WE START WITH YES.

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ADVANCEMENTS IN FUEL SPRAY AND COMBUSTION MODELING WITH HIGH-PERFORMANCE COMPUTING RESOURCES

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Project ID # ACS075

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

OVERVIEW

Timeline

Project start: April 1st 2012
Part of 2017 lab call

Partners

Argonne National Laboratory
Mathematics and Computing Science
Leadership Computing Facility
Advanced Photon Source
Convergent Science Inc. {CRADA}
Cummins Engine Company {CRADA}
General Motors R&D
Lawrence Livermore National Laboratory
Sandia National Laboratory
Advanced Engine Combustion (AEC)
Co-Optima
Advanced Computing Tech Team (ACTT)
University of Connecticut
University of Perugia (Italy)
Several University FOAs

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 15: 525 K
FY 16: 490 K
FY 17: 370 K*
* Note: reflects reduced spending rate

OBJECTIVES AND 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:

- Fuel spray and nozzle-flow models
- Detailed chemistry based combustion models
- Fine mesh => grid-convergence
- Improved load-balancing algorithms with METIS
- High-fidelity turbulence models: LES based

+

- High-Performance Computing

Towards Predictive Simulation of the Internal Combustion Engine

- Develop reliable engine modeling capability with fewer tuning constants
- Sub-models published in open-literature and available to the industry through software packages
- Develop "engineering best practices" for industry to use these high-fidelity models

RELEVANCE – NEED FOR SPEED AND AVAILABILITY TO OEMS*

- **Nozzle flow and Spray research**
  - In-nozzle flow and fuel spray in the near nozzle region plays a central role in combustion and emission processes
  - *One-way coupling* allows high-fidelity nozzle flow simulations to be effectively coupled with near-nozzle simulations
  - *One-way coupling* approach validated for gasoline and diesel sprays is now available for OEMs through CONVERGE
- **Combustion modeling using detailed chemistry**
  - Accurate chemical kinetics for fuel surrogates are key for predictive combustion modeling
  - We developed a Tabulated Flamelet model (TFM) that allows us to include both detailed chemical kinetics and turbulence chemistry interaction in a cost-effective manner
  - TFM is currently available through UDFs that can be ported to any academic or commercial code
- **High-Performance Computing (HPC)**
  - Current state-of-the-art for engine simulations in OEMs involve up to 50 processors (approx.) only on clusters: high throughput computing allows ~10k such simulations in a matter of weeks for engine design on Mira
  - These HPC advancements are now available for OEMs through CONVERGE v2.3 or custom made executables on Mira

Cluster

Super-Computer

* DOE-VTO workshop to identify roadmap for CFD organized by Leo Breton in 2014

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SIMULATION APPROACH: SUB-MODEL DEVELOPMENT

Modeling Tool	CONVERGE
Smallest and largest characteristic grid size(s)	**Finest grid size simulations:** **2.5 µm for nozzle flow (35 million cells)** **~30 µm for GDI and diesel Sprays (20 million cells)** **~60 µm for spray combustion (30 million cells)**
Turbulence-chemistry interaction (TCI) model	**Tabulated Flamelet model (TFM)** **Homogeneous Reactor based model (HR)**
Turbulence model(s)	LES: Dynamic Structure sub-grid scale model ✓ Extensive nozzle flow and GDI spray simulations
In-nozzle Flow	**Homogeneous Relaxation Model (HRM)** ✓ Diesel and gasoline injectors ✓ Extended for multi-component fuels
Spray models	Volume of Fluids (VOF) approach for phase-tracking **Coupled Eulerian-Eulerian Near Nozzle Model** **one-way coupling approach**
HPC Developments for simulations on MIRA	**Capability Computing: Scalability on 8k processors** **Capacity Computing: ~10k simulations in 1-2 weeks**

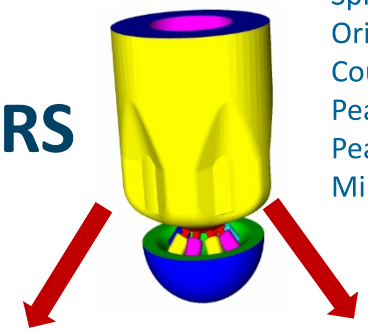
Extensive Validation using experimental data from Engine Combustion Network (Courtesy Lyle Pickett et al.) and X-ray data (Courtesy Chris Powell et al.)

MILESTONES FOR FY 17

- Nozzle flow and Spray Research (CRADA with Cummins and CSI)
  - Validation of *one-way coupling* approach against diesel and gasoline nozzle flow and spray data {100% complete: December 2016}
- Combustion Modeling with Detailed Chemistry
  - Multi-component (4-component) diesel surrogate mechanism development and reduction followed by validated engine simulations (with TFM) against optical engine data from Sandia {50% Complete}
  - Robust validation of TFM against single and multi-component constant volume data for diesel surrogates from Sandia ECN data. Model implemented in Converge code. {60% complete}
- High-Performance Computing
  - Identify computational bottlenecks for scaling high-fidelity nozzle flow and spray simulations on Mira {0% complete}

All the newly developed models and key findings are published in journal papers and peer-reviewed conference proceedings so that academia, OEMs, and other software vendors can benefit from our work. Several OEMs and software vendors have engaged with us through the VERIFI program

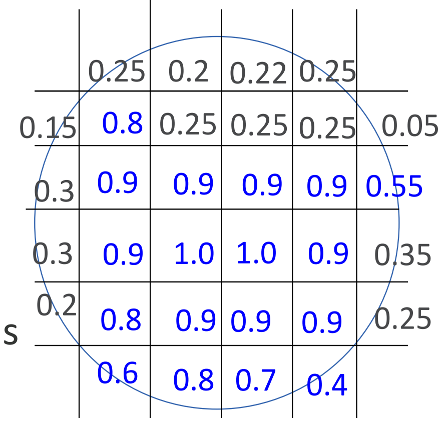
ACCOMPLISHMENT: *ONE-WAY COUPLING* FOR MULTI-HOLE INJECTORS



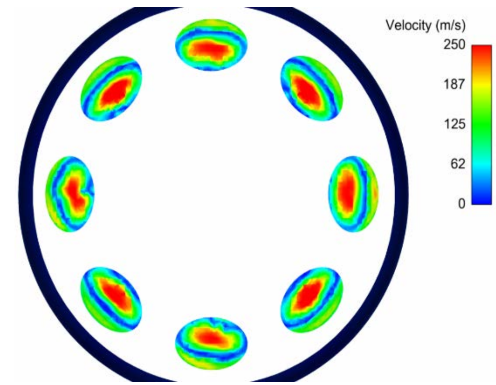
Spray G: ECN injector
Orifice dia. = 165 µm
Counter-bore dia. = 388 µm
Peak needle lift = 45 µm
Peak cell count ~4.5 millions
Min. cell size = 15 µm

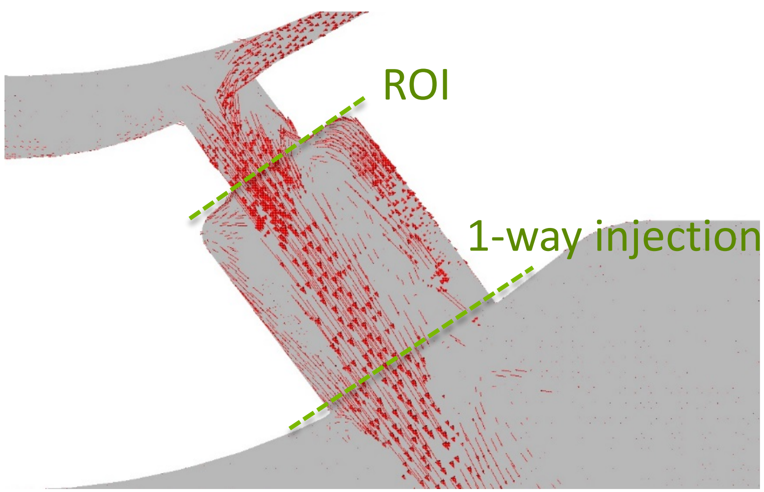
- Rate of Injection (**ROI**) profile allows us to provide the same mass flow rate at the hole exit for each orifice => **plume-to-plume variations cannot be captured**
- In-nozzle flow simulations provide information on hole-to-hole variations ***one-way coupling*** approach allows:
  - Different mass flow rate and discharge coefficient per orifice
  - Capture effects of backflow of chamber gas into the counter-bore (**partial hydraulic flip**) and its influence on the ensuing spray

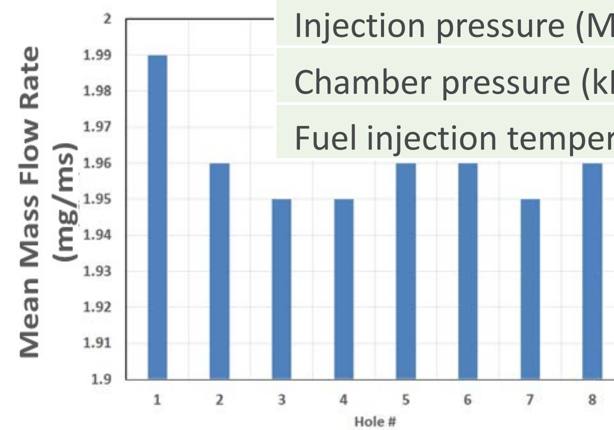
Liquid Volume fraction at counter-bore exit



Velocity at counter-bore exit







Injection pressure (MPa)	20
Chamber pressure (kPa)	600
Fuel injection temperature (K)	363

