014)**

  - ❏ Identify numerical "best-practices" for open and closed cycle, multi-cylinder Caterpillar engine simulations {10% complete: September 2014}

Simulation Approach: Sub-Model Development

Modeling Tool	**CONVERGE** Source code access for spray and High Performance Computing Algorithms
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)	Finest grid size**: 5 µm for nozzle flow; ~30 µm for Spray; 100 µm for engine**; simulations
Total grid number	**50 millions is the highest cell count run** ⬅
Parallelizability	**Good scalability on up to 1000 processors**
Turbulence model(s)	RANS: RNG k-ε; **LES: Smagorinsky, Dynamic Structure**
Spray models	**Eulerian-Eulerian Near Nozzle Model** ⬅ Lagrangian Models: Breakup: KH-RT without breakup length concept Multi-component evaporation: Frossling correlations Drag-law: Dynamic model
In-nozzle Flow	**Homogeneous Relaxation Model (HRM)** ⬅
Time step	Variable based on spray, evaporation, combustion processes
Turbulence-chemistry interactions model	Direct Integration of detailed chemistry: well-mixed model **Representative Interactive Flamelet (RIF) Model** ⬅
Time discretization scheme	PISO (Pressure Implicit with Splitting of Operators)

Extensive Validation using experimental data from Engine Combustion Network
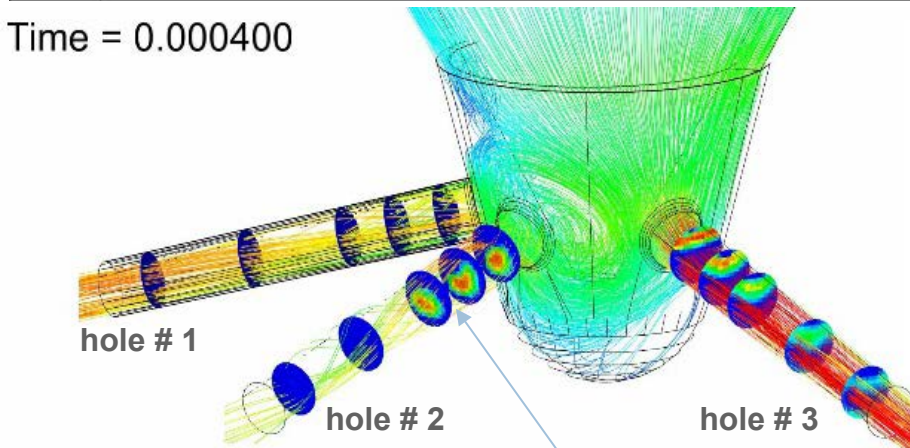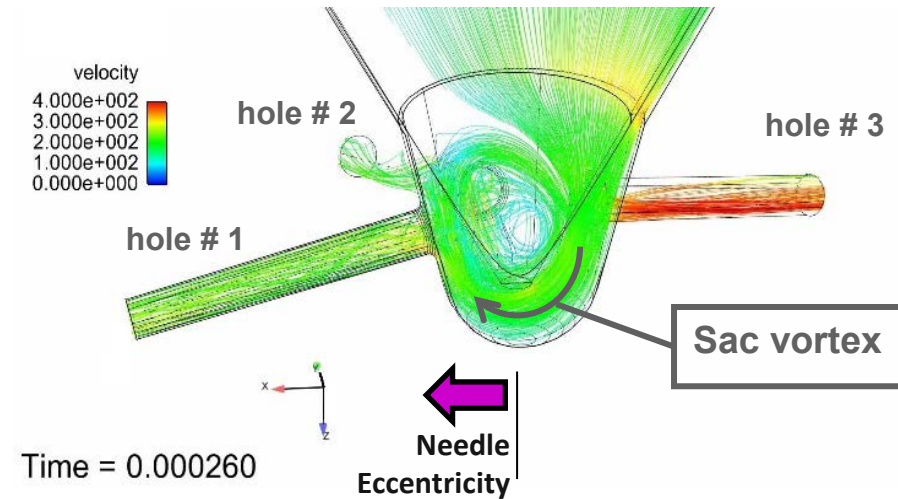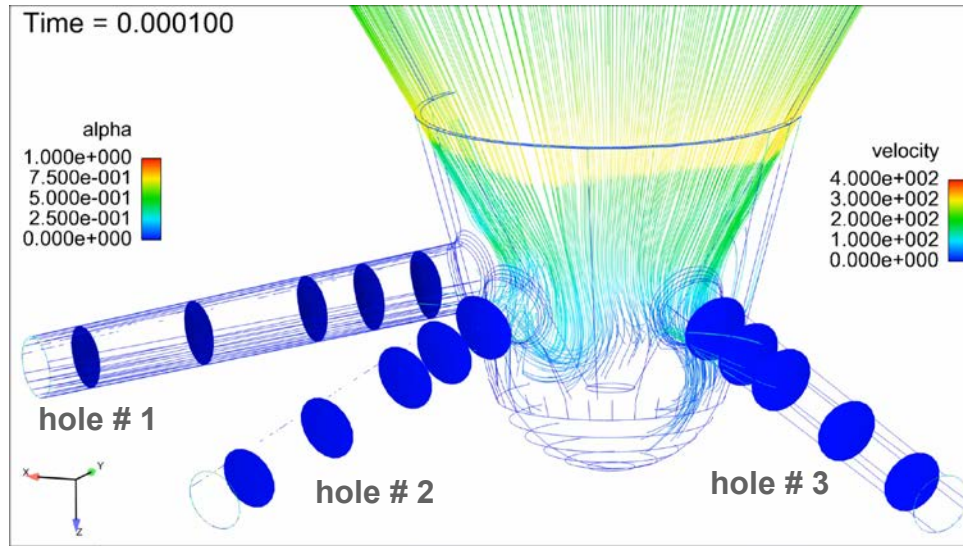(Courtesy Lyle Pickett et al.) and X-ray data (Courtesy Chris Powell et al.)

Technical Accomplishments

Plume-to-Plume Variations

Time = 0.000100

alpha
1.000e+000
7.500e-001
5.000e-001
2.500e-001
0.000e+000

velocity
4.000e+002
3.000e+002
2.000e+002
1.000e+002
0.000e+000

hole # 1
hole # 2
hole # 3

velocity
4.000e+002
3.000e+002
2.000e+002
1.000e+002
0.000e+000

hole # 2
hole # 3
hole # 1

Sac vortex

Needle Eccentricity

Time = 0.000260

Time = 0.000400

hole # 1
hole # 2
hole # 3

"String type" cavitation

- Swirling jet coming out from hole #2
- Half cross section blocked for hole #3

Time = 0.000260 s

alpha
1.000e+000
7.500e-001
5.000e-001
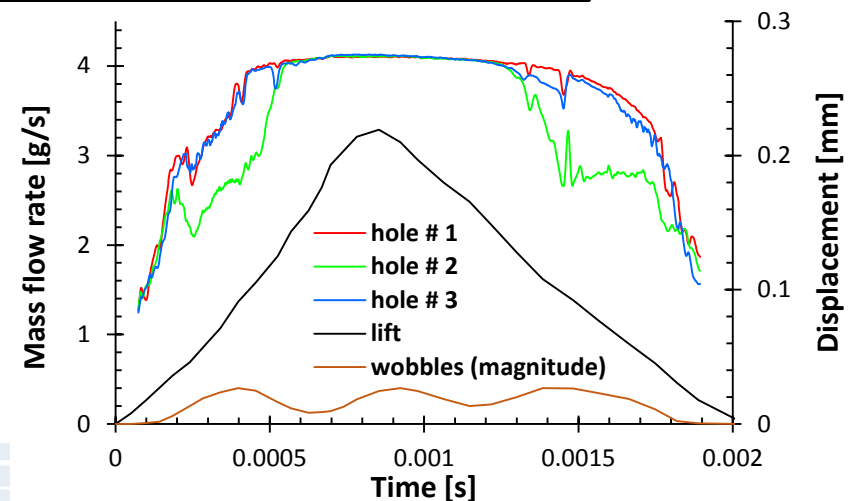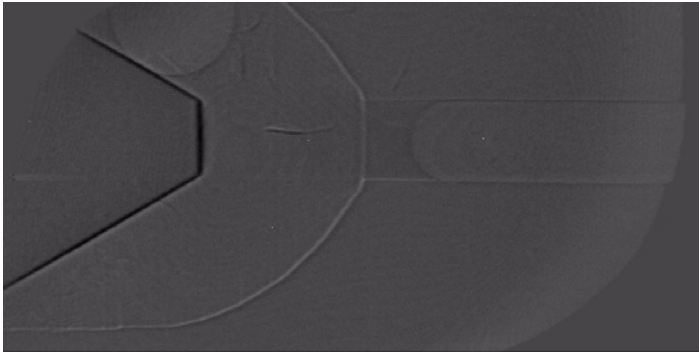2.500e-001
0.000e+000

