PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Fuel Injection and Spray Research

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Annual Merit Review, 22 June 2021

Project ACE143

Overview: Experiments and Simulations of Injection and Sprays

- **Timeline**
  - Most projects started mid-2019, two are new this year
  - Projects end in 2023, 46% complete
- **Budget**

Task	Description	FY20	FY21
A.E.04 Powell	ANL, Free Spray and Wall Film X-ray Experiments Powell, Sforzo, Tekawade	$200k	$441k
O.E.04.01 Wissink	ORNL, New Injector Procurement and Characterization Wissink	$0	$125k
S.M.04.01 Nguyen	SNL, Free Spray Modeling Nguyen, Tagliante, Pickett	$100k	$50k
S.M.04.02 Tagliante	SNL, Spray Accuracy Toolkit Tagliante, Nguyen, Pickett	$0	$125k
S.E.04.01 Pickett	SNL, Free Spray and Wall Film Optical Experiments Pickett, Manin, Karathanassis, White, Tagliante, Strickland	$380k	$380k
A.M.05.02 Ameen	ANL, High-Fidelity Spray and Combustion Models in Nek5000 Ameen, Colmenares Fernandez	$350k	$310k

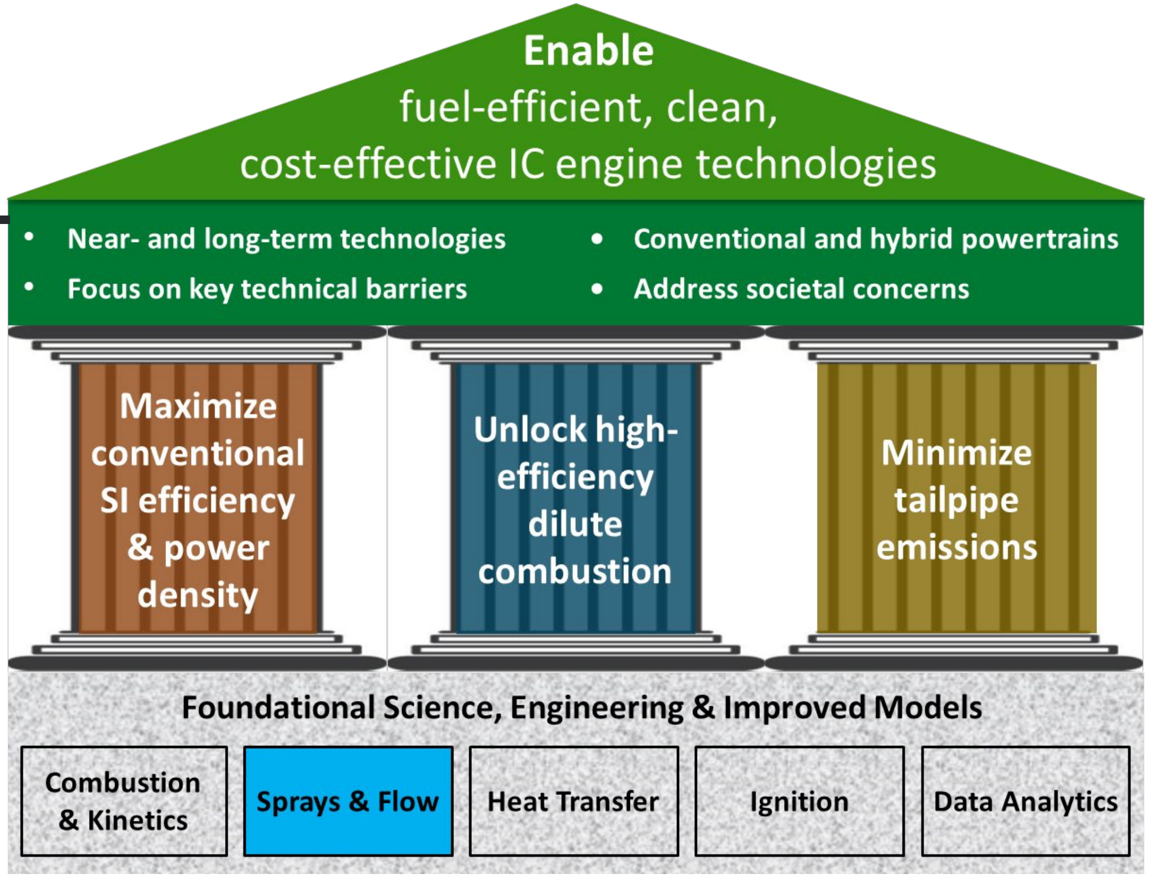
Budgets above reflect each project's total for PACE, rather than the share of the work discussed in this presentation
See complete PACE budget in Reviewer Slides

- **Contributes to all PACE major outcomes**
  - Minimizing emissions at all operating conditions, including cold-start with potential film combustion
  - Predicting free-spray and wall-impinging sprays, ultimately producing combustible mixtures at the spark plug for efficient (including dilute) combustion
  - Avoiding liner and piston liquid impingement, with implications on knock and premixed ignition
  - CFD spray and film combustion model improvement for engine design/optimization
- **Partners**
  - PACE, a DOE-funded consortium of 6 National Laboratories working towards a common goal
  - PACE sprays team coordinates tasks and sets direction
  - 15 Industry partners in the AEC MOU.
  - Engine Combustion Network, Spray G (20+ partners)
  - CONVERGE Working Group: Universities, Labs, Convergent Science Inc

Relevance: Major Outcomes of PACE and the Role of the Sprays Team

Improved understanding and modeling of sprays, films, and mixture formation addresses

- **Ability to Predict and Mitigate Knock and Pre-ignition at High Load**
  - Simulation and experiments characterizing free sprays, wall impingement, and mixture formation
- **Overcome Barriers to Lean/Dilute Combustion**
  - Measurements and modeling of mixture formation under lean/dilute conditions
  - Measure and model spray variability
- **Minimize tailpipe emissions**
  - Experiments and modeling including multiple injections at cold-start conditions
  - Modeling of spray-wall interactions, films, vaporization, heat transfer, wall-film soot
  - How to create a combustible mixture at the spark plug on Cycle 1?