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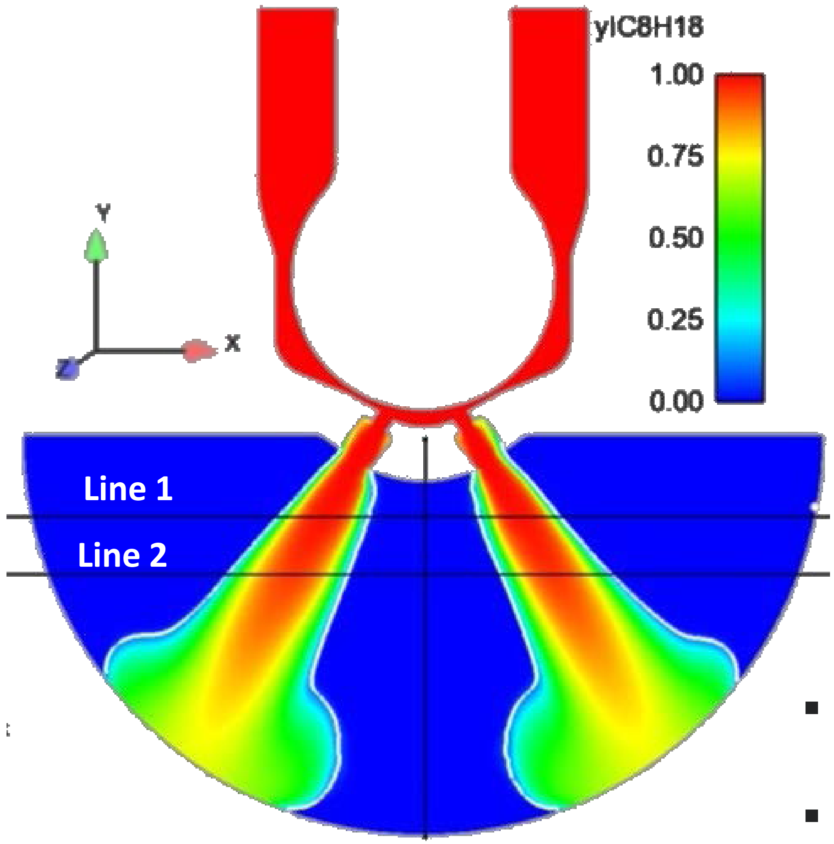
ACCOMPLISHMENT*: PLUME CONE-ANGLE AND TARGETING ESTIMATED FROM NOZZLE FLOW SIMULATIONS

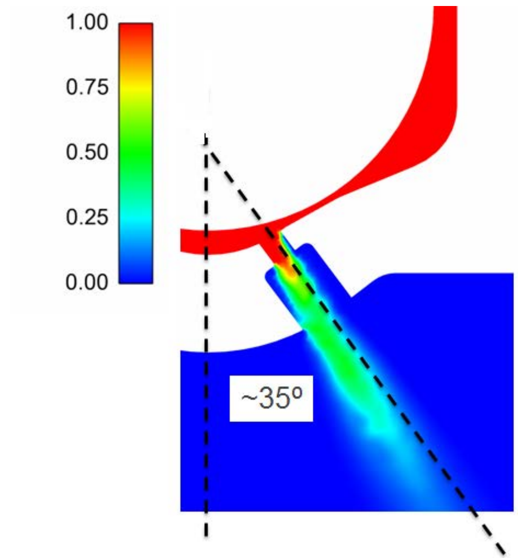


Ensuing jets are clearly not round jets, but rather elliptical in nature

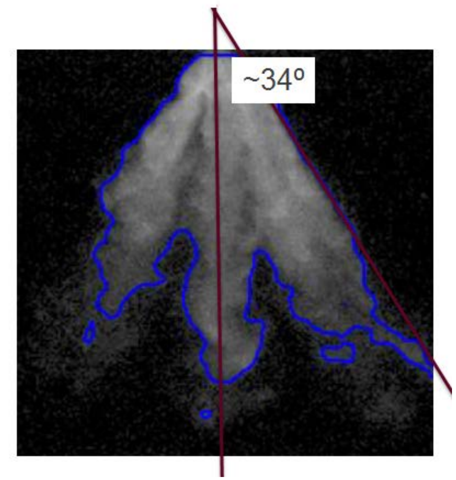
X-Y = 21^{o} Z-Y = 29^{o}

@ 0.5 ms from SOI

Effective Spray Cone Angle ≈ 25^{o}



Experiments by Manin et al. JSAE 2015



Simulations reveal that plume targeting angle is different from the geometrical drill angle of 37°

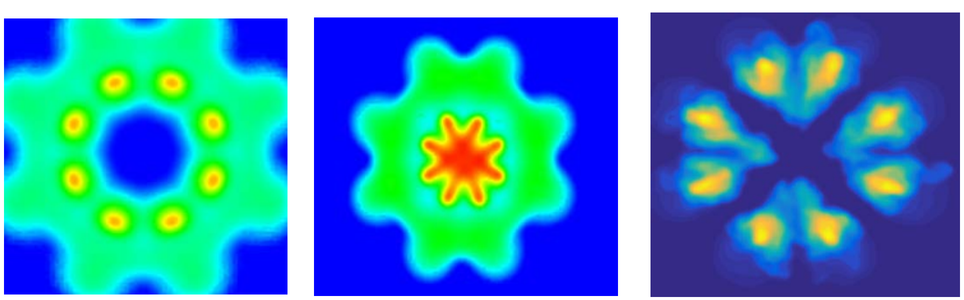
- Nozzle flow simulations allow us to predict transient information of spray cone angle variation
- Nozzle flow simulation enable us to predict accurate spray targeting information, consistent with experimental observations
- Transient plume cone angle and spray targeting information will provide improved boundary conditions for Lagrangian spray calculations

*Selected as an ACEC accomplishment

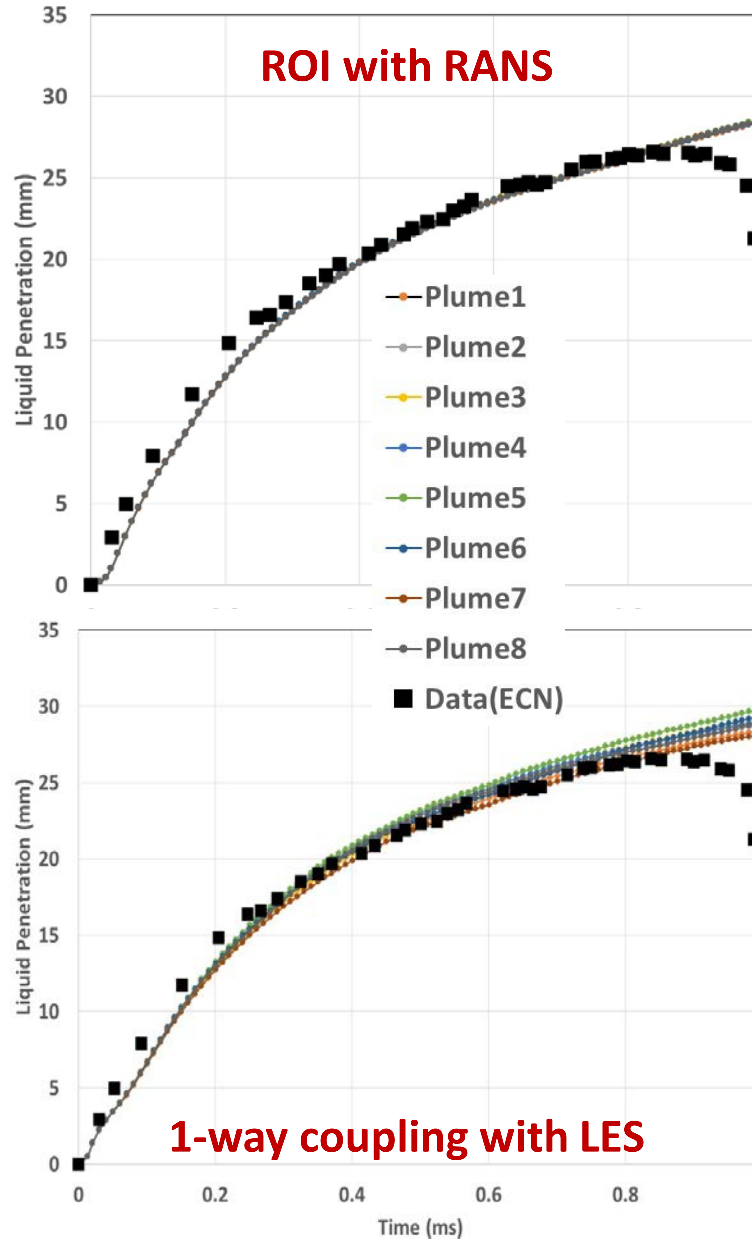
ACCOMPLISHMENT: LES *ONE-WAY COUPLING* IS MORE PREDICTIVE THAN ROI APPROACH

- Experimental data for validation is obtained from the Engine Combustion Network at Sandia. Under these conditions, plume merger is not expected at 0.7 ms from SOI
- One-way coupling demonstrates liquid penetration differences up to 10% between the plumes which is not captured with the ROI approach
- Higher-fidelity turbulence model (LES) in conjunction with one-way coupling approach can capture the experimental trends accurately