1
2
3

8
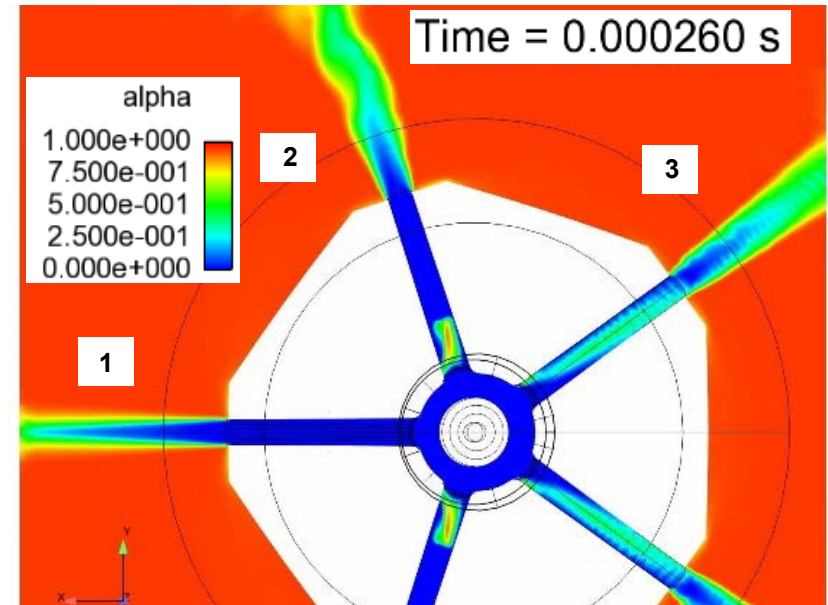
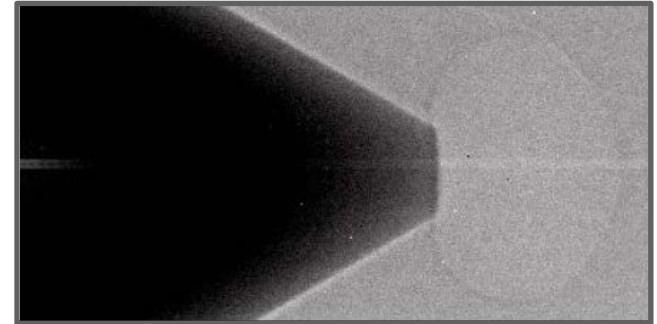# Needle wobble Resulting in Plume-to-Plume Variations
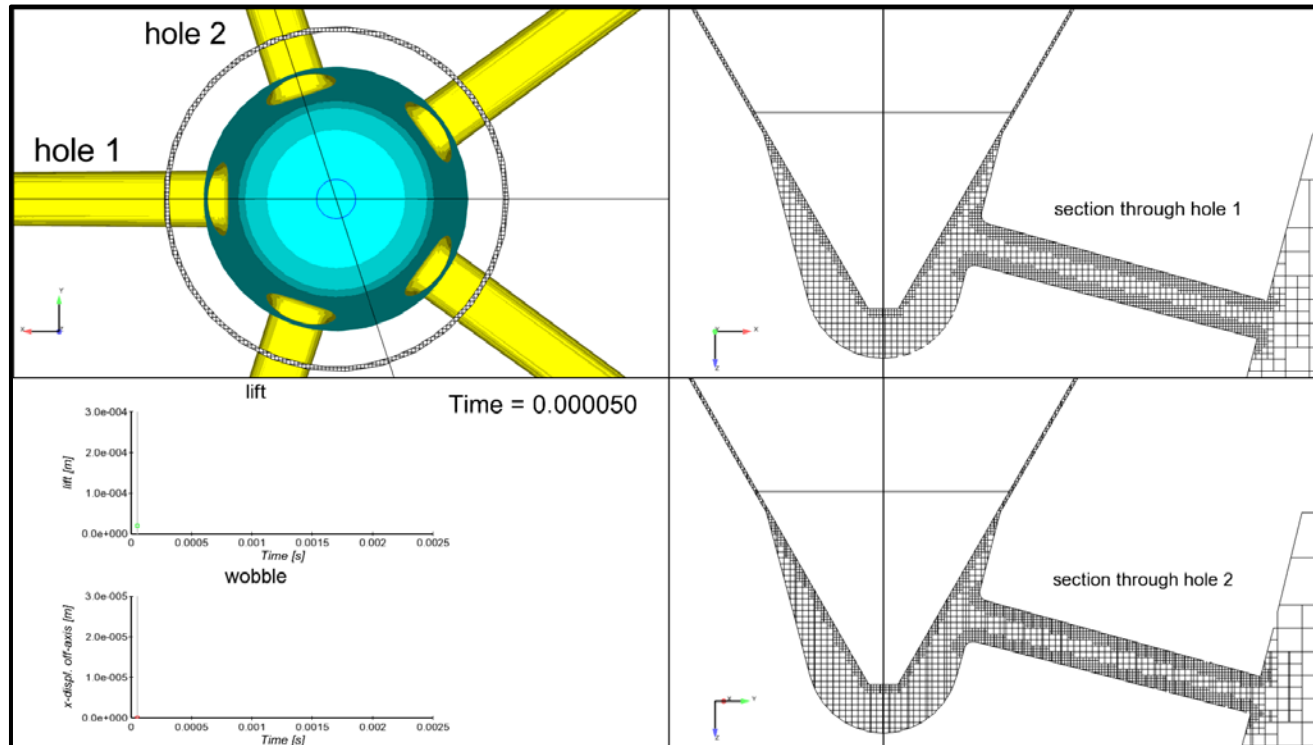
- ❖ First of its kind simulations accounting for needle lift and **off-axis motion**
- ❖ High temporal and spatial resolutions
- ❖ Geometry Information: Payri et al. SAE Paper No. 2009-24-0025
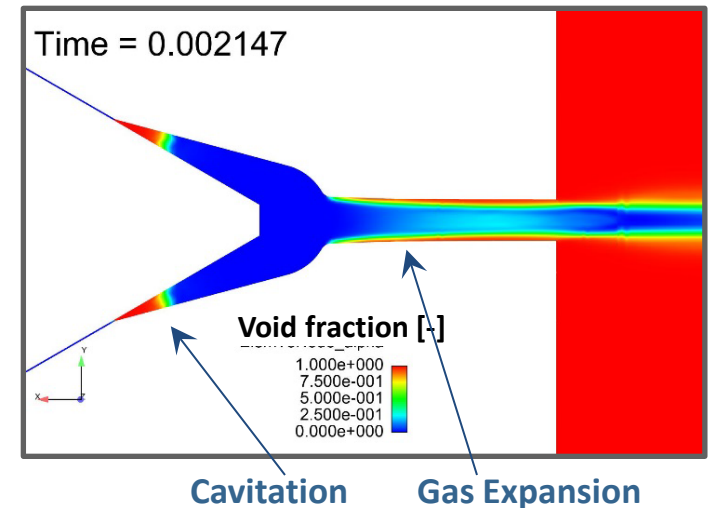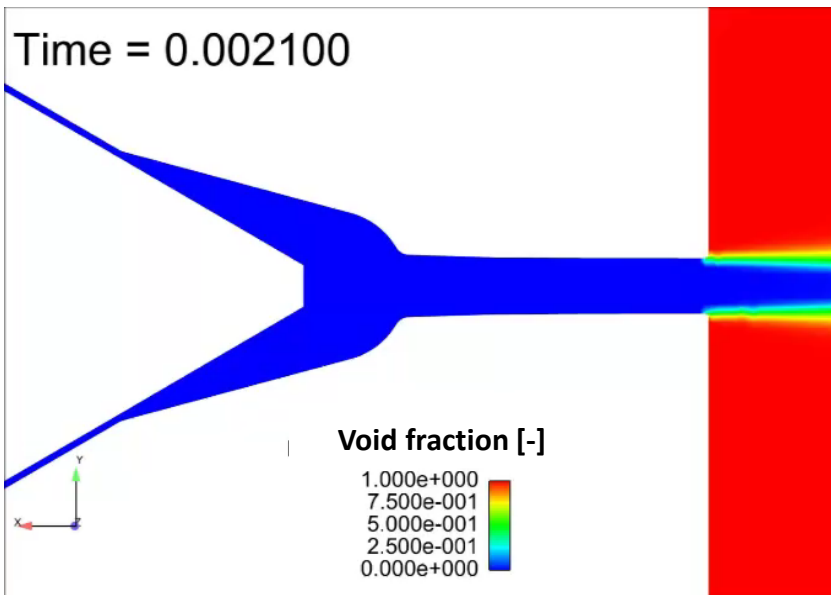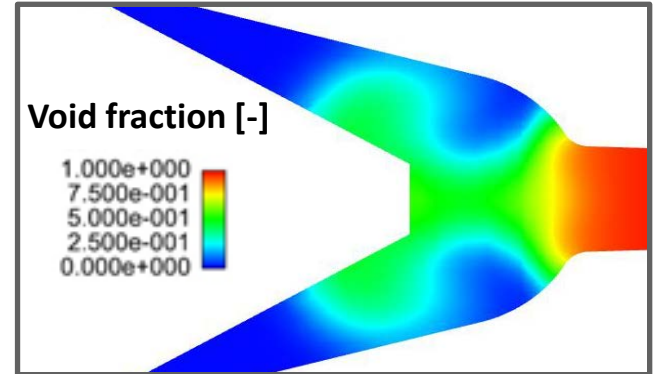- ❖ **Significant hole-to-hole variations during needle transients**

Needle Transient: End-of-Injection

Movie Courtesy: Dr. Chris Powell (Argonne)

Time = 0.002100

Void fraction [-]

1.000e+000
7.500e-001
5.000e-001
2.500e-001
0.000e+000

Experiments

Simulations

Void fraction [-]

1.000e+000
7.500e-001
5.000e-001
2.500e-001
0.000e+000

Time = 0.002147

Void fraction [-]