Milestones, FY2020 and FY2021 (1)

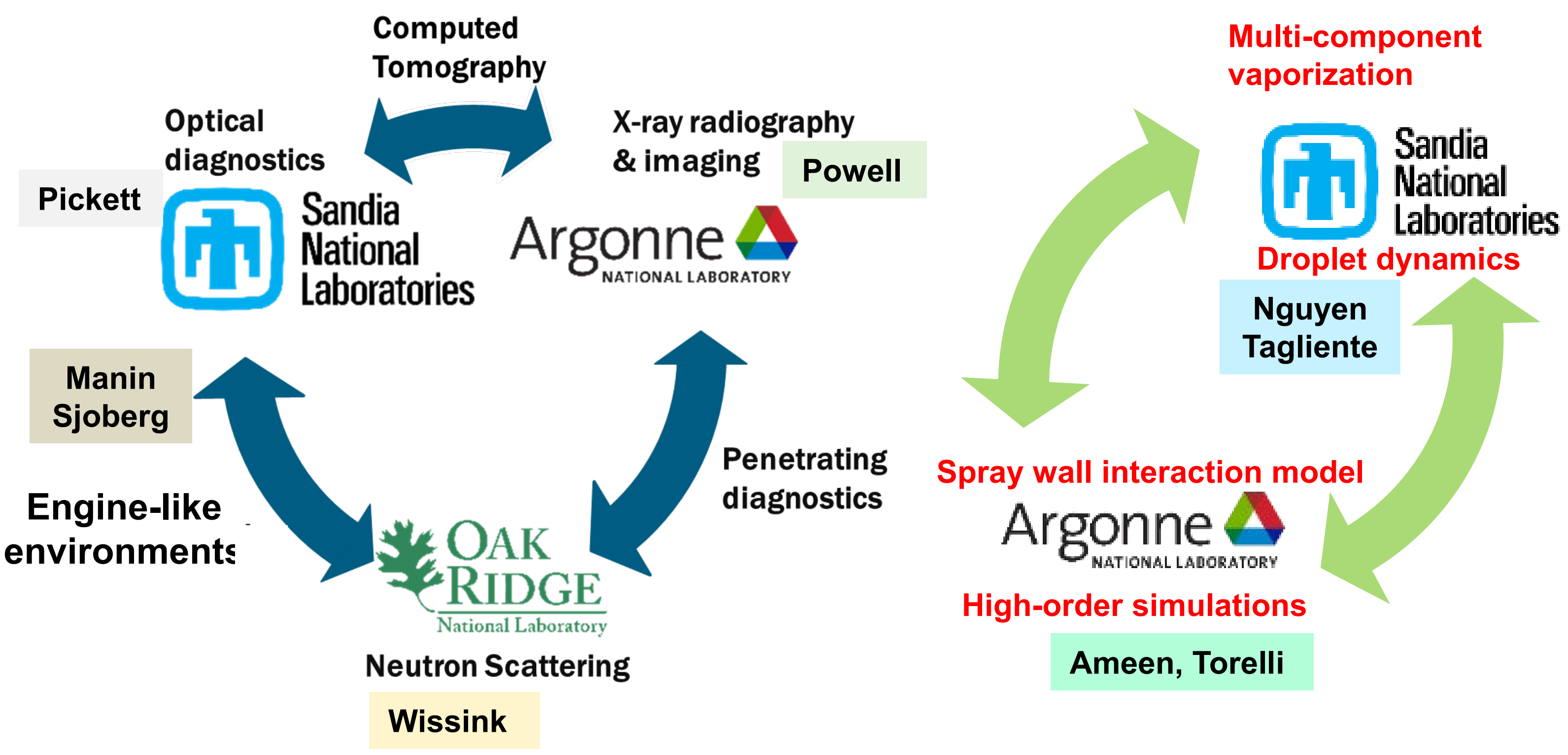
Month / Year	Task	Description of Milestone or Go/No-Go Decision	Status
Nov 2020	S.E.04.01 Pickett	In spray chamber, measure 3D liquid volume fraction using PACE surrogate fuels compared to RD5-87	Complete
Mar 2021	S.M.04.01 Nguyen	Perform free-spray Lagrangian simulations including tip counterbore geometry	Complete
Mar 2021	A.E.04 Powell	X-ray measurements quantifying the fuel distribution of GDI sprays impacting a wall	Complete

Milestones, FY2020 and FY2021 (2)

Month / Year	Task	Description of Milestone or Go/No-Go Decision	Status
Jun 2021	S.E.04.01 Pickett	In spray chamber, measure 3D liquid volume fraction with injector and conditions applicable to Sandia SIDI engine	On Track
Jun 2021	A.M.05.01 Ameen	High-fidelity LES of evaporating ECN Spray G simulated using Nek5000	On Track
Sept 2021	S.M.04.02 Tagliante	Development of full "accuracy test" toolkit (scripts and workflow) with merit functions for free sprays	On Track
Jun 2021	A.E.04 Powell	Dataset of measurement results including free-spray and wall-film measurements will be archived online.	On Track
Sept 2021	O.E.04.01	Report on the progress made toward transitioning PACE to higher pressure injectors to spray team, PACE leadership, and DOE	On track

Overall Approach: Collaborative Measurements and Simulations

Experiment



Simulation

- **Focusing on gasoline free spray phenomena**
- **Free sprays must remain a focus to**
  - Predict and understand wall impingement
  - Predict and understand sprays in engines
- **Coordinated design of experiments and simulations**
- **Complementary diagnostics and modeling approaches**
- **Deliver detailed validation data for CFD simulations**

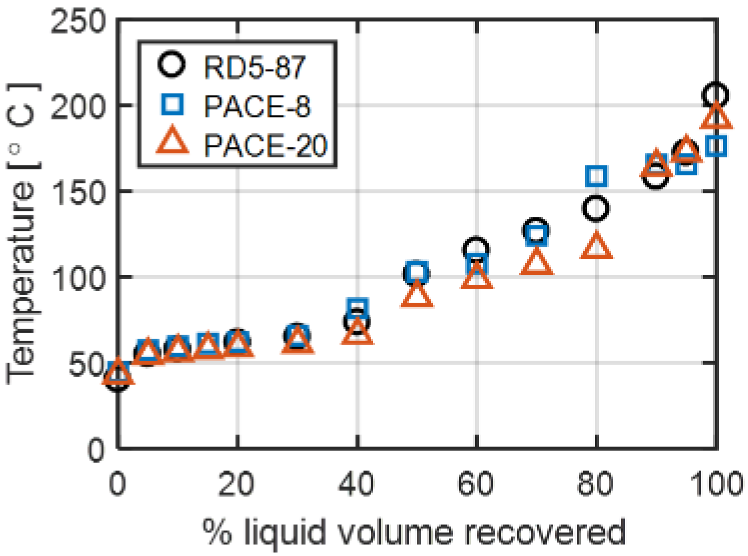
PACE Sprays Team meets biweekly coordinate over 90 current tasks:

Free-spray target conditions: chosen for joint PACE research to "lay" the foundation for wall-film research at similar conditions