ROI with RANS | One-way coupling with RANS | One-way coupling with LES

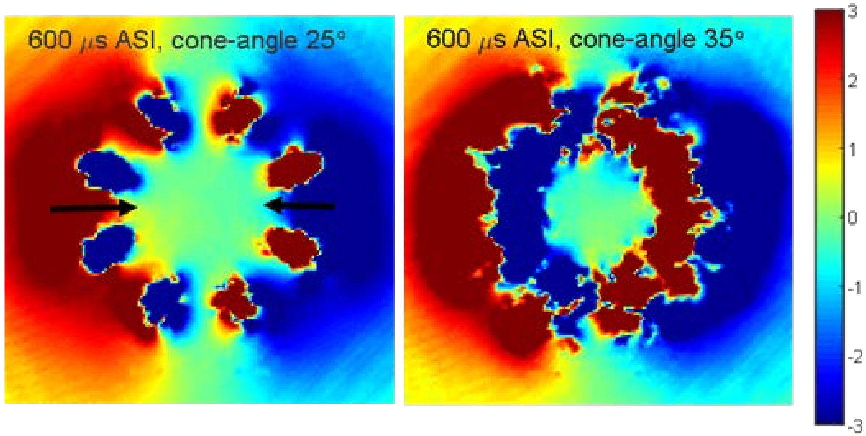


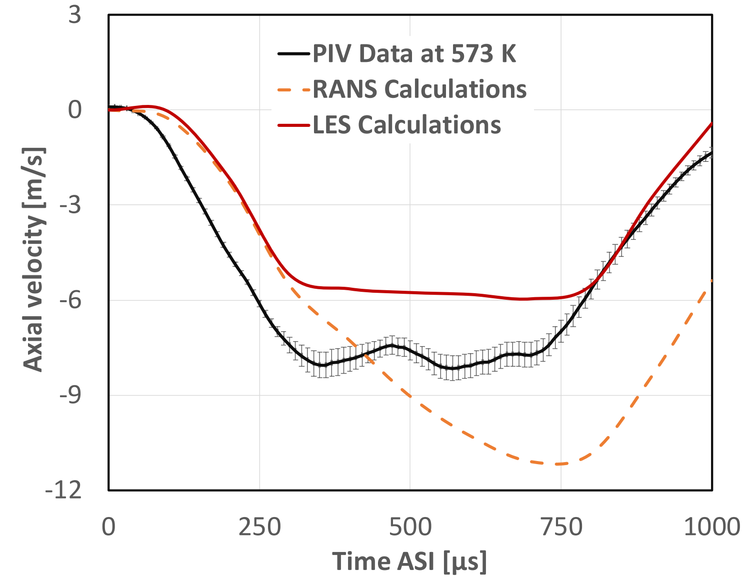
Density (kg/m^3) contours at 15 mm from injector tip at 0.7 ms from SOI



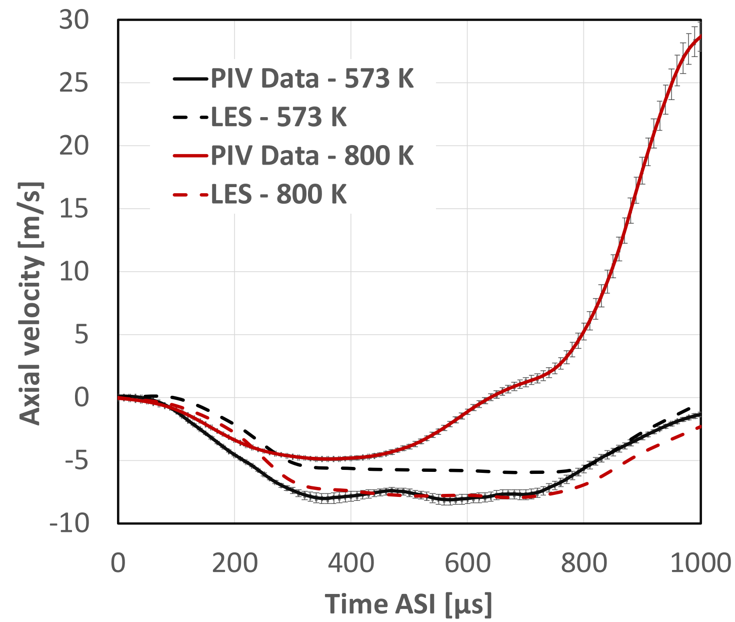
ACCOMPLISHMENT: LES EXPLAINS THE PHYSICS OF PLUME COLLAPSE IN GDI SPRAYS

Horizontal radial velocities predicted with LES @ 573 K





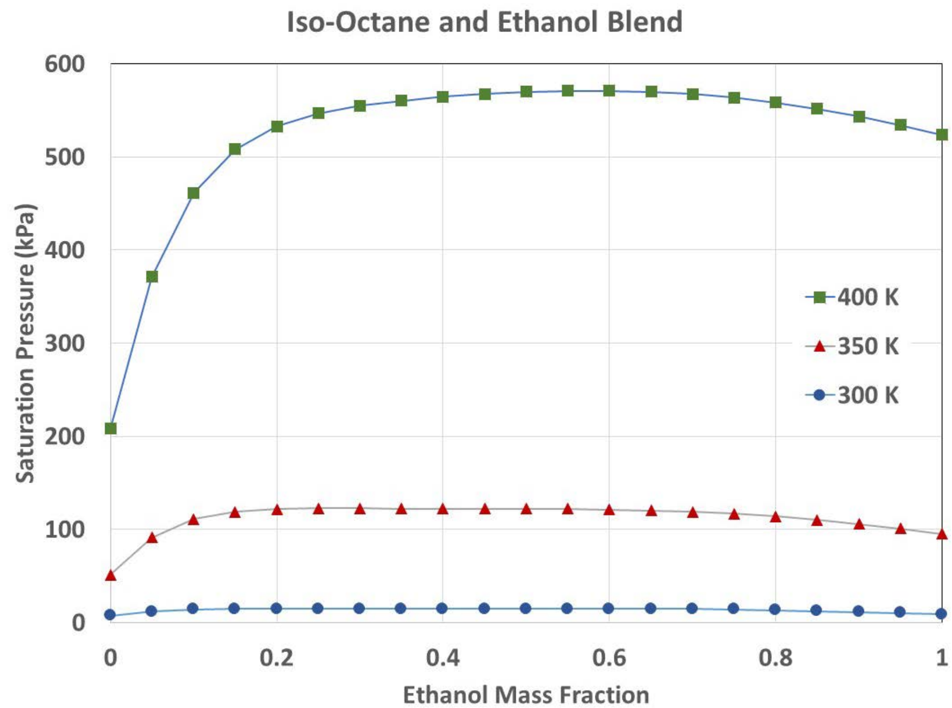
- LES (25° plume cone angle): Plumes do not contact. The arrows indicate a flow of ambient gas between plumes into the central recirculation zone. This equilibrates pressure and sustains the recirculation zone without spray collapse. But the strength of the recirculation zone is weaker compared to PIV data
- LES (35° plume cone angle): Results are closer to experiments. No break between plumes for radial ambient gas entrainment. Strong central recirculation zone exists at the moment, but pathway to equilibrate pressure is blocked by merged plumes
- Simulations are currently unable to capture the influence of high-temperature evaporation effects

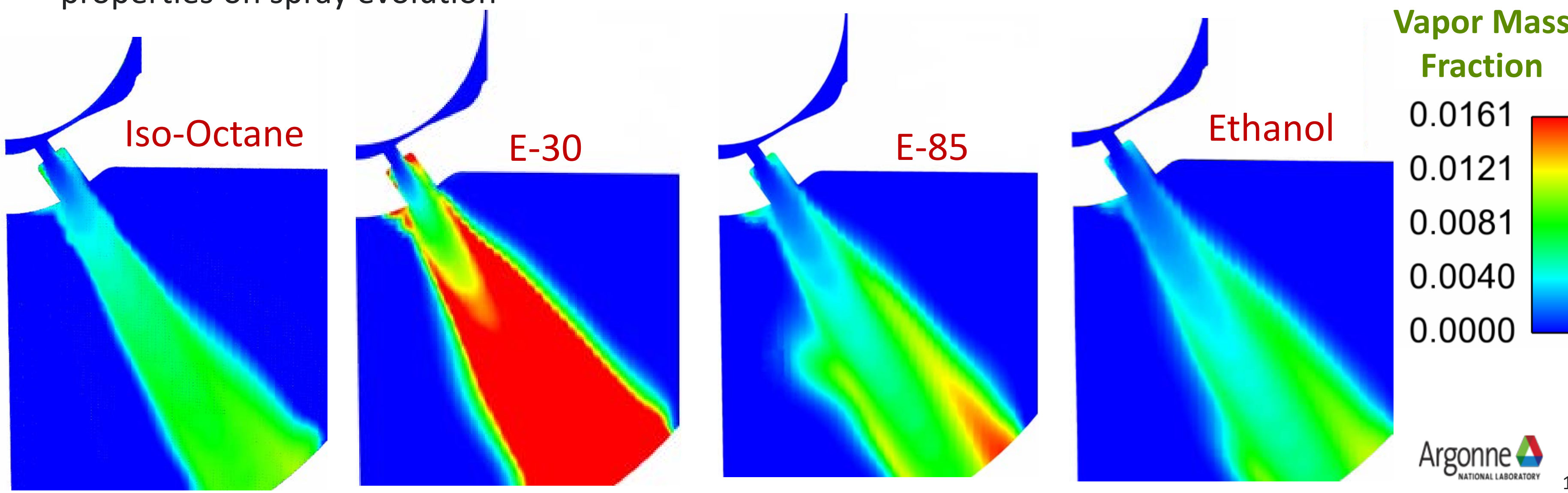


Joint publication with Pickett and co-workers: Panos Sphicas et al. (SAE Journal 2017-01-0837)