1.000e+000
7.500e-001
5.000e-001
2.500e-001
0.000e+000

Cavitation   **Gas Expansion**
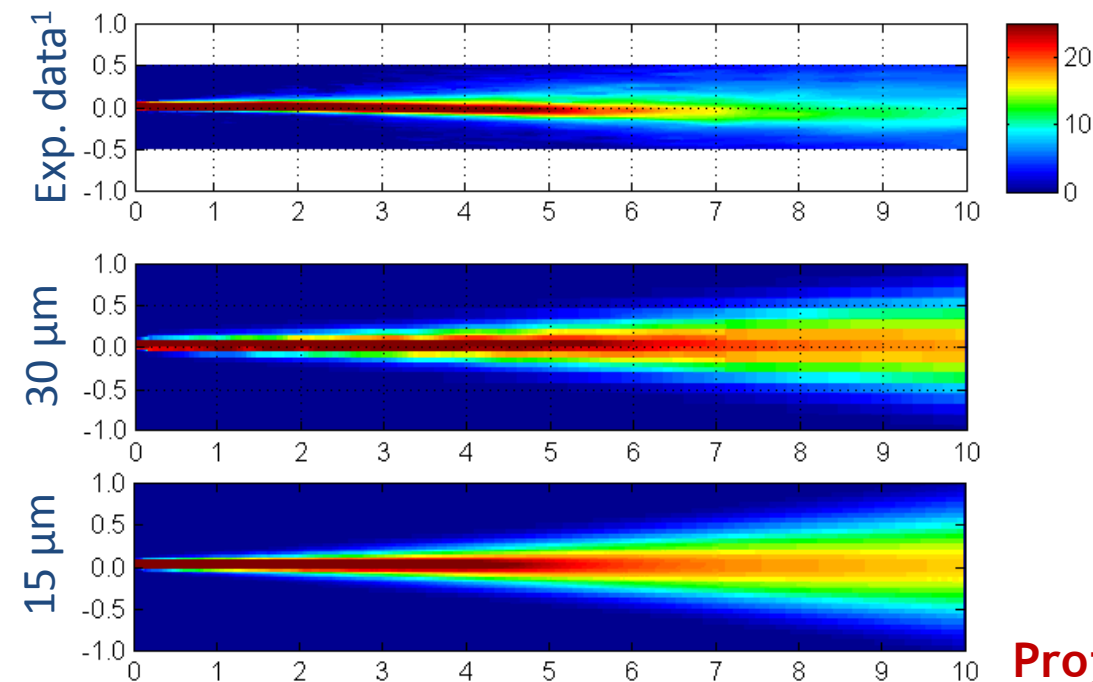
- **High-fidelity "first-of-its kind" simulations**
- Minimum cell size = 5 µm, More than 20 million cells
- Minimum time step size = 1 E-9
- <u>S</u>**imulations explain the physics behind ingested gas in the sac**

Validation of Coupled Eulerian Spray Model

Projected Density at 0.51 ms (µg/mm^2)

X = 2.0 mm

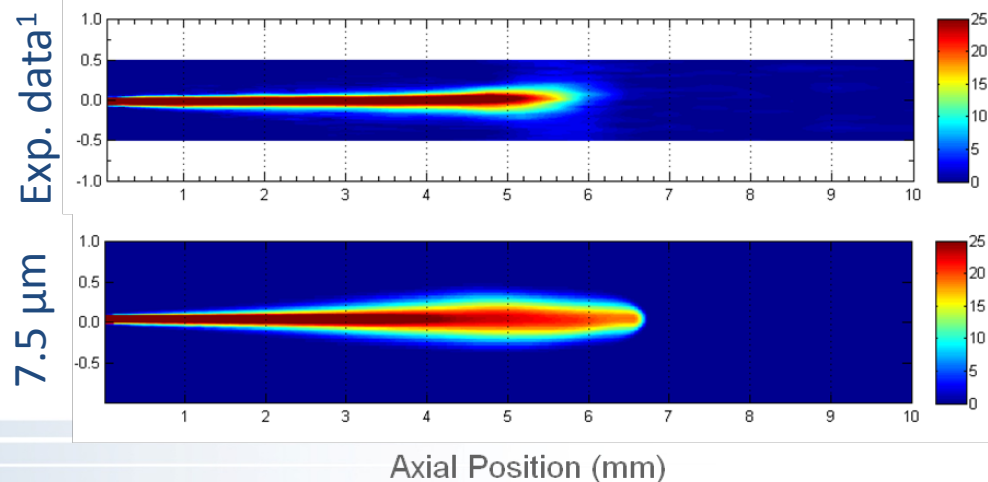

Projected Density at 0.022 ms (µg/mm^2)
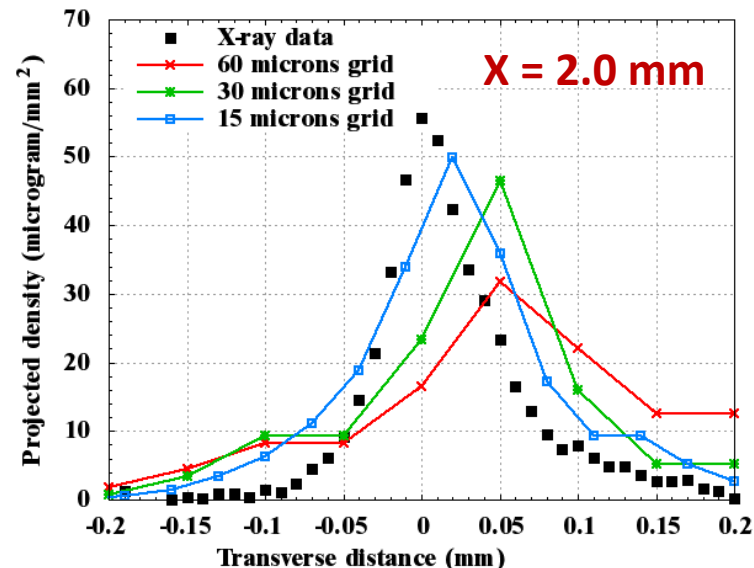
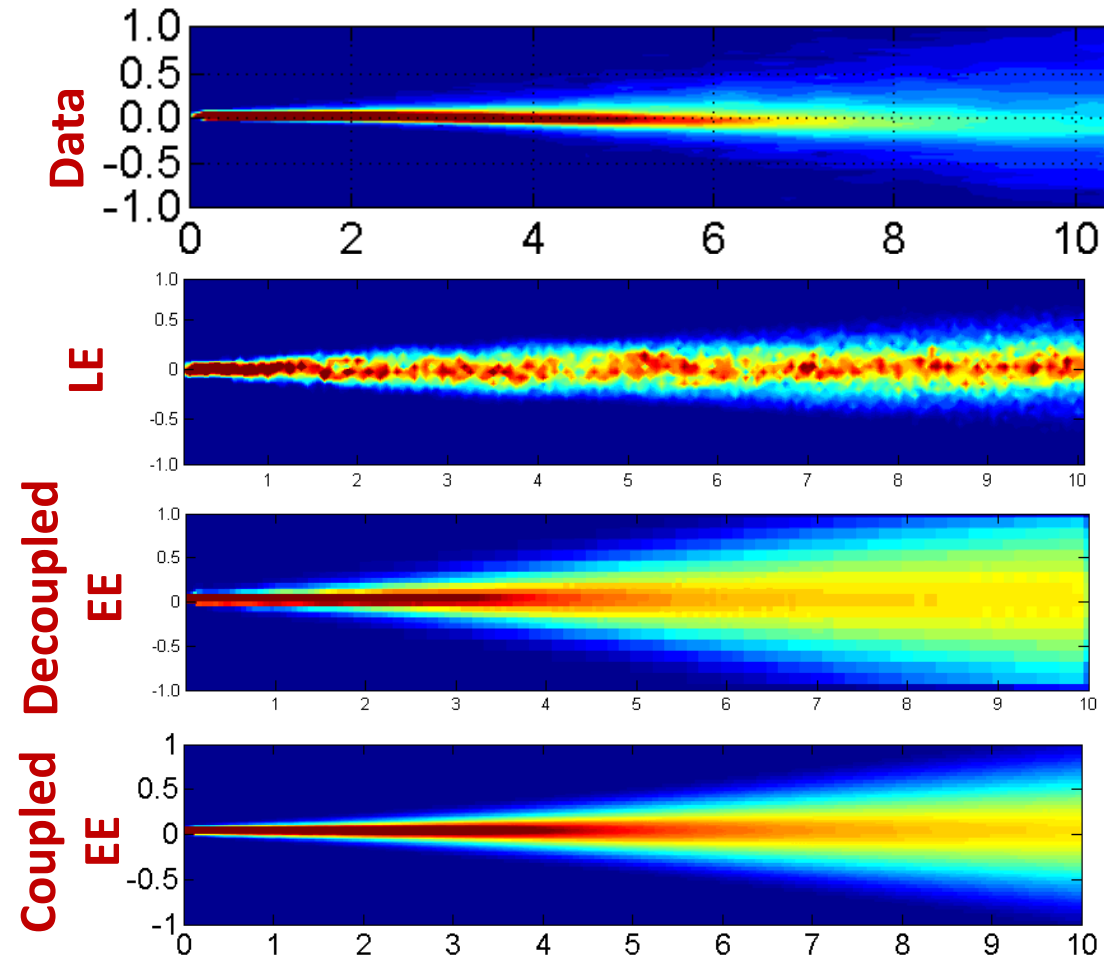Spray A (ECN) nozzle data:
- **Diameter = 90 mm**
- **Injection Pressure = 1500 bar**
- **Back Pressure = 60 bar**
- **Fuel: n-dodecane**