PACE free-spray conditions for GDI applications

	T_{amb} [K]	P_{amb} [kPa-a]	ρ_{amb} [kg/m³]	T_f [K]	p_{inj} [MPa]	$T_{inj,hyd}$ [ms]	m_{inj} [mg]
G1	573	600	3.5	363	20	0.780	10
G2	333	50	0.5	363	20	0.780	10.1
G3	333	100	1.01	363	20	0.780	10.1
G2-cold	293	50	0.57	293	20	0.780	10.6
G3-cold	293	100	1.15	293	20	0.780	10.6
G3-double	333	100	1.01	363	20	0.462 0.900 dwell 0.327	6.1 + 4

Overview
- **Injector: ECN Spray G, 8-hole unit provided by Delphi**
- **Fuel: iso-octane/E00, 3-component/ PACE-20, 9-component fuel**
- **Ambient: 100% N2**



<u>Importance of operating conditions</u> (many are ECN conditions)
G1: injection late during compression
- **knock control, lean dilute combustion, cold start**

G2: intake injection commonly encountered
- **flash-boiling; modeling weaknesses demonstrated**

G3: intake injection at 1 bar
- **standard patternator and other SAE J2715 data available**

double injection and cold fuel are applicable to cold start

PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Approach: O.E.04.01 (Wissink)
Injector Characterization & Distribution

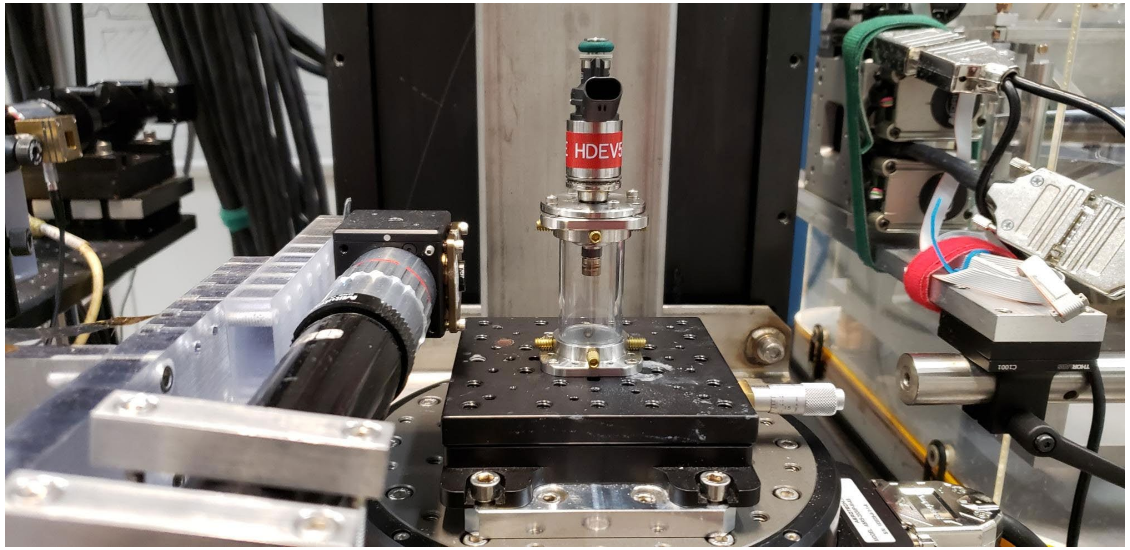
- Support the acquisition, characterization, and distribution of gasoline direct injectors for the PACE engines and related spray chamber experiments. Using a matched and characterized set of injectors will ensure alignment between various experimental and modeling efforts within PACE.
- A key limitation of the production HDEV5 injectors is the relatively low operating pressure of 200 bar. This task will investigate pathways to support the transition to 500 bar injectors which will retain similar spray pattern and geometric compatibility with the production injectors.

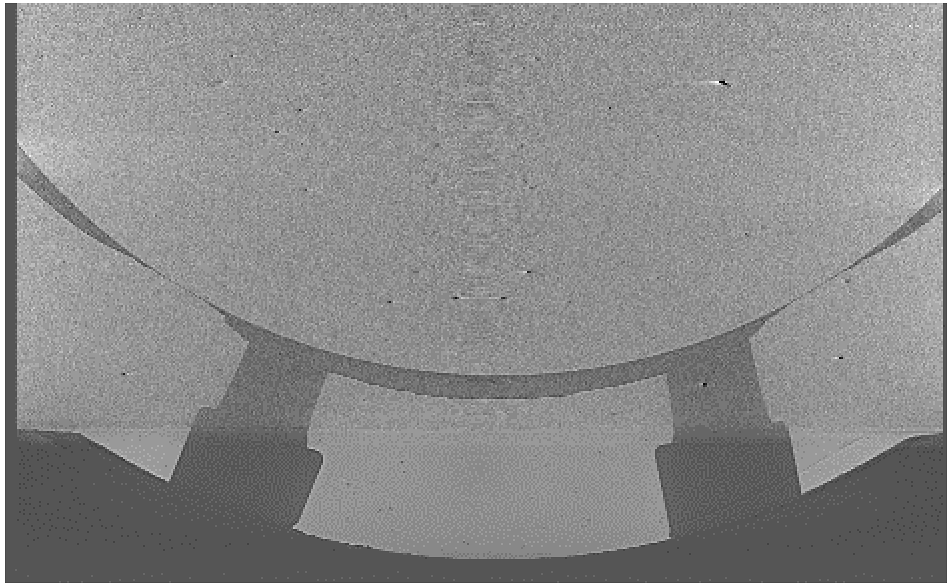
Technical Accomplishments and Progress: O.E.04.01 (Wissink)
Procurement, Characterization & Distribution of new High Pressure Injectors

- **Surveyed PACE PIs regarding needs for injectors, drivers, and fuel pumps**
- **Ford has approved the request for Bosch to use the spray pattern from the 2.3L Ecoboost in custom high-pressure injectors**
- **Have progressed through several iterations of scope with Bosch Motorsport**
  - Qty 25 HDEV 5.2 500 bar injectors with spray validation of match to production injector
  - Qty 11 injector drivers
  - Laser light section patternation of 1-25 injectors (depending on price, may use 3rd party)
  - Needle lift measurement of 1 injector
  - Plan to issue subcontract in FY21 Q3 and receive injectors in Q4.
- **Depending on remaining funds after injector purchase, may re-commission rate of injection meter at ORNL to perform rate shape characterization**
- **Characterization efforts coordinated with Spray Team partners at SNL and ANL**

Approach and Technical Accomplishment: A.E.04 (Powell)
Free Spray and Wall-Film X-ray Experiments