ACCOMPLISHMENT: FUEL EFFECTS ON FLASH-BOILING

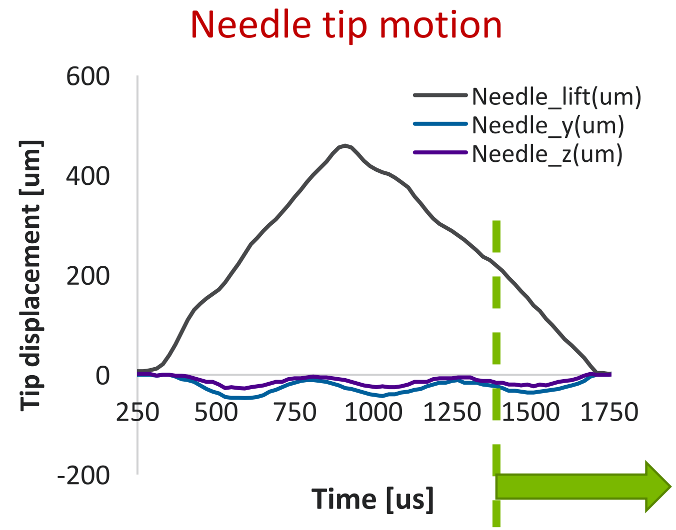
- Single Component Homogenous Relaxation Model (HRM) for flash-boiling shown by our group in previous AMRs was modified to account for multi-component effects
- In-nozzle flow simulations under flash-boiling conditions shows that the extent of vapor formation is similar for the pure components (iso-octane and Ethanol). Blends are more volatile than the individual component owing to their higher saturation pressures
- Multi-component HRM will allow us to accurately capture the effect of fuel properties on spray evolution

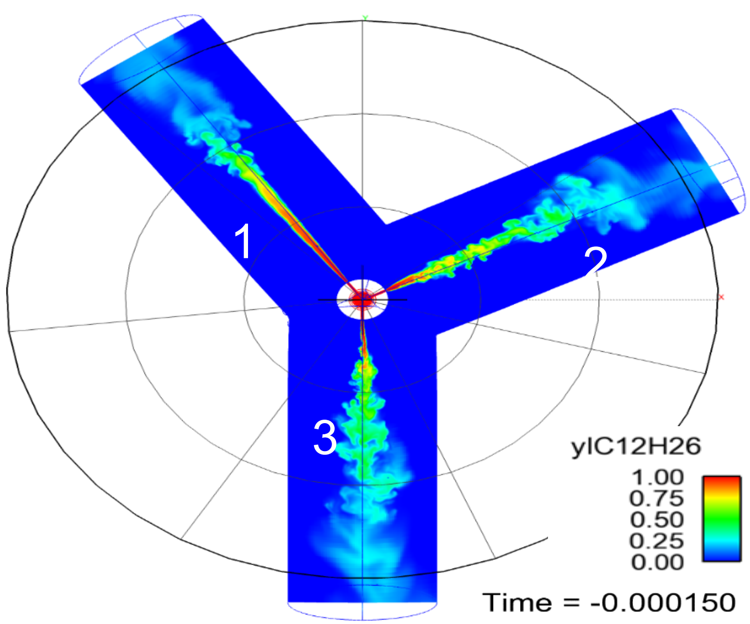


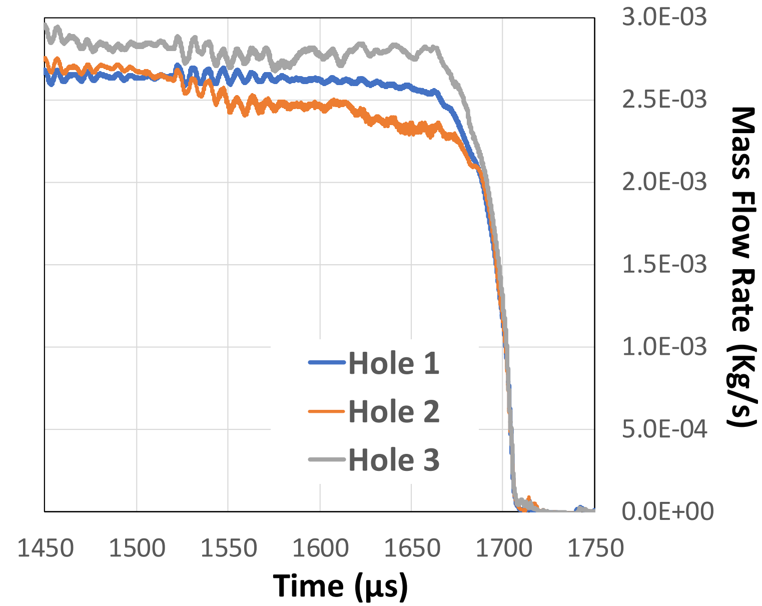


ACCOMPLISHMENT: PLUME-TO-PLUME VARIATION IS CAPTURED DURING EOI

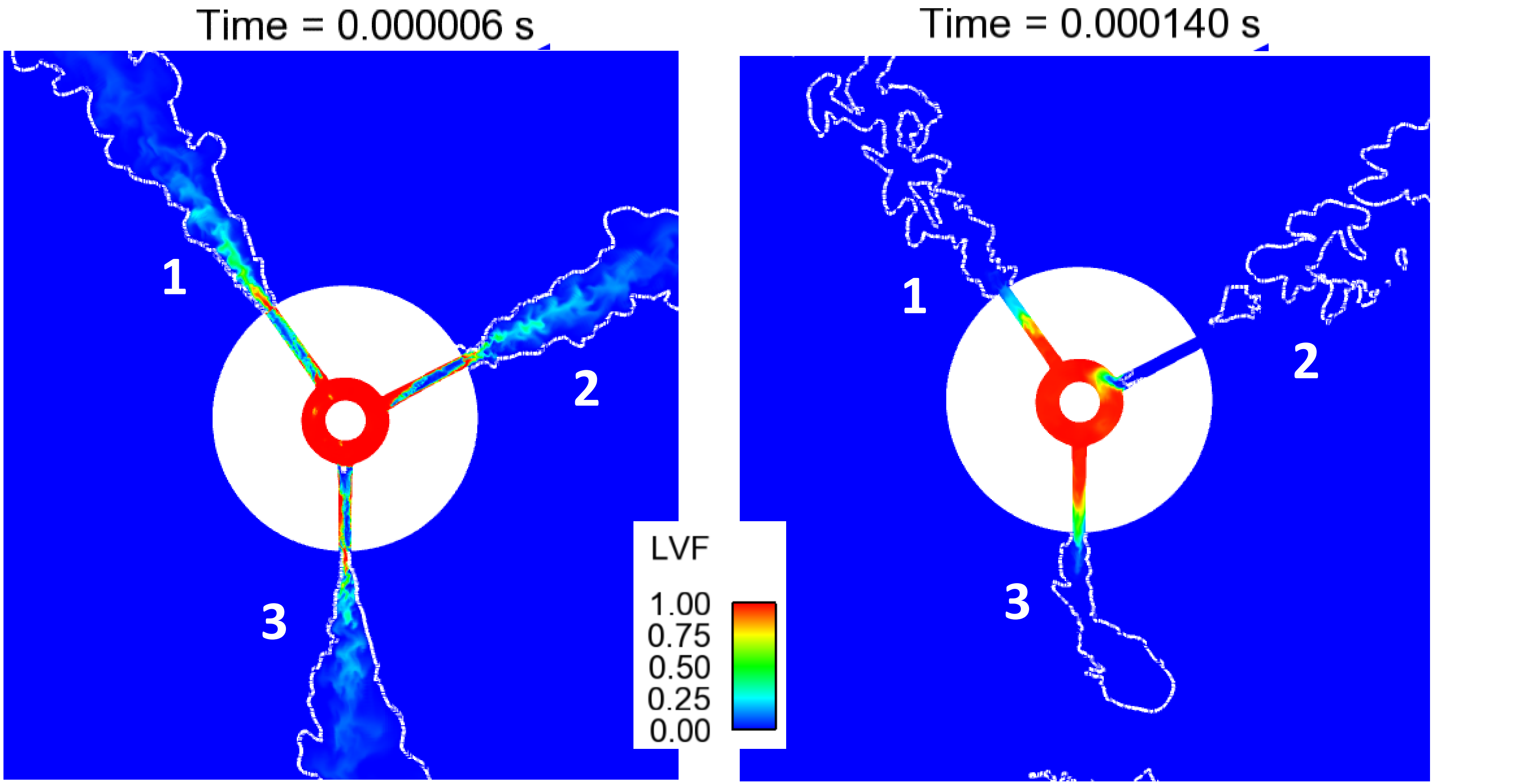
- Our previous AMR presentations have shown EOI transients for single hole injectors
- A multi-hole Spray B injector from ECN is simulated in order to capture the EOI transients (in collaboration with Prof. Michele Battistoni, University of Perugia)
- The needle lift and off-axis motion profile is obtained from x-ray measurement at APS (courtesy Dr. Chris Powell and co-workers)
- Plume-to-plume variations in spray structure and mass flow rate are predicted by simulations owing to the needle off-axis motion and injection transient







ACCOMPLISHMENT: SOI TRANSIENTS, SAC RESIDUALS AND DRIBBLES FOR SPRAY B INJECTOR PREDICTED



Grid size = 2.5 µm, 35 Million cells - Simulated time = 0.450 ms; About 3 months on 256 cpus

- High-fidelity simulation reveal SOI transients in ECN Spray B injector showing asymmetries in sac region due to needle off-axis motion
- Fuel dribble phenomenon is also captured wherein plume 3 is observed to be significantly different from other plumes