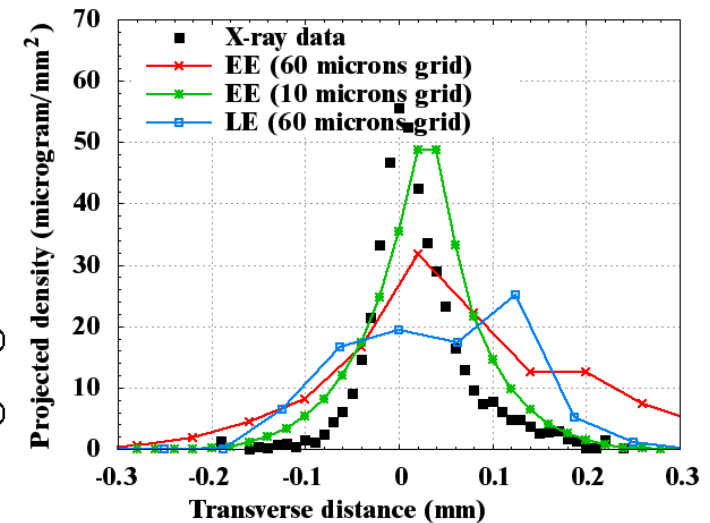1) Kastengren , Powell et al., Atomization and Sprays (2014)

Axial Position (mm)

Comparison of Eulerian and Lagrangian Approaches

❖ Coupled EE model is 3 times more expensive than decoupled EE model
❖ Coupled EE model is about 5 times more expensive than the LE model for the same resolution

❖ Eulerian (EE) model is better than traditional Lagrangian (LE) approach in the near nozzle region
❖ Lagrangian simulations: 62.5μm minimum resolution; blob injection model; 300K parcels
❖ Decoupled EE simulations perform as well as coupled EE model for this case. This shows that if the Rate of injection is reliable, perhaps decoupled EE model is sufficient.

Approach: Diesel Surrogate Mechanism Development

Detailed Mechanism (from LLNL)
2885 species, 11754 reactions

~ 18 times reduction

DRG – X

↓

DRGASA

↓

Isomer Lumping

↓

**Skeletal Mechanism
163 species, 887 reactions**

Computational time scales:

- with $N^2 \sim N^3$ of number of species
- Linearly with number of reactions

Range of operation:
- ✓ Pressure: 1-100 atm
- ✓ Equivalence ratio: 0.5-2.0
- ✓ Initial temperature: 700 – 1800 K

➢ n-dodecane (77%) + m-xylene (23%) used as a surrogate for diesel fuel: **SR23 surrogate**
➢ Reduced model is available for Engine Combustion Network modeling studies
➢ Mechanism development and reduction performed in collaboration with **Prof. T. Lu at University of Connecticut and Dr. W.J. Pitz at LLNL**
➢ Mixture properties obtained from **NIST**
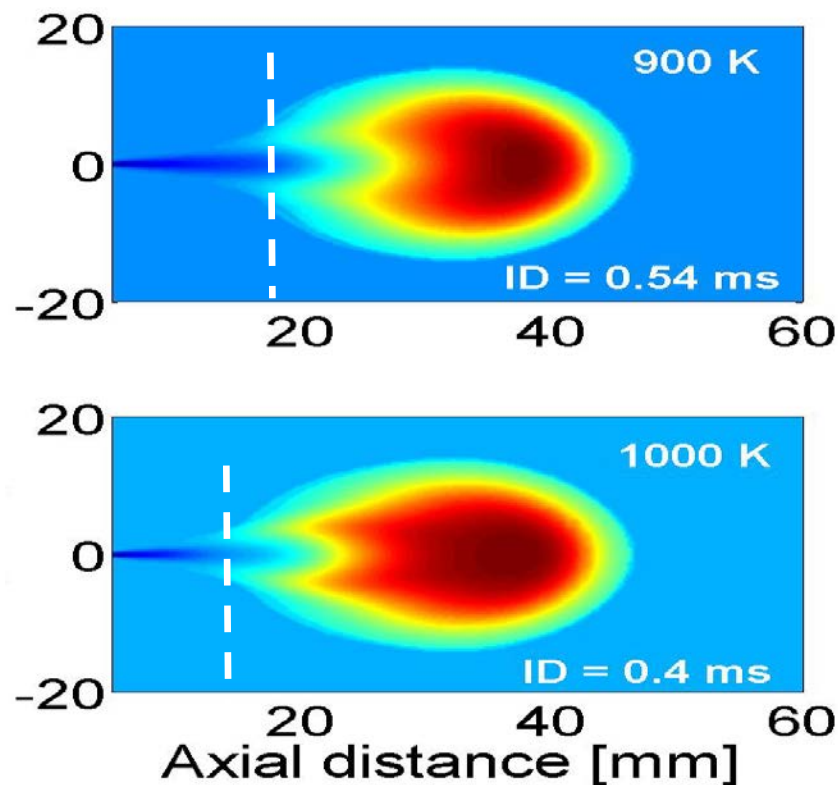➢ **All reduced mechanisms available at:**

www.transportation.anl.gov/engines/multi_dim _model_combustion.html

Symbols: Detailed Mechanism
Lines: Reduced Mechanism
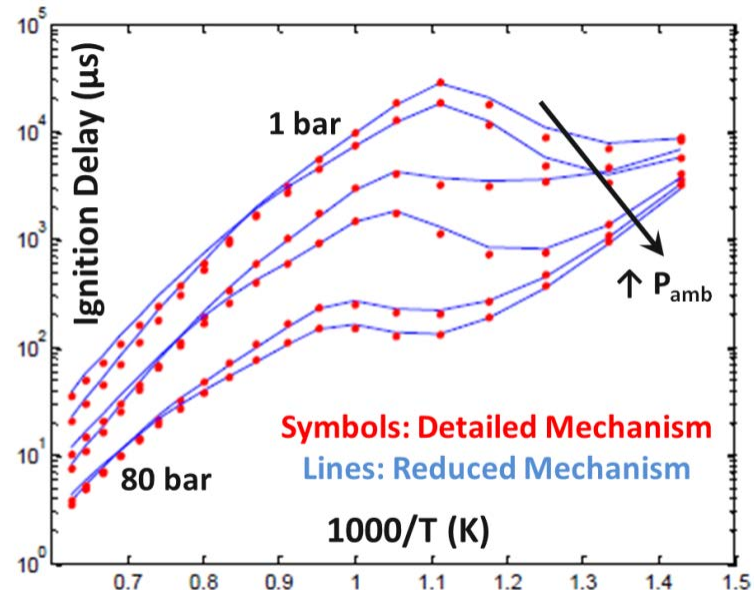
Multi-Component Mechanism Validation
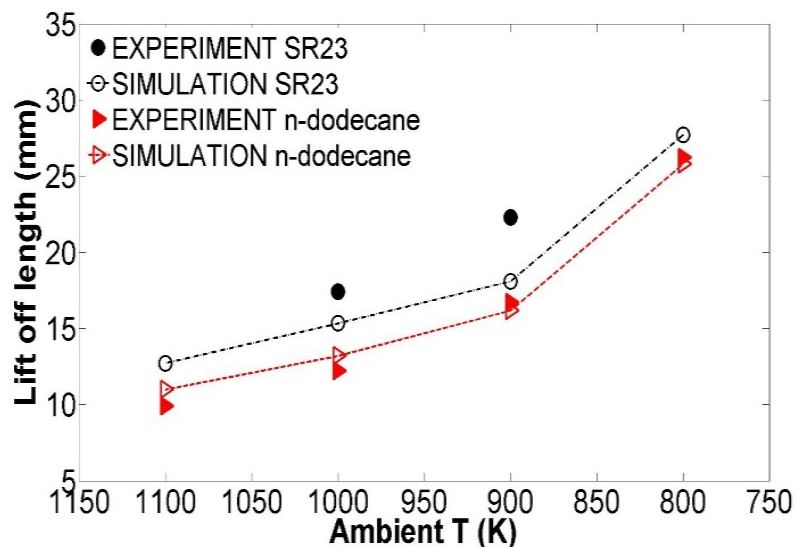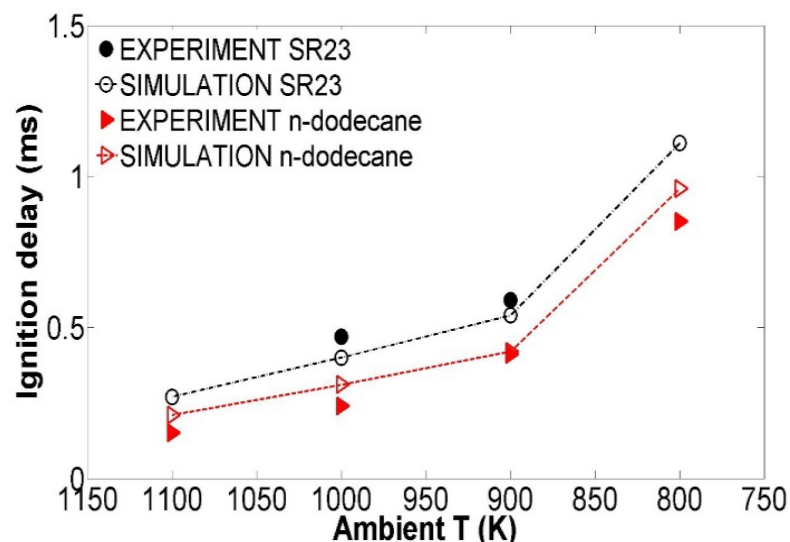
Temperature Contours at 1.5 ms