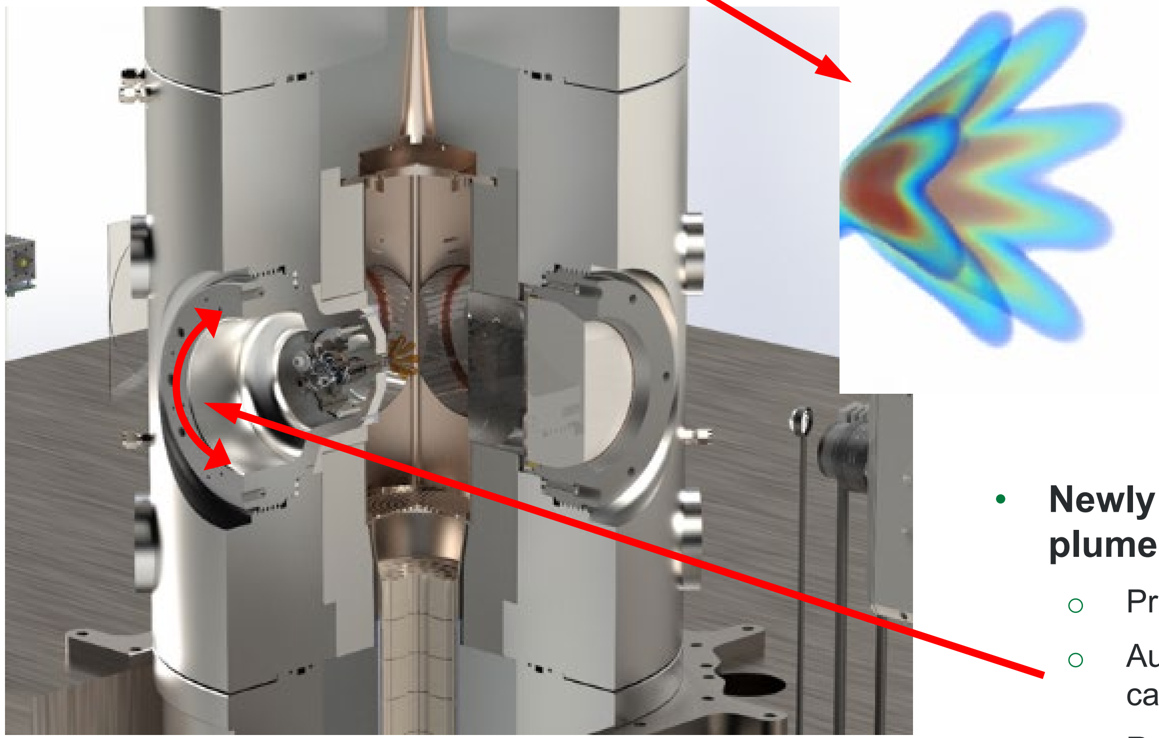
- **At the start of FY2020, the highest priority task was design, fabrication, and measurements in a new chamber for X-ray measurements of spray/wall interactions**
- **COVID delayed significant progress on this task**
- **Instead, we moved forward with measurements of the production HDEV5 injectors for the new PACE engines: 2020 Ford 2.3 l EcoBoost**
- **Five injectors were procured and scanned**
  - Will allow assessment of hole-to-hole and injector-to-injector variations
  - These statistics will help to understand any variability in baseline PACE engine data
- **High-resolution measurements of nozzle geometry will enable high-fidelity simulations of internal flow**
- **Future measurements will focus on the more modern, higher pressure HDEV 5.2**





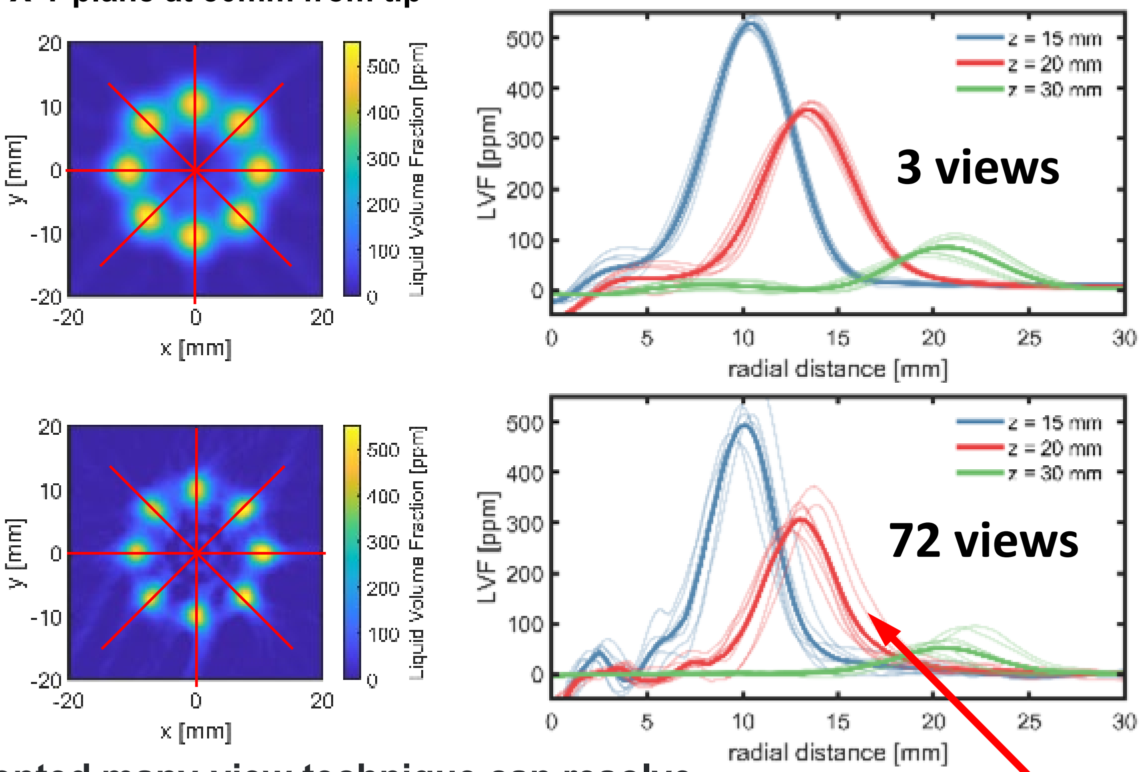
Approach S.E.04.01 (Pickett)
New Capability for 3D Measurements of Liquid Volume Fraction

- **SNL continuous flow vessel allows for high-repetition rate injection experiments at engine-relevant conditions**
  - Combining Diffuse Back-Illuminated (DBI) extinction imaging from multiple viewing angles through Computed Tomography (CT) enables 3D reconstruction of the spray Liquid Volume Fraction (LVF) distribution