APPROACH: TFM MODEL* FOR REDUCING COMPUTATIONAL COST WITH LARGE MECHANISMS

- Salient features: Incorporate history effects in tabulated combustion models. Current versions of tabulated models do not account for the history effects
- Advantage: High fidelity model with significantly lower computational cost
- No "progress variable" assumption
- Role of Turbulent Chemistry Interaction (TCI) captured

* Software Invention # SF-16-159

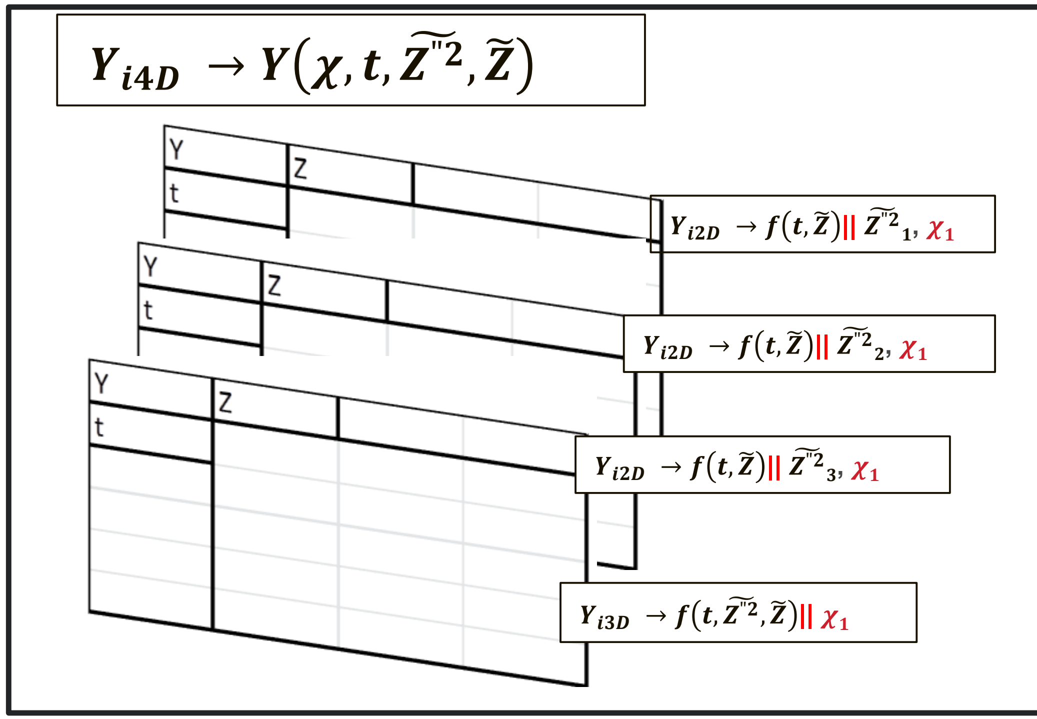
Multidimensional chemistry tabulation

Flamelet Equation: $\rho \frac{\partial Y_i}{\partial t} = \rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i$

$$Y_i \rightarrow Y\left(\chi, t, \widetilde{Z''^2}, \widetilde{Z}\right)$$

Scalar dissipation rate (TCI term):

$$\widetilde{\chi} = C_x \frac{\varepsilon}{k} \widetilde{Z''^2}$$

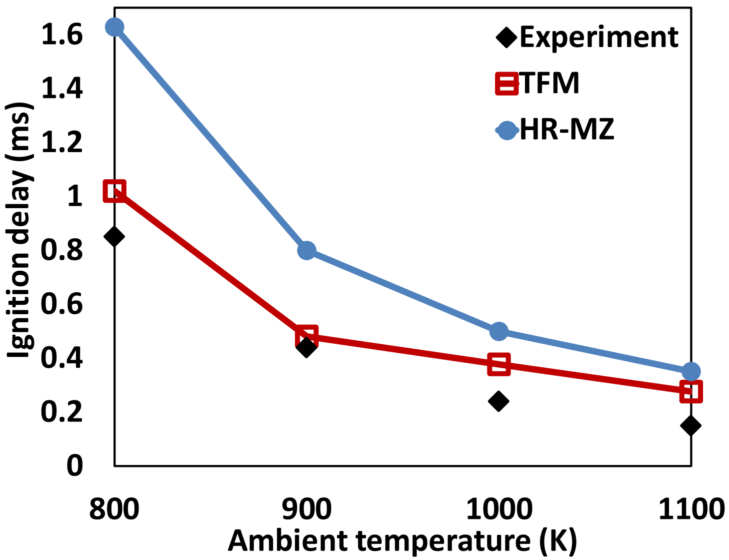


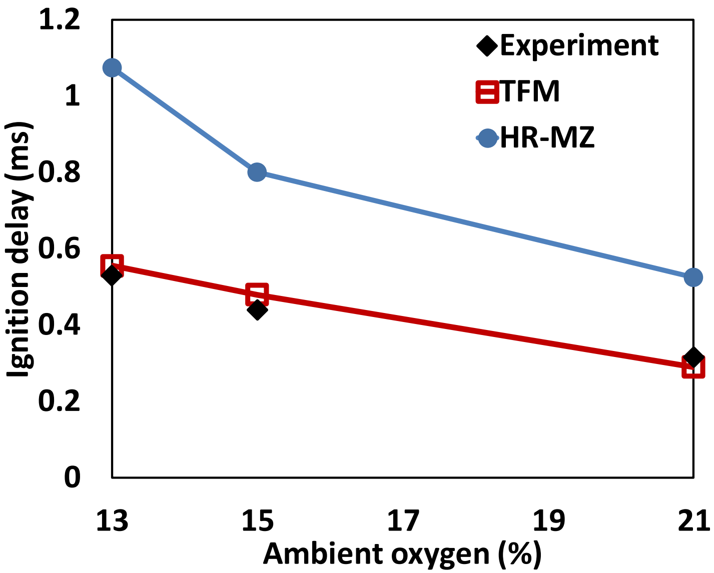
Tabulation features:

- Multidimensional table generation
- Each dimension can be calculated independently
- Large scale parallelization with no communication overhead
- **Best speed-ups obtained for large chemistry mechanisms**