- Experimental data from Kook et al. {Fuel 2012}, Sandia National Laboratory
- **Simulations can predict the ignition delay very well**
- Simulations tend to under predict flame lift-off length
- N-dodecane results are shown for comparison with the SR23 surrogate
- **Multiple Representative Interactive Flamelet model used for turbulence chemistry interactions**

Future Work: Implement update kinetics from Pitz et al. (LLNL) to improve flame lift-off length predictions

Diesel Engine Simulations using HPC Tools
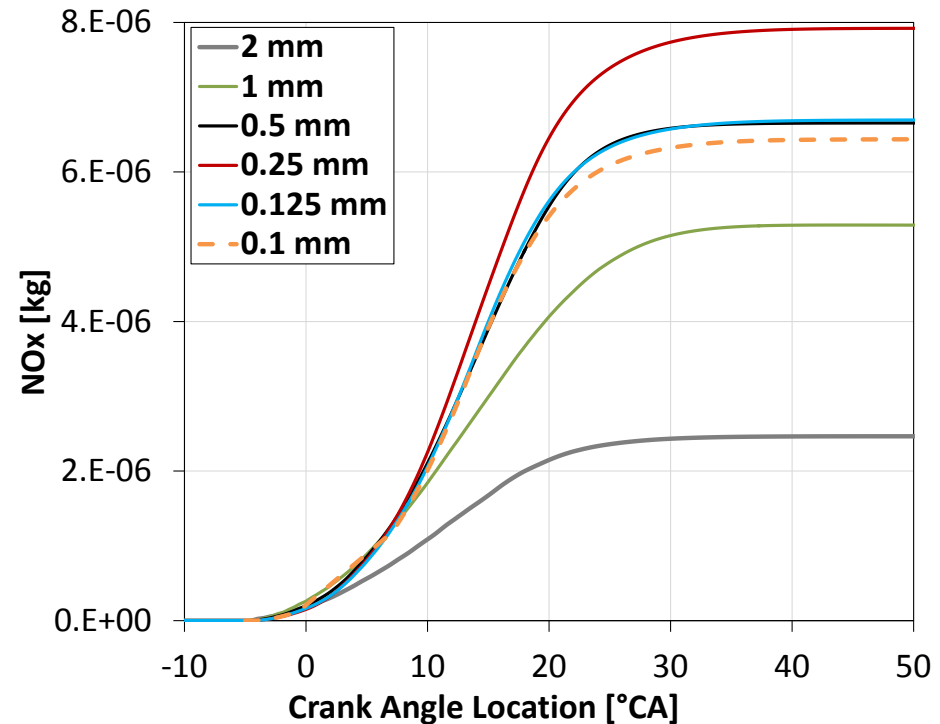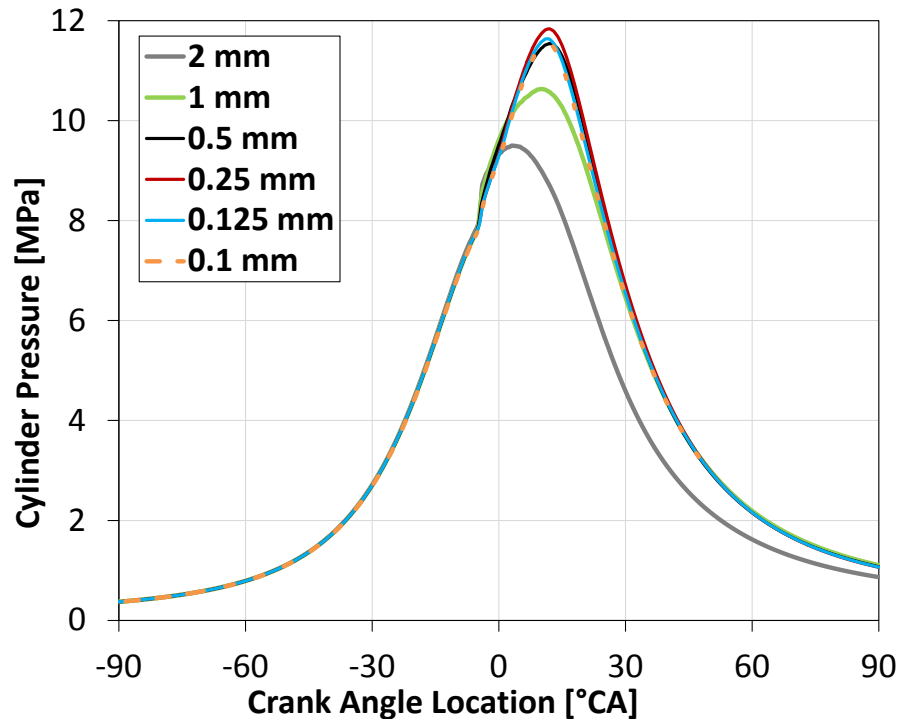
Minimum cell size (mm)	Peak Cell-count	Wall clock time
0.5	2.5 million	14 hours on 64 cores
0.25	9 million	3.5 days on 64 cores
0.125	34 million	13 days on 256 cores
0.1	50 million	14 days on 512 cores

- Single cylinder Caterpillar Engine simulated
- Many parameters such as pressure, heat release rate, grid converge at coarse resolutions of 0.5 mm
- NOx emissions grid converge below 0.125mm

Largest diesel engine simulation performed!!

Typical engine simulation in industry done on 24-64 processors

Collaborations

Argonne National Laboratory
Engine and Emissions Group: (Provide data for model validation)
Chemical Science and Engineering Group: (Mechanism development and reduction)
Leadership Computing Facility (Improving Scalability of CONVERGE, HPC resources)
Mathematics and Computing Science: (HPC resources)

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

Cummins (Provide experimental data, alpha testing of new models)

Caterpillar Inc. (Testing and implementation of HPC tools)

Sandia National Laboratory (Provide experimental data through the ECN)

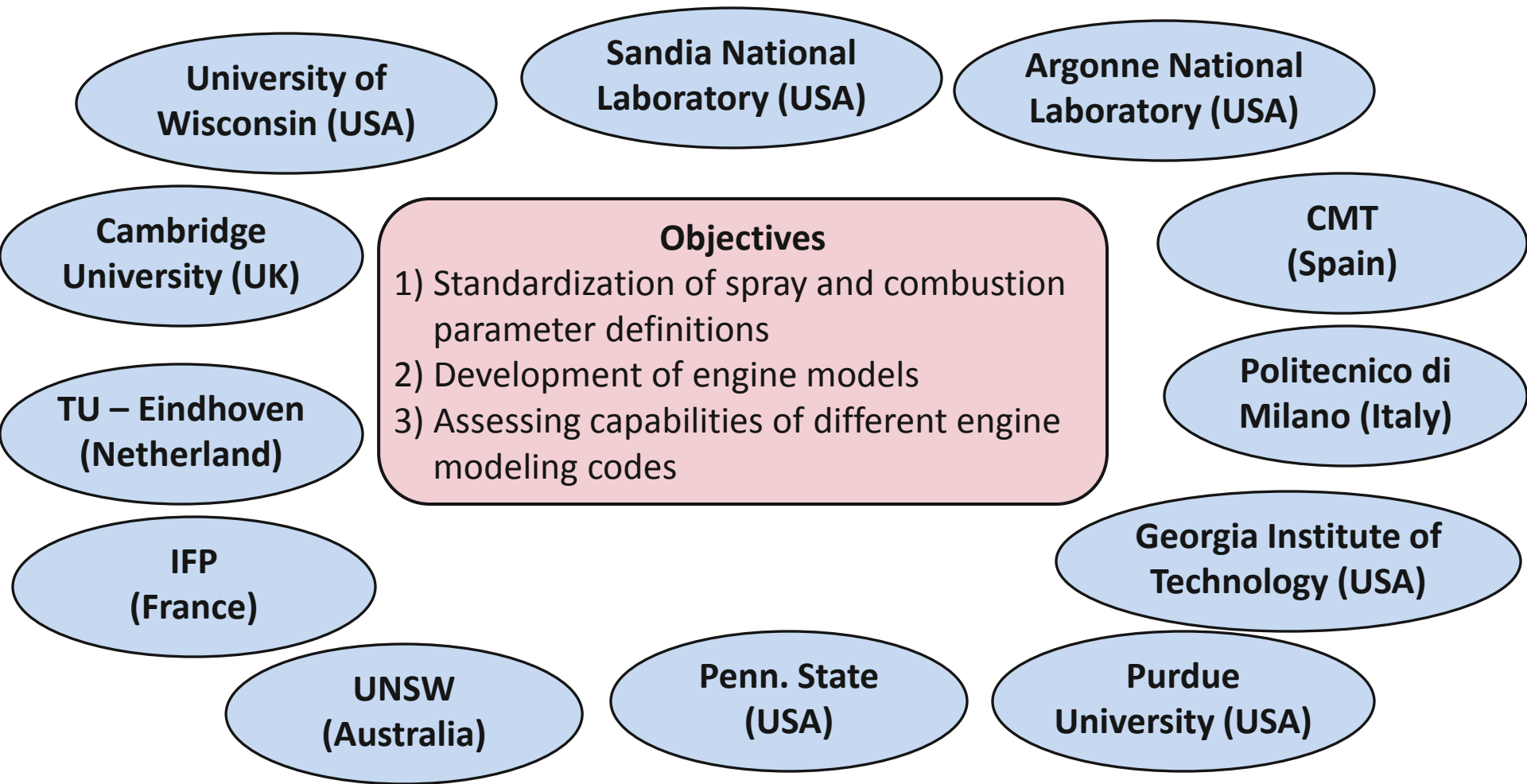**Lawrence Livermore National Laboratory (Mechanism development)**