ECN G1 – EEE gasoline

X-Y plane at 30mm from tip | **Cuts through plume centers**

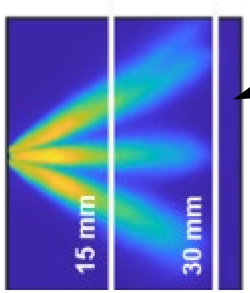


- **Newly implemented many-view technique can resolve plume-to-plume variations and asymmetric sprays**
  - Prior campaigns were limited to 3 viewing angles
  - Automatic rotation mount for injectors allows many views per test case
  - Recent campaigns with many (72 views) demonstrate capabilities of the many-view CT technique

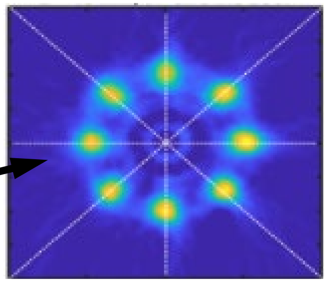
Plume-to-plume variations in location and width

Technical Accomplishment S.E.04.01 (Pickett)
New Capability for 3D Measurements of Liquid Volume Fraction

- **Used 3D CT methods to characterize PACE multi-component gasoline surrogates relative to RD5-87**
  - Validated that **proposed PACE surrogates behave like research gasoline blends in free spray experiments** with ECN spray G injector and conditions
- **Characterized plume-to-plume variations in symmetric spray G injector free sprays**
  - Despite symmetric hole pattern, CT measurements showed spray G injectors produced plume-to-plume deviations in liquid density
  - Observations are both informing CFD modeling inputs and offering target for simulation results
- **Many-view CT allows for characterization of sprays from injectors with non-symmetric hole patterns**
- **Operating profile of continuous flow vessel recently expanded to ambient pressures up to 40 bar and temperature up to 900 K**

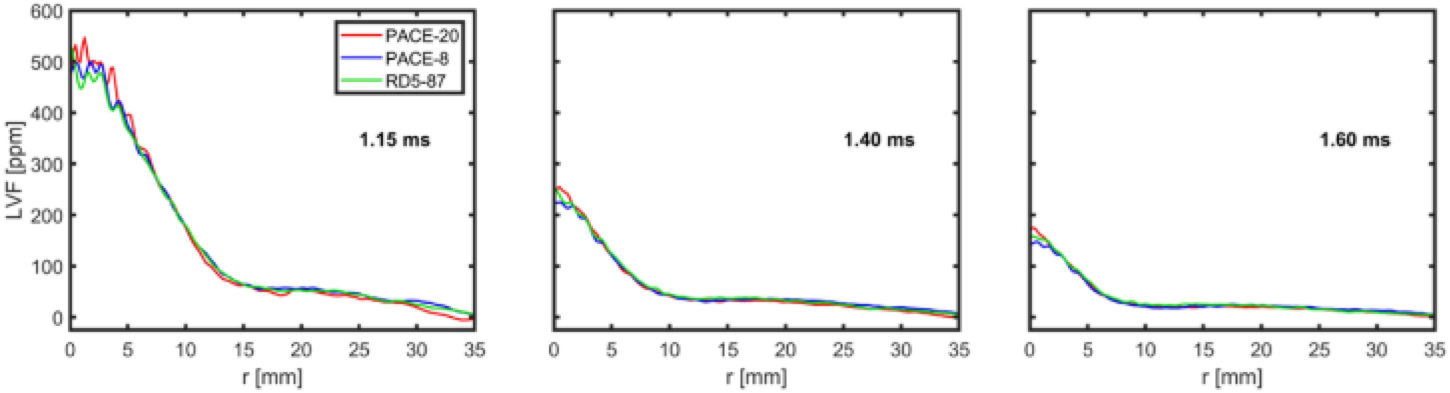


Results show LVF at 30 mm plane



Plumes from spray G injector show differences in local liquid density

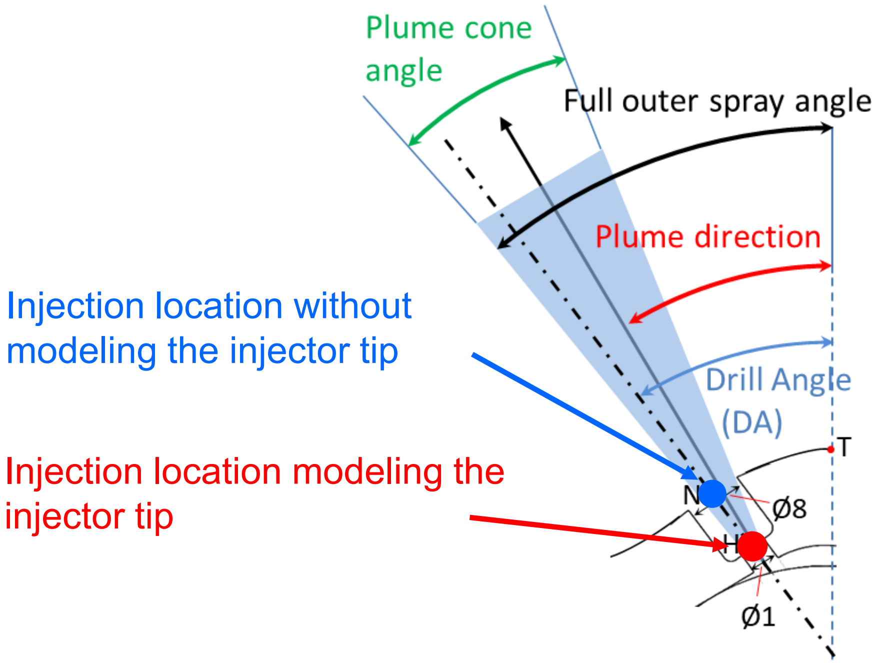
Average radial Liquid Volume Fraction (LVF) distributions