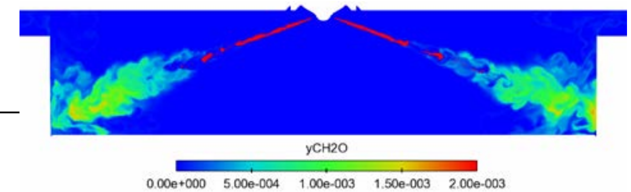
ACCOMPLISHMENT: EXTENSIVE VALIDATION OF TFM

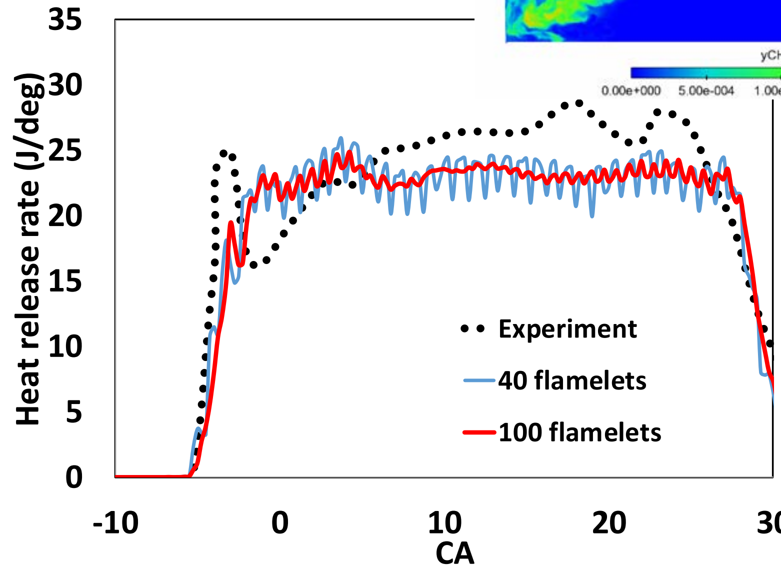
Spray Flame Simulations





Engine Simulations





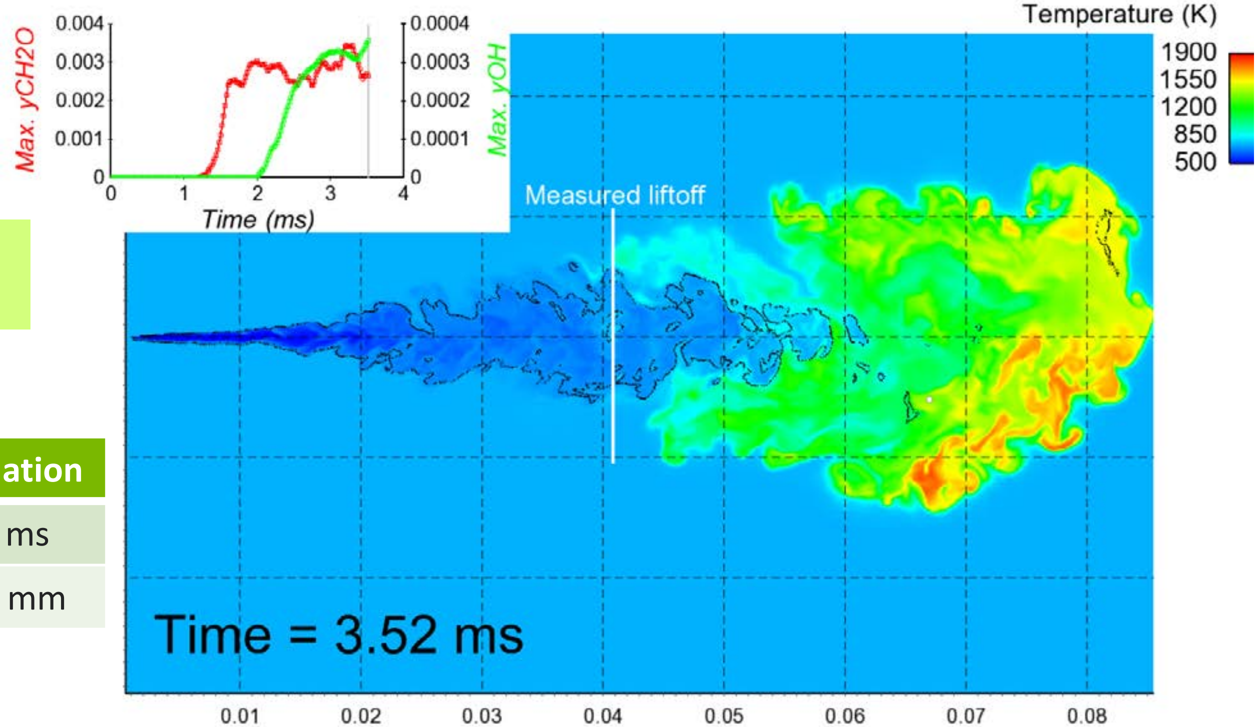
- Extensive validation has been performed against experimental spray flame data from ECN (n-dodecane fuel) and optical engine data (Methyl Decanoate fuel) from C.J. Mueller at Sandia. These have been published in journal and conference papers
- In spray flame simulations, the TFM is demonstrated to be more accurate than state-of-the-art model in commercial code. **The computational cost for TFM is 50-75% lower, depending on the ambient conditions**
- **Best practices for mesh size, TFM table granularity etc. have been published**

ACCOMPLISHMENT: IGNITION AND FLAME STABILIZATION UNDER LTC CAPTURED WITH TFM

Modeling challenges @ 750 K

- Long injection duration – 6 ms
- Large ignition delay > 2 ms

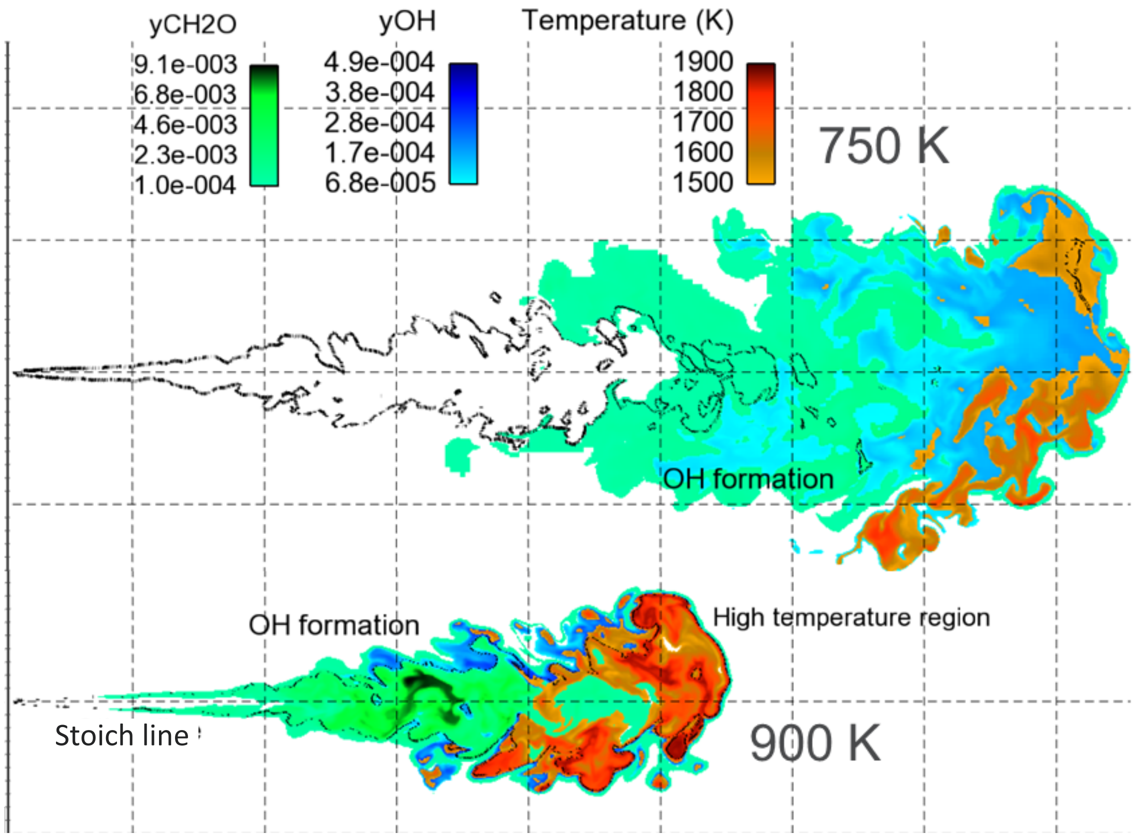
- CH_2O formation starts at 1.2 ms
- OH formation observed at 2 ms



	Experiment	Simulation
Ignition delay	1.79 ms	2.1 ms
Liftoff length	40.8 mm	37.3 mm

- 750 K low-temperature (ambient) condition is simulated with the TFM approach together with high-fidelity LES turbulent model (developed and validated and shown in our previous AMR presentations). Experimental data is obtained from ECN
- It should be noted that under this low-temperature condition, simulation groups at ECN have not been able to capture auto-ignition and flame stabilization phenomenon. This is due to the fact that the coupled effects of mixing and TCI are more pronounced under these conditions.
- TFM can capture TCI effects and provides insights on the flame stabilization phenomenon at the 750 K condition

ACCOMPLISHMENT: INSIGHTS INTO THE FLAME STABILIZATION MECHANISM AT 750, 900 K CONDITIONS



- Ignition not observed with homogeneous reactor model at 750 K and over-estimated at 900 K
- TCI is observed to play a key role in species diffusion from the first stage ignition, thereby enhancing the main ignition, especially under LTC. TFM can capture this effect
- Significantly lower temperatures and species concentration at 750 K compared to 900 K
- At 750 K, CH_2O formation starts at significantly lean regions due to longer ignition delays leading to more mixing compared to 900 K
- Similar conclusions are drawn for OH as well

In order to understand the role of TCI at lower temperatures, unsteady flamelets are simulated with our flamelet code with different scalar dissipation rates (χ_{st}), i.e., with χ_{st}=0 (homogeneous reactor) vs χ_{st} = 2 s^{-1}

- Lean regions (ϕ<1) do not ignite with homogeneous reactor assumption
- Scalar dissipation leads to diffusion of radical species enhancing ignition in the lean regions

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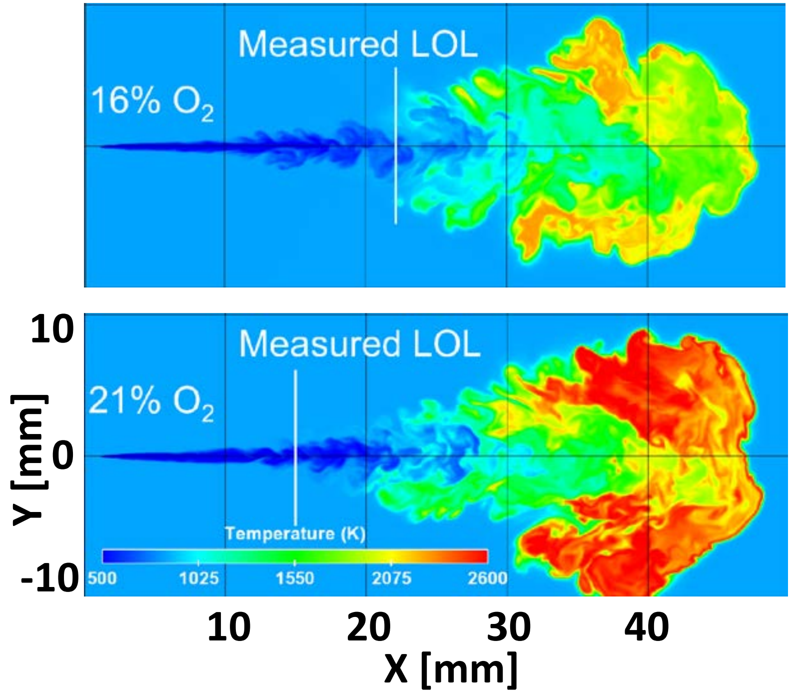
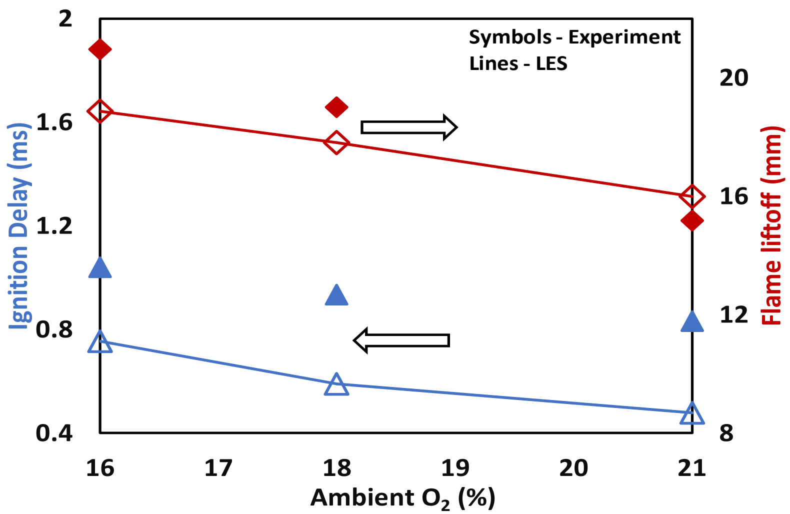
ACCOMPLISHMENT: LES WITH 4-COMPONENT DIESEL SURROGATE MECHANISM