University of Connecticut (Mechanism Reduction)

University of Perugia (Visiting Scholar: Cavitation and Spray Modeling)

Politecnico di Milano (Spray and Combustion modeling using OpenFOAM)

Engine Combustion Network Organization

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 engine modeling codes

TU – Eindhoven (Netherland)

Politecnico di Milano (Italy)

IFP (France)

Georgia Institute of Technology (USA)

UNSW (Australia)

Penn. State (USA)

Purdue University (USA)

- ❑ Topic 1 (Near nozzle flow and sprays): Som (leader), Pei and Xue (Organizers)
- ❑ Accelerated the development of models due to the availability of high-fidelity data
- ❑ Motivated experiments to measure parameters that they would not measure otherwise

Response to Previous Year Reviewer Comments

1. How does this work couple with the validation in real application?

We have simulated the **Chrysler Dual Fuel Engine** (AMR 2014 presentation by Ron Reese, Chrysler LLC.) and the **Gasoline compression ignition engine** (AMR 2014 presentation by Dr. Steve Ciatti, Argonne) to demonstrate the use of our approaches on real applications. We have also **published 2 papers on these engine simulations, focusing heavily on the validation aspect**.

2. It is unclear how successful the high fidelity approach is towards becoming more predictive.

The high-fidelity approaches are typically grid-convergent. Hence, the **grid size is not a tuning parameter anymore in simulations**, thus reducing a degree of uncertainty in the calculation. The **high-fidelity simulations (EE model) has only one constant compared to the lower fidelity (LE model) which has multiple constants** for simulating spray breakup.

3. It is unclear on what the plan is to transfer the findings of this work to engineering models that can be used for engine design.

All the models developed in this program are **available for the engine designers through the CONVERGE code**. These models are typically more expensive than the standard Lagrangian models, but do offer more insights into the spray processes. Our **grid-convergence studies have also shown that coarse mesh simulations can provide useful insights at a reasonable cost**

4. What is the long term vision of this activity?

The long term vision is to develop spray and combustion models for diesel and gasoline fuels of interest. Since the models will be robust, high-performance computing tools will also be developed in parallel to ensure reasonable computational costs. **The ultimate goal is to provide the industrial partners predictive modeling approaches at reasonable computational cost (also keeping in mind that the computational power is growing rapidly)**

# Remaining Challenges and Barriers

❖ Nozzle flow and spray simulations:

  ❖ EE models need a primary breakup model, since the turbulence mixing based models only capture mixing but not spray breakup

  ❖ In order to accurately resolve the flow field in the needle seat region and at the walls, **more grid resolution is desirable**. This is quite challenging with the current approach of using the cut-cell gridding algorithms

  ❖ Nozzle flow simulations need to **account for liquid compressibility effects and temperature variations**. Current simulations are performed assuming isothermal conditions inside the nozzle

  ❖ In order to capture the initial transients, coupled simulations need to start with very low needle lift values, which also necessitates the using of very fine resolutions in the needle seat region

Grid = 2.5 μm

❖ The quest for better and more representative chemical kinetic models will require the use of a three component mixture for diesel fuel => continue collaborative research with Pitz et al. from LLNL
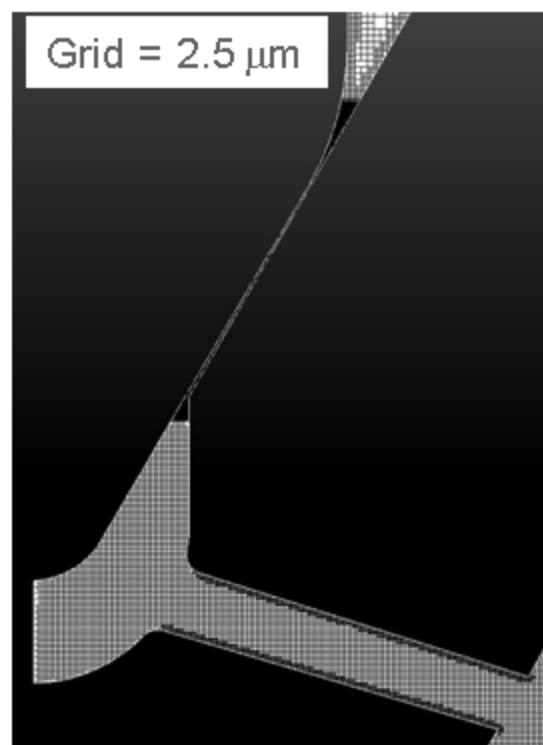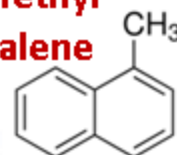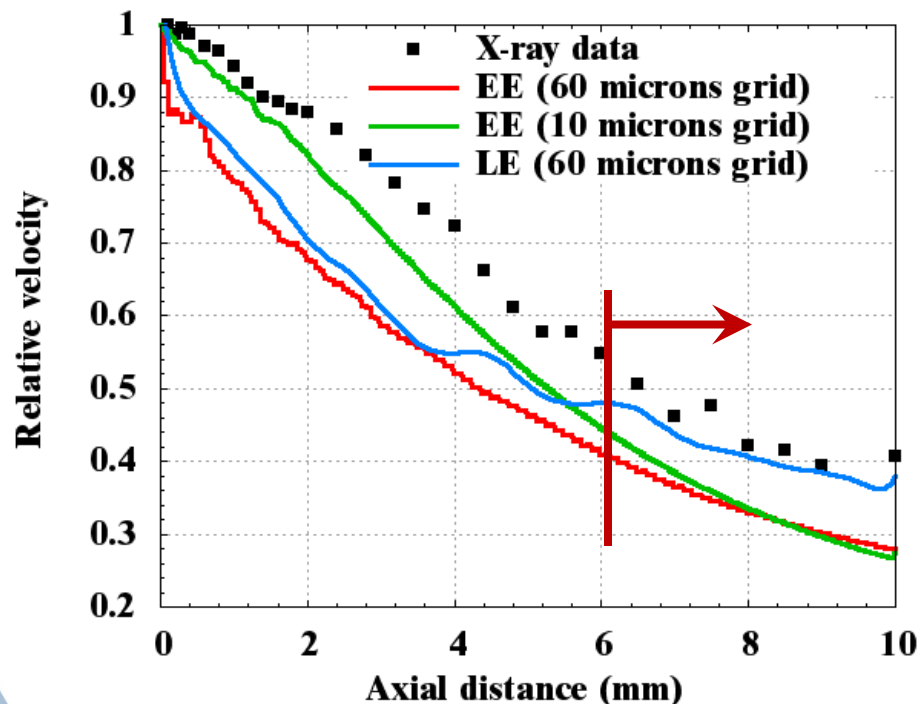
N-Cetane

iso-Cetane
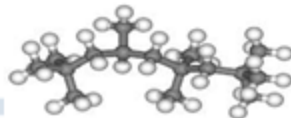
Alpha Methyl Naphthalene   CH$_3$

Future Work - 1

1) Determine how many LES injections are necessary to mimic all experimental characteristics for combustion simulations
   - Already performed 20 injections for Spray A
2) Transition to a Eulerian-Lagrangian spray model
   - Perhaps 6 mm downstream would be a good location for transition

**Relevance Index*: A criteria for determining when to end LES spray realizations**
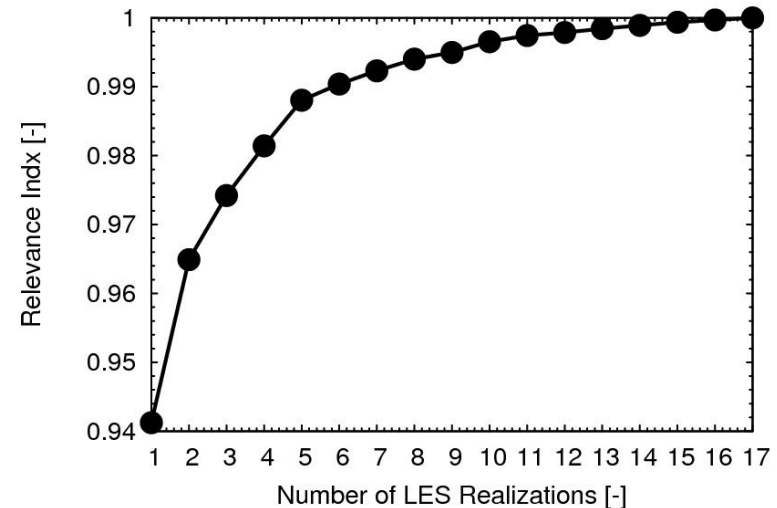
$$f_{u,v} = \frac{(u,v)}{\| u \| \| v \|}$$

* Analysis performed by Dr. Siddhartha Banerjee and Dr. Bing Hu at Cummins Engine Company as part of the CRADA

Future Work - 2

3) In-nozzle flow simulations with Cummins specific hardware (CRADA)
   – X-ray phase contrast imaging in-progress to obtain relevant boundary conditions