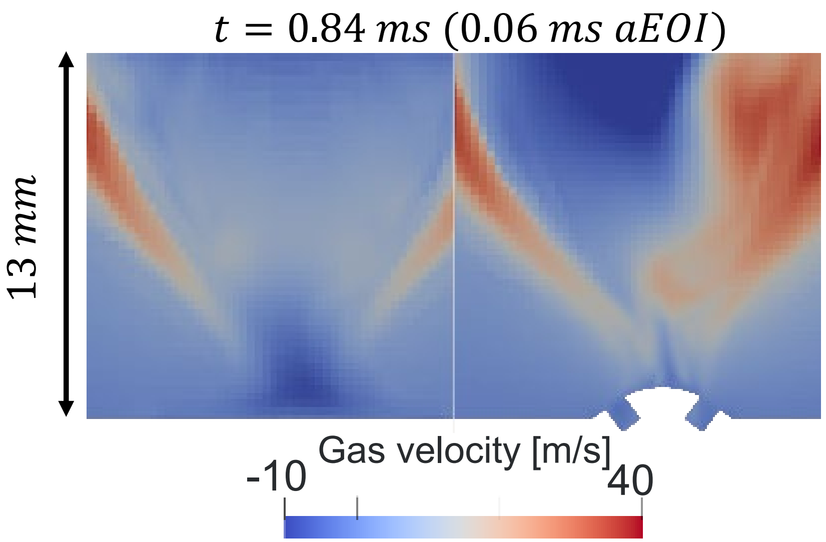


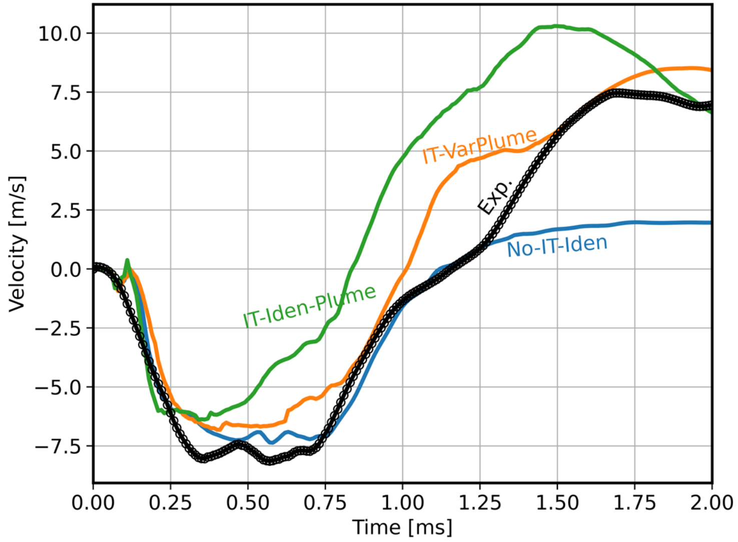
ECN G2 Conditions

Technical Accomplishment: S.M.04.01 (Nguyen)
Inclusion of Injector Geometry Improves Air Entrainment Even with RANS Calculations

- **Current standard practice ignores the injector tip geometry**
  - Often, parcels are often generated away from the domain boundary
  - This could influence entrainment, plume direction, cone angle…



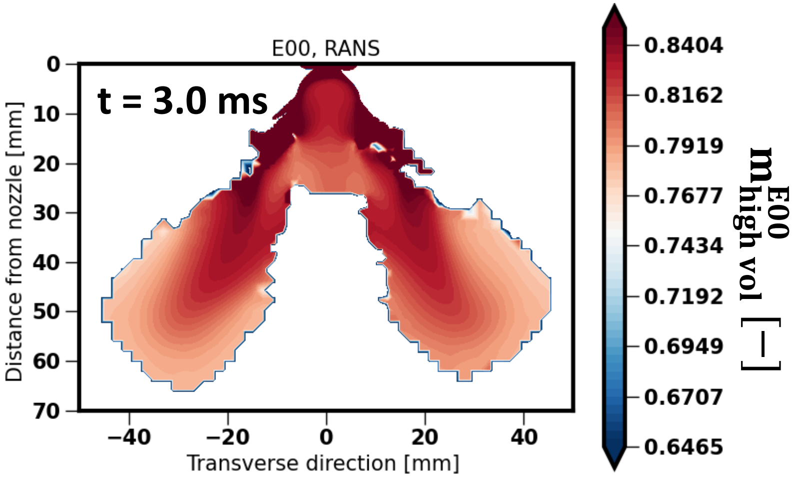


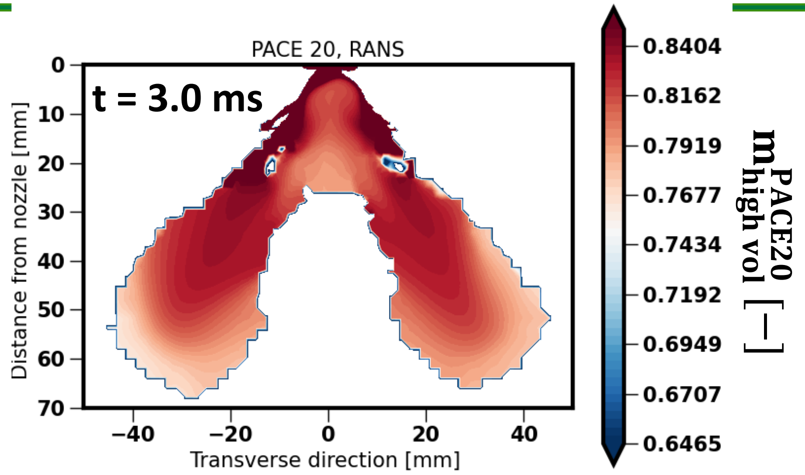


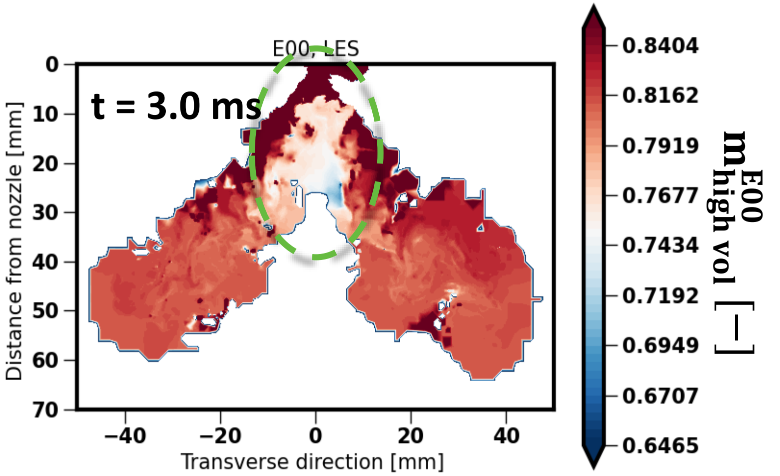
Modelling the injector tip geometry + hole-by-hole variation improves the air entrainment dynamics between the plumes

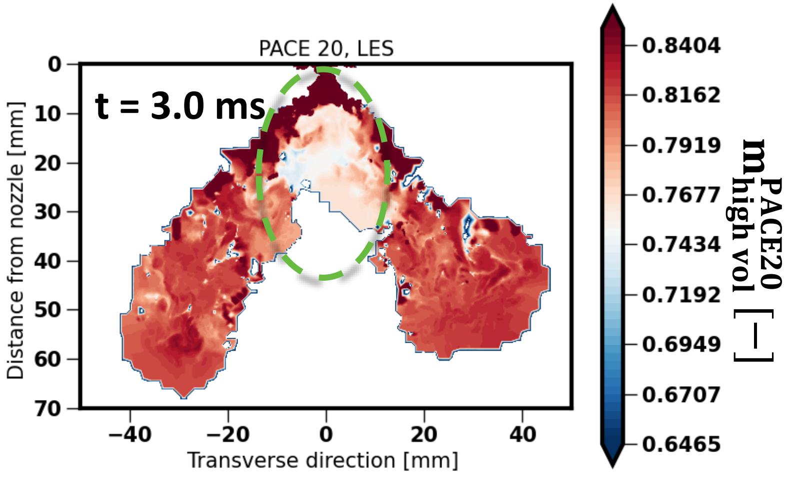
Technical Accomplishment: S.M.04.01 (Nguyen)
LES of Multi-Component Gasoline Surrogate