- V0A surrogate (4-component diesel surrogate, CRC AVFL-18a) mechanism developed by **W.J. Pitz et al. at LLNL** was reduced to ~ 1000 species for 3D CFD simulations
- Analytical Jacobian for the mechanism generated in collaboration with **Prof. T. Lu and Mr. Chao Xu at University of Connecticut**
- The ~1000 species mechanism was tabulated for TFM calculations together with high-fidelity LES
- ~1000 species mechanism CFD simulations are unprecedented and will offer more insights into combustion processes compared to ~100 species mechanisms

Temperature Contours



Experimental data from ARL (M. Kweon, J. Temme, and V. Coburn)



- LES calculations were performed with our previously identified best practices (AMR 2015 and 16)
  - ~ 22 million cells with min. cell size of 62.5 µm, dynamic structure LES model with multiple realization averaging
- Ignition delay and flame lift-off length are currently under-predicted with the CFD simulations
  - Possible causes could be the detailed chemistry mechanism as well as spray-mixing predictions

COLLABORATIONS

Argonne National Laboratory

Engine and Emissions Group: (Provide data for model validation)
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)

GM R&D (In-nozzle flow and spray simulations for GDI injectors)

Sandia National Laboratory (Provide experimental data)

Lawrence Livermore National Laboratory (Mechanism development)

University of Connecticut (Mechanism Reduction)

University of Perugia (ECN Spray B In-nozzle Flow Simulations)

Presentations at Advanced Engine Combustion (AEC) Working group
Active role in Advanced Computing Tech Team (ACTT) by ASCR
Engine Combustion Network Participation and Data Contribution

***Toolkit Development* in "Co-Optima" is leveraging our developments**
- **FT037, FT052, FT053, FT054, FT055**

Three University FOAs are leveraging our developments
- **S.Y. Lee ACS108; C.F. Lee ACS106; A. Agrawal ACS107**

COLLABORATIONS THROUGH VERIFI

Based on the capabilities developed under this program, we have established the Virtual Engine Research Institute and Fuels Initiative (VERIFI)

VERIFI is designed to provide HPC solution for industrial problems of interest using either clusters of leadership class supercomputer such as Mira

3rd workshop in November 2017

Understanding and Predicting Cyclic Variability in Engines

FY 16 & 17

GE

aramco

GT Gamma Technologies

Small Business Vouchers Pilot
U.S. DEPARTMENT OF ENERGY

CONVERGENT SCIENCE

HPC4 MANUFACTURING

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy
ADVANCED MANUFACTURING OFFICE

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DELPHI

RESPONSE TO PREVIOUS YEAR REVIEWER COMMENTS

Overall the reviewers were positive about the progress of this project

Explain the novelty of the cavitation work compared to the current state-of-the-art.

Cavitation model (HRM) is now fairly standard and available in many commercial and academic codes. Our work is unique due to the resolutions we are able to add for LES calculations and consequently capturing new physics. For e.g., cavitation at low needle lifts due to needle eccentricity was first observed by us, to the best of our knowledge!

Apply LES and new turbulent combustion model to selective engine to assess the improvements compared to RANS and homogenous reactor models.

Authors are currently modeling the heavy duty optical engine from Sandia (from C.J. Mueller) with this goal. The aim is to understand tradeoffs in accuracy vs. run-time between different approaches.

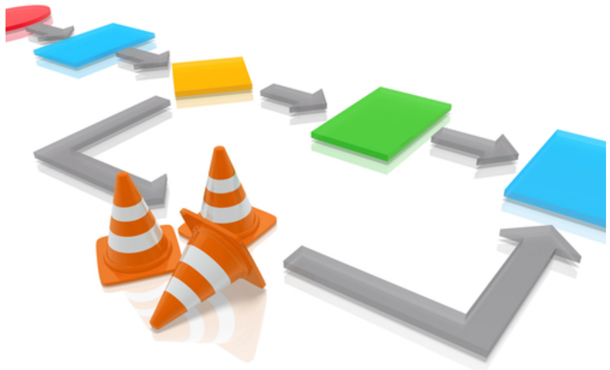
How have the previous AMR findings being used, such as, needle wobble effects, optimized mechanisms, injector dribble predictions etc.?

The reduced optimized mechanism has been used by other researchers contributing to ECN work across the world. Strategy to capture needle wobble effects is now in Cummins simulation workflow. The injector dribble calculation, especially for multi-hole injector still remain extremely expensive to be used as a product design tool.

HPC work is code specific. It is crucial to avoid (in reality or perception) any unfair subsidies for product development to a particular software vendor.

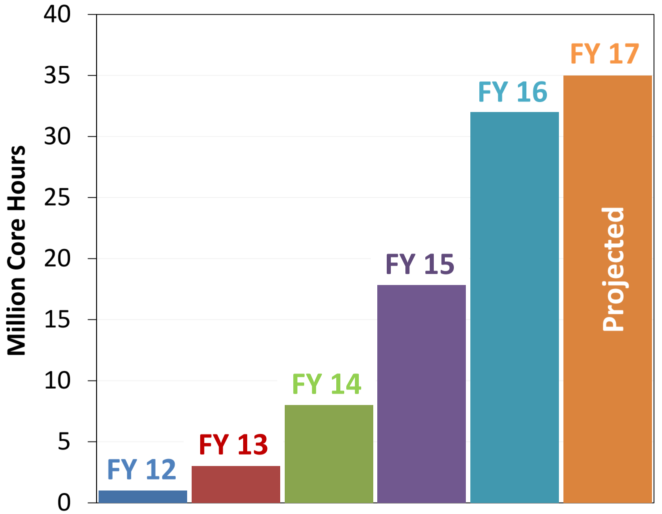
The details of our work demonstrating the use of HPC for engine simulation has all been made available publicly. The platform chosen for those demonstrations was based on input from our industry collaborators, and the vendor’s willingness to work closely with our researchers. We recognize that this work does become code specific, and we believe that we have offered to perform the same HPC optimization to all software vendors in the ICE simulation space. Additionally, in another area of our work we are in discussion with multiple software vendors to implement TFM into their codes.

REMAINING CHALLENGES AND BARRIERS



- Work-flow: More efficient "workflow" to ensure that code improvements and model developments reach industrial partners in a more timely fashion
  - Model development and validation time-scale is usually 6-9 months
  - Commercial code releases are usually once a year

- Computing time: High-fidelity calculations that need to be performed to develop 'best practices' for industry are expensive. The need for multi-cycle realizations with LES also increase simulation time extensively
  - Our computing needs have grown from FY12 (1-2M core hours) to FY16 (~30M core hours)
  - Computing time from ASCR is not guaranteed since ALCC and INCITE awards are extremely competitive



- High-fidelity experimental engine data: We not only need experimental data for boundary conditions from our experimental collaborators but we need uncertainty in these boundary conditions and measured data. Note that the simulations calculate results based on some averaged inputs from experiments and do not account for the experimental uncertainties that can be significant

FUTURE WORK*

1) Improve multi-component evaporation models, especially for GDI applications
2) Integrate the multi-component flash boiling model with LES and compare against x-ray radiography data from APS at Argonne
3) Extend the *one-way coupling* approach and couple with the new TFM combustion solver to predict the influence of nozzle flow on combustion and emissions
4) CRADA project with Cummins and CSI (FY16-FY18)
   - Develop cavitation erosion model for diesel injectors: validation against published data in literature
   - Development of fluid structure interaction model to predict needle transients: validation against x-ray measurements of needle lift and wobble
   - Develop "engineering best-practices" to enable industry use these high-fidelity models
   - Scale the expensive coupled nozzle flow and spray simulations on supercomputer to reduce runtime

5) Robust validation of the 4-component diesel surrogate mechanism (from LLNL) against and TFM against:
   - Constant volume chamber data from ARL (Improve predictions of ignition delay and flame LOL)
   - Optical engine data from Sandia (in collaboration with C.J. Mueller)
   - Understand and report run-time vs. accuracy trade-off of turbulence models and detailed kinetic mechanisms

* Any proposed future work is subject to change based on funding levels

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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**
  - In-nozzle flow simulations shown to guide plume targeting and provide estimation of spray cone angle which is critical to Lagrangian calculations of GDI sprays
  - One-way coupling demonstrated to capture plume to plume variations
  - Multi-component blends can cause more flash boiling than the constituent individual components
  - Validated LES set-up was able to provide insights into the physics of plume collapse
  - EOI transients and injector dribbles can be captured for multi-hole injectors, provided sufficient spatial and temporal resolution is used along with a LES turbulence model
  - TFM is demonstrated to be more predictive at lower computational costs compared to homogenous reactor based models used in literature
  - TFM captures ignition delays and flame liftoff lengths under LTC conditions, where traditional homogeneous models fail. Diffusion of species is understood to be critical under these conditions
  - For the first time, 4-component diesel surrogate simulations with large chemistry mechanism (~1000 species) was performed with LES. This was possible due to the unique tabulation approach of TFM
- **Collaborations and coordination**
  - with industry, academia, and national laboratories; through ECN with researchers world-wide
  - through VERIFI collaborations with light-duty, heavy-duty, software vendors, and energy companies