Phase-Contrast Imaging at the Advanced Photon Source at Argonne

Lift vs. wobble amplitude
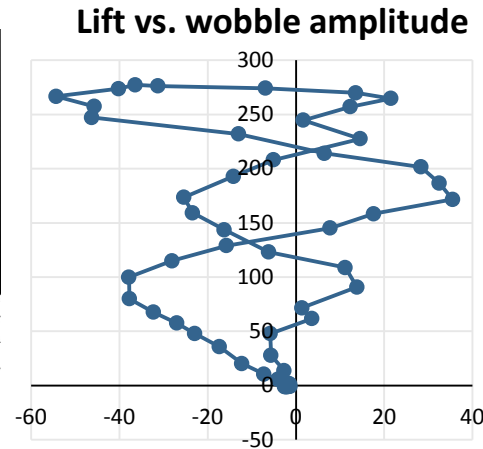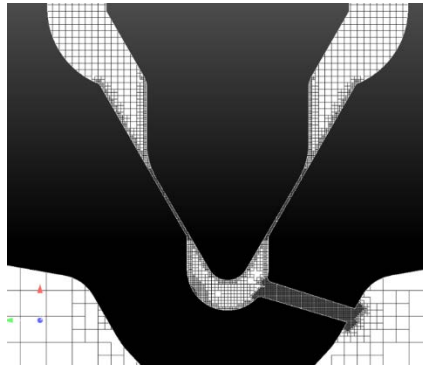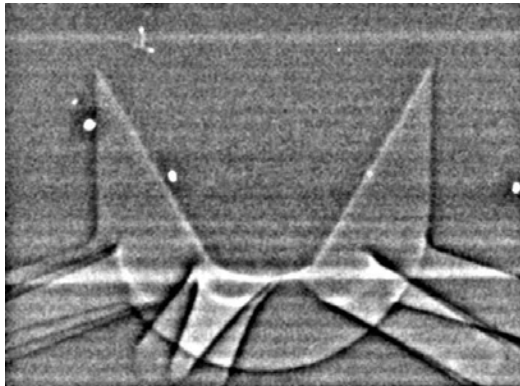
9-hole Cummins injector

4) HPC enabling multi-cylinder Caterpillar Engine Simulations (CRADA)
   - How many simulations are needed to wash out the influence of initial guesses in open cycle engine simulations?
   - What is the appropriate resolution for multi-cylinder simulations keeping in mind accuracy and computational costs?
   - What resolution is necessary for flow through ports and plenums to capture the fluid dynamics characteristics?

Summary

❑ **Objective**
  ➢ Development of predictive spray, turbulence, and combustion models aided by high-performance computing tools and comprehensive validation

❑ **Approach**
  ➢ Coupling expertise from DOE Office of Science on fundamental chemical kinetics, industrial partners, and HPC resources for development of robust engine models

❑ **Technical Accomplishment**
  ➢ Effect of *needle off-axis motion* quantified with in-nozzle simulations
  ➢ Coupled Eulerian Spray model developed and implemented in CONVERGE
  ➢ End-of-Injection transients explored and understood with high-fidelity simulations
  ➢ Multi-component surrogate model for diesel fuel developed and tested
  ➢ HPC resources enabled simulation of the largest diesel engine case showing grid convergence of both combustion and emission characteristics of interest

❑ **Collaborations and coordination**
  ➢ with industry, academia, and national laboratories in US
  ➢ through ECN with researchers world-wide

❑ **Future Work**
  ➢ Transition to an Eulerian-Lagrangian approach for comprehensive spray modeling
  ➢ Development and validation of realistic diesel surrogate chemical kinetic model
  ➢ Identify numerical "best practices" for multi-cylinder simulations with HPC resources

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.)

Eulerian Mixture & Cavitation Model

Mixture Model equations (homogeneous multi-phase model)

Continuity: $\dfrac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{v} = 0$

mixture density: $\rho = \displaystyle\sum_{i=1}^{n} \alpha_i \rho_i$

Momentum: $\dfrac{\partial \rho \vec{v}}{\partial t} + (\nabla \cdot \rho \vec{v})\vec{v} = -\nabla p + \nabla \cdot \bar{\bar{\tau}} + \rho \vec{f}$

volume & mass fractions: $\alpha_i \rho_i = Y_i \rho$

Species: $\dfrac{\partial \rho Y_i}{\partial t} + (\nabla \cdot \rho Y_i)\vec{v} = \nabla \cdot (\rho D_i \nabla Y_i) + S_i$

void fraction: $\alpha_g = \dfrac{Y_g / \rho_g}{\sum Y_i / \rho_i}$

(plus: Energy, Turbulence)

Mass transfer: Homogeneous Relaxation Model (HRM) [1,2]

The model accounts for non-equilibrium heat transfer phenomena, using an empirical correlation

Hypothesis: finite rate of relaxation to equilibrium

$$\frac{dY_v}{dt} = \frac{Y - \bar{Y}_v}{\Theta}$$

Exponential relaxation of the vapor quality Y to the equilibrium table value $\bar{Y}_v$ over a timescale Θ.

$$\bar{Y}_v = \frac{h - h_l}{h_v - h_l} \qquad \Theta = \Theta_0 \alpha^a \psi^b \qquad \psi = \left| \frac{p_{sat} - p}{p_{crit} - p_{sat}} \right|$$

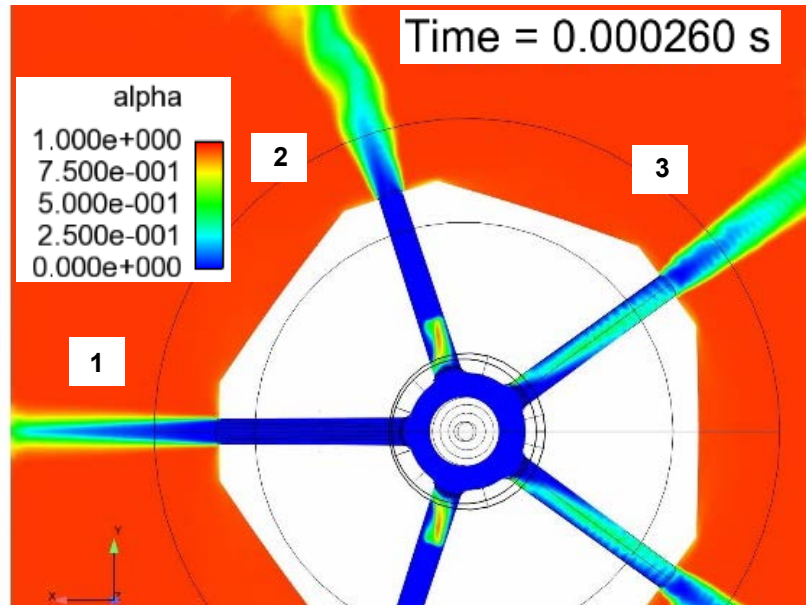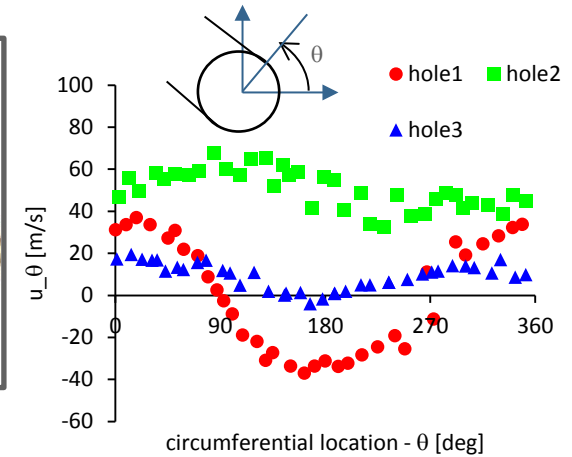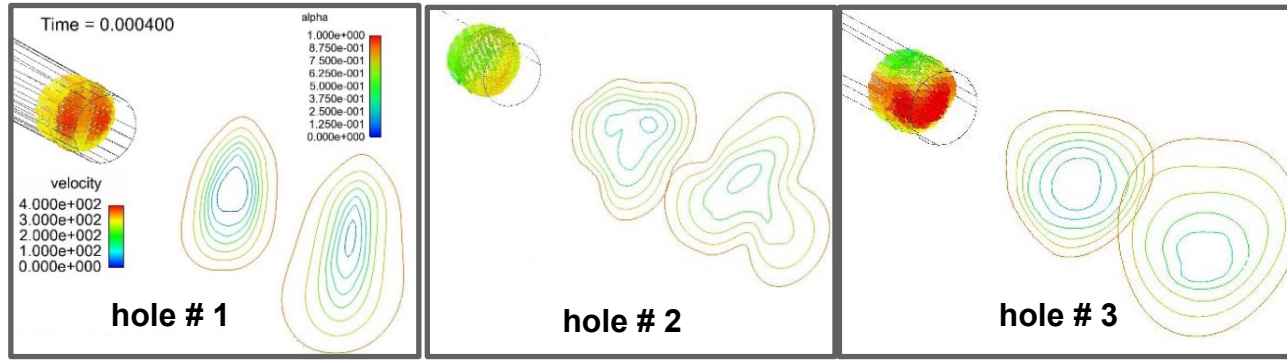## Mixture: 1. liquid + 2. vapor + 3. air