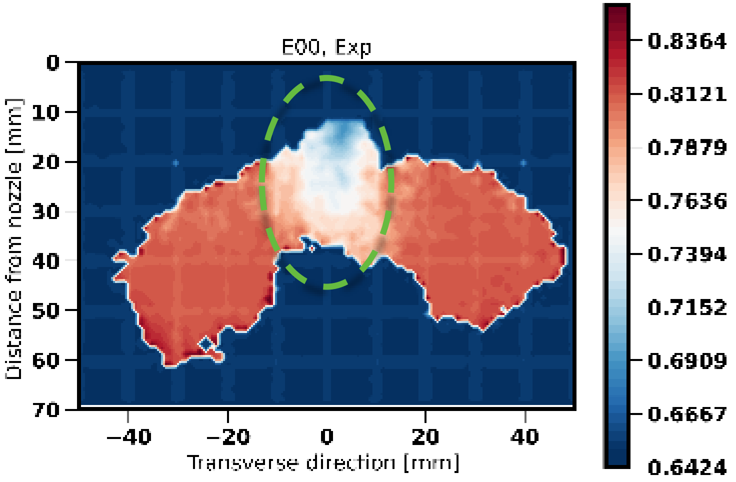
- **Comparison between IFPen cut plane mixing measurement of high volatility component ($y_{i-C_8H_{18}} + y_{n-C_5H_{12}}$) for E00 at 3 ms ASOI.**
- **PACE 20 high volatility components include any hydrocarbon less than C8**
- **Region with value between 0.7 and 0.8 indicates strong preferential evaporation**
- **LES is more capable to evaluate preferential evaporation compared to RANS**











$$m^{E00}_{high\ vol} = \frac{m_{i-C_8H_{18}} + m_{n-C_5H_{12}}}{m_{n-C_{11}H_{24}} + m_{i-C_8H_{18}} + m_{n-C_5H_{12}}}$$

E00 Composition

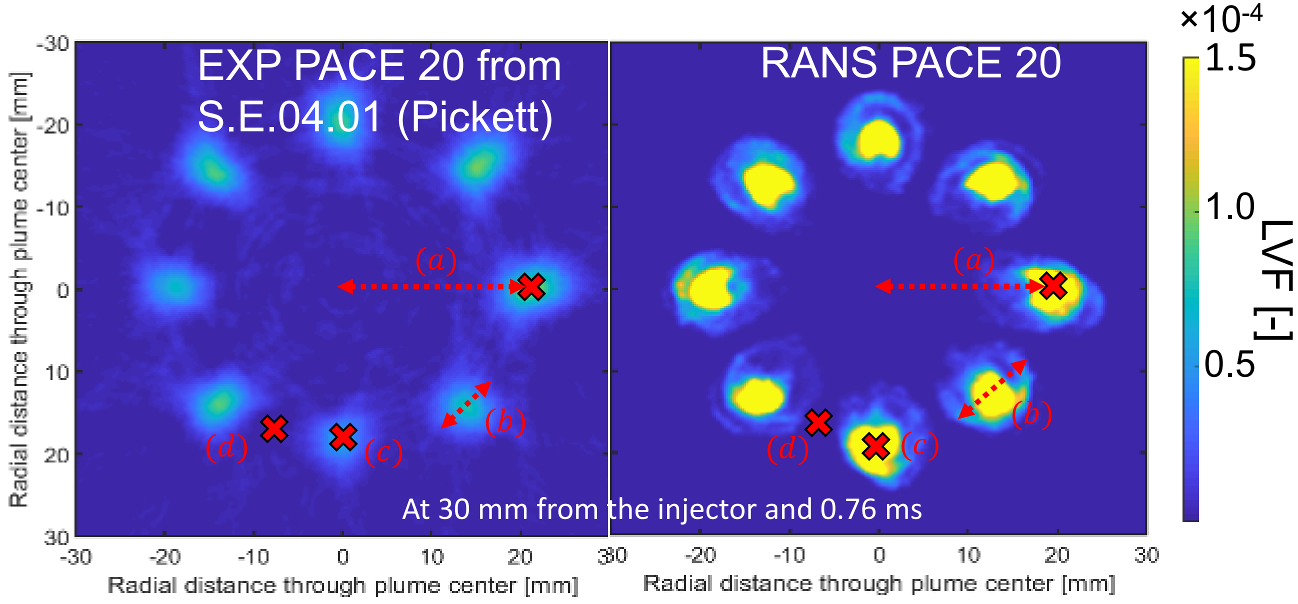
Species	$i\text{-}C_8H_{18}$	$n\text{-}C_5H_{12}$	$n\text{-}C_{11}H_{24}$
Mass fraction	0.47	0.33	0.2