Technical Back-Up Slides

EULERIAN MIXTURE & CAVITATION MODEL

Mixture Model equations (homogeneous multi-phase model)

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

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

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

(plus: Energy, Turbulence)

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

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

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

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

$$\frac{dY_v}{dt} = \frac{Y - \overline{Y_v}}{\Theta}$$

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

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

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**

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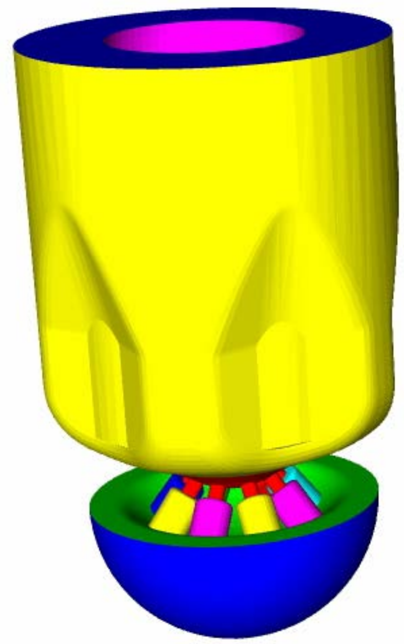
GDI NOZZLE FLOW AND SPRAY SIMULATION CONDITIONS

Pressure Inlet

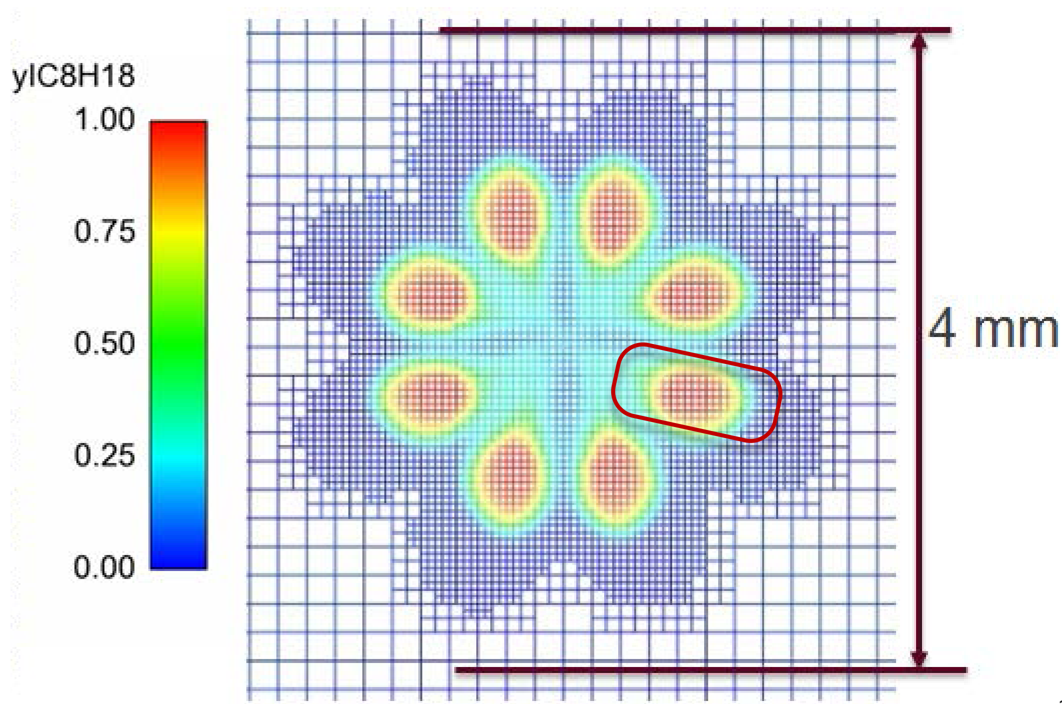


Pressure Outlet

Orifice dia (D_1) – 165 µm; $L_1/D_1 \approx 1$
Counter-bore dia (D_2) – 388 µm; $L_2/D_2 \approx 1.2$

Parameters	Spray G (Non-Flashing)	Spray G2 (Moderate Flashing)	Spray G3 (Intense Flashing)
Injection pressure (MPa)	20	20	20
Chamber pressure {P_{ch}} (kPa)	600	53	100
Fuel injection temperature {T_{fuel}} (K)	363	363	413
Degree of superheat {ΔT} (K)	N/A	12.34	40.68
Pressure ratio (R_P)	0.13	1.48	2.83

Base Grid (µm)	Min. Grid (µm)	Cell Count (millions)
180	22.5	1.4
140	17.5	2.8
120	15	4.5



EXPERIMENTAL CONDITIONS FOR COMBUSTION SIMULATIONS

Spray flame experiments 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/

Heavy duty optical engine experiments

Parameter	Quantity
Cycle	4-stroke CIDI
Bore	125 mm
Stroke	140 mm
Connecting rod length	225 mm
Piston bowl diameter	90 mm
Piston-bowl depth	16.4 mm
Swirl ratio	0.59
Squish height	1.5 mm
Displacement	1.72 L
Injector	Cat CR 350
Compression ratio	12.3:1

C.J. Mueller & co-workers, *Energy and Fuels*, 2014

4-component diesel surrogate:
n-hexadecane, isohexadecane, Trans-decalin, 1-methylnaphthalene

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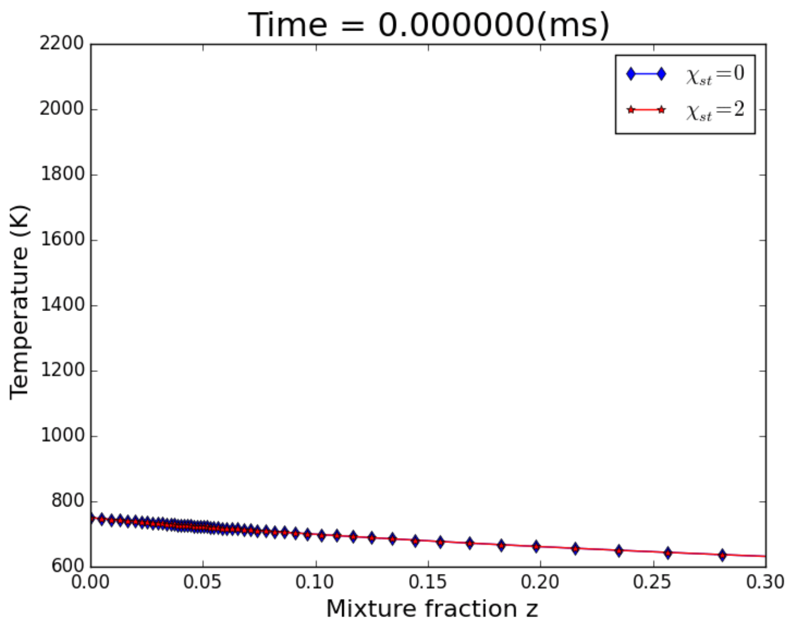
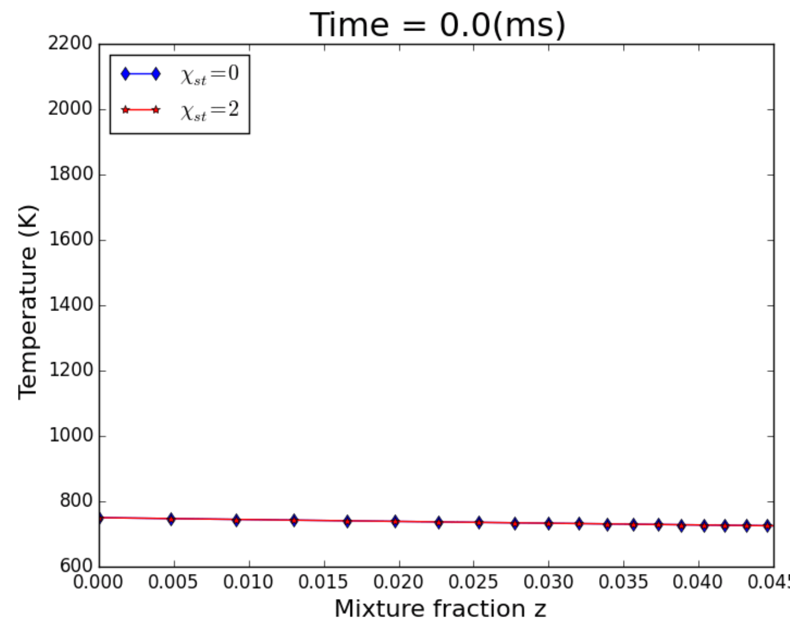
ROLE OF SCALAR DISSIPATION RATE UNDER LOW-TEMPERATURE CONDITIONS





Lean region (Z=0 – 0.045)

- Ignition not observed with homogeneous reactor with 103 species mechanism.
- Unsteady flamelets simulated with $\chi_{st}=0$ (homogeneous reactor) vs $\chi_{st} = 2\ s^{-1}$.
  - Lean regions (φ<1) do not ignite with homogeneous reactor assumption.
  - Diffusion of species in Z space lead to ignition.

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: ~ 768,000 – core super-computer

operated by the Leadership Computing Facility

Fusion Cluster

MIRA Super-Computer

We gratefully acknowledge the computing resources provided by the ASCR Leadership Computing Challenge (ALCC) award of 60 million core-hours on Mira supercomputer at the ALCF at Argonne National Laboratory