1. Schmidt, D. P., et al., *Int. J. of Multiphase Flow*, 2012
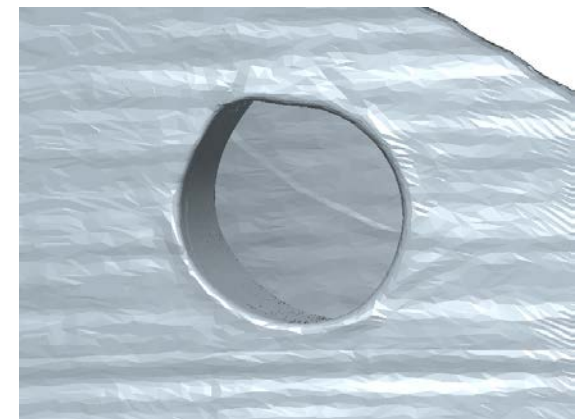2. Bilicki and Kestin, *Proc. Roy. Soc. Lond. A.*, 1990

Further Details About Eulerian Mixture Model

- ❑ VOF method used to model the internal nozzle two-phase flow with cavitation description closed by the homogeneous relaxation model
- ❑ Eulerian single velocity field approach by Vallet et al. (2001) is implemented for near-nozzle spray simulations
  - *Large scale flow features* dominate rather than the small scale structures under the high Reynolds and Weber number conditions
- ❑ This approach considers the liquid and gas phases as a complex mixture with a highly variable density to describe the dense spray region
  - Mean density is obtained from Favre-averaged liquid mass fraction: $\dfrac{1}{\bar{\rho}} = \dfrac{\tilde{Y}}{\rho_l} + \dfrac{1 - \tilde{Y}}{\bar{\rho}_g}$

- ❑ The liquid mass fraction is transported with a model for the *turbulent liquid diffusion flux into the gas*:

$$\frac{\partial \bar{\rho}\tilde{Y}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{Y}}{\partial x_i} = -\frac{\partial \overline{\bar{\rho}u_i'Y'}}{\partial x_i} - \bar{\rho}\dot{\tilde{Y}}_{evap}$$

- ❑ *Closure for the liquid mass transport is based on a turbulent gradient flux model*:

$$\overline{\bar{\rho}u_i'Y'} = \frac{\mu_t}{Sc_t}\frac{\partial \tilde{Y}}{\partial x_i}$$

- ❑ Void fraction (α) $= \begin{cases} 0 & \text{if the computational cell is filled with pure liquid} \\ 1 & \text{if the computational cell is filled with pure gas} \\ (0,1) & \text{if the computational cell is filled with both liquid and gas} \end{cases}$

* Xue, Som, et al. SAE Journal of Fuel and Lubricants, 2014

Needle wobble: near-nozzle hole-to-hole variation

hole # 1

hole # 2

hole # 3

u_θ [m/s]

circumferential location - θ [deg]

- hole1 - hole2 - hole3

Time = 0.000260 s

alpha
1.000e+000
7.500e-001
5.000e-001
2.500e-001
0.000e+000

2   3

1

Spray B – hole #3 (ECN3) [1]

High res. Tomography [2]

- ✓ «Non regular» liquid distributions in the near-nozzle region
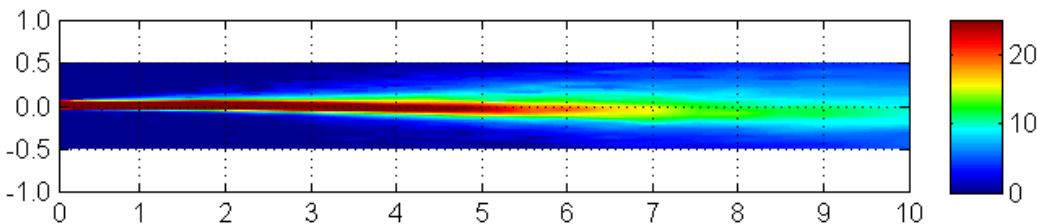- ✓ Demand for near-nozzle validation data

1. **Pickett L. et al. (ECN3, 2014)**
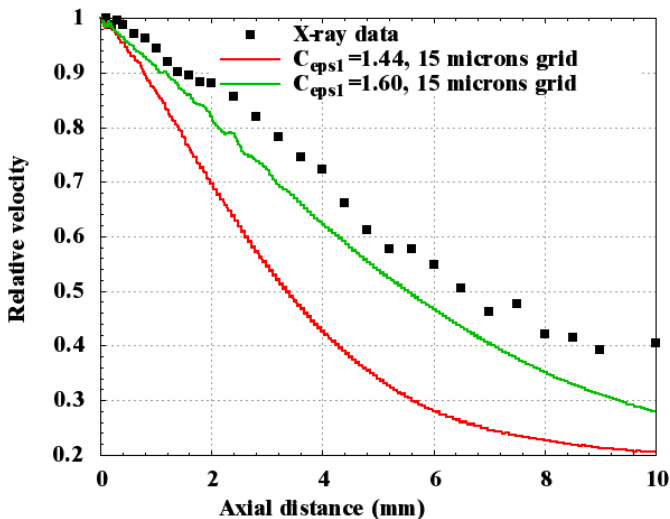2. **courtesy of Peter Hutchins, Infineum Ltd**

26

Eulerian spray model: Turbulence Model Constant
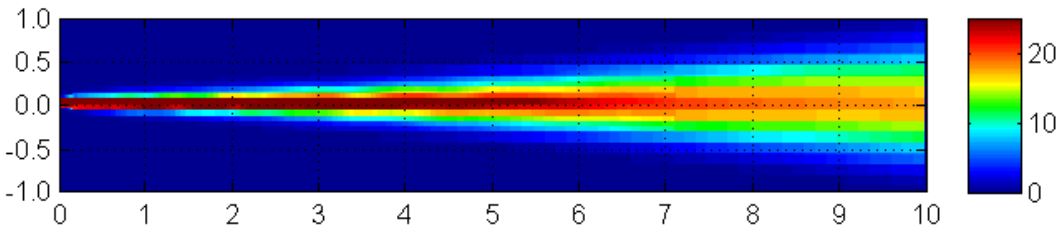
Projected mass at 0.51 ms ASOI (μg/mm^2)

Experimental Data
Powell et al. Argonne National Laboratory

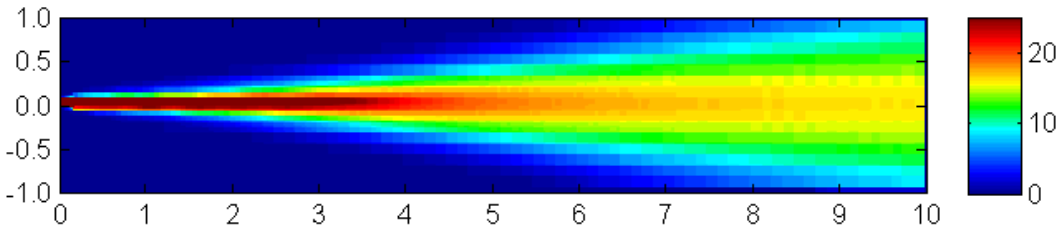
Mass-averaged spray velocity along spray axial distance at 0.51 ms ASOI

C_{eps1} = 1.60 (round jet correction[1])

C_{eps1} = 1.44 (standard model constant)

1. Pope, S. B., *An explanation of the turbulent round-jet/plane-jet anomaly*, AIAA Journal (1978)

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.

❑ <u>Data available for :</u> Spray penetration, liquid length, vapor penetration, mixture fraction, ignition delay, flame lift-off length, soot distribution , high-speed movies
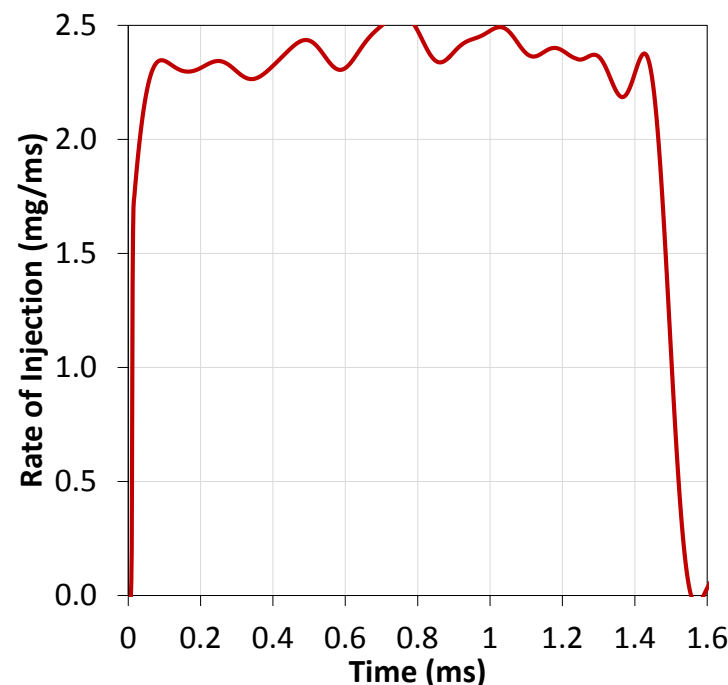
Computational Resources

We gratefully acknowledge the computing resources provided at Argonne National Laboratory

- Fusion: ~ 2,500 - core computing cluster

- Blues: ~ 5,000 - core computing cluster

operated by the Laboratory Computing Resource Center

- Vesta: ~ 33,000 – core super-computer

- Mira: ~ 758,000 – core super-computer

operated by the Leadership Computing Facility

Fusion Cluster

MIRA Super-Computer