PACE20 Composition

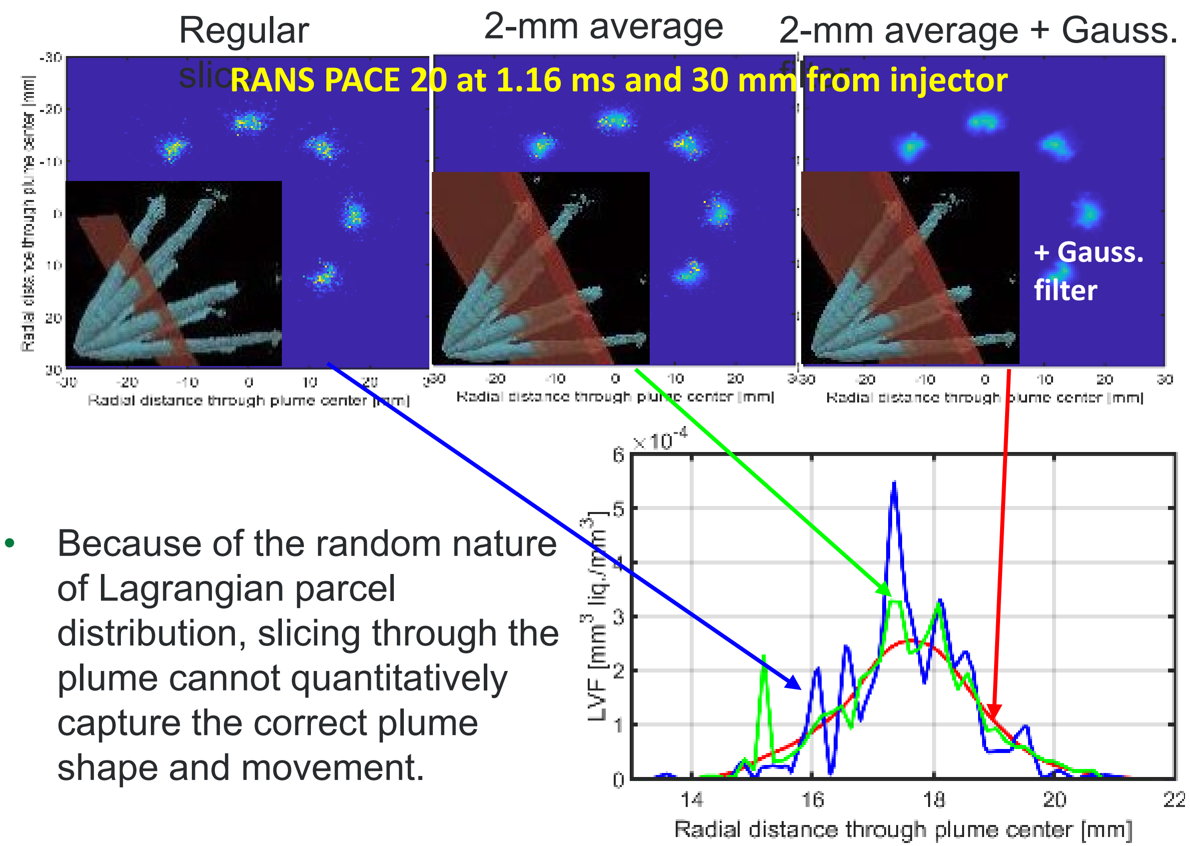
Species	C6H12-1	C7H8	CPT	$i\text{-}C_8H_{18}$	$n\text{-}C_5H_{12}$	$n\text{-}C_7H_{16}$	T124MBZ	TETRA	ETHA
Mass fraction	0.05	0.11	0.11	0.23	0.12	0.11	0.14	0.04	0.10

Technical Accomplishment: S.M.04.02 (Tagliante)
New Post-Processing Techniques Enable Development of Merit Function

- **A merit function testing the accuracy of CFD will help to quantify comparisons and track progress**
- **A number of criteria can be compared:**
  - (a)- Plume center location
  - (b)- Plume cone width
  - (c)- LVF in the plume center
  - (d)- LVF between plumes
  - (e)- Liquid length
  - Liquid velocity
  - Gas velocity
  - SMD or surface area
  - Vapor mass fraction
  - Vapor axial penetration



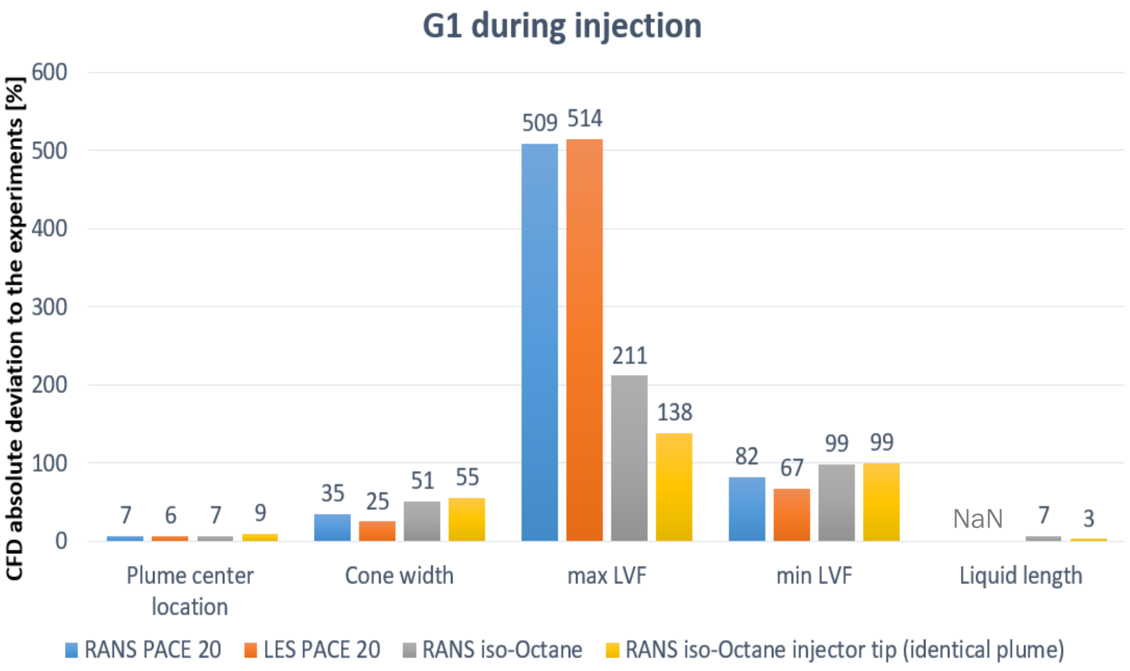
- **Post-processing of each criteria must be carefully defined**
- **Example: use Sandia's new 3D Liquid Volume Fraction to evaluate the performance of the CFD**



- Because of the random nature of Lagrangian parcel distribution, slicing through the plume cannot quantitatively capture the correct plume shape and movement.

- Slicing through the plumes using a 2-mm finite width enhances plume resolution while reducing the scattering around edges of the plume + a Gaussian filter is applied

Technical Accomplishment: S.M.04.02 (Tagliante)
Initial Steps for Development of a Merit Function for Sprays

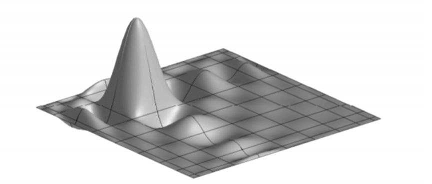


- **The merit function takes into account experimental uncertainties in the optical thick zone by a weighting function depending on the axial location.**
- **Because the merit function treats each plume separately it can be used on injectors with asymmetric plumes**

- All the simulations capture the plume center location well
- The cone width is underestimated for all simulations, especially for iso-octane
- Large overestimation of the LVF in the center of the plume for PACE 20. Simulations of iso-octane also overestimate the LVF but to a minor degree compared to PACE 20.
- Taking into account the injector tip improves the prediction of the LVF in the plume center
- Work on merit function will continue, incorporating more parameters

Approach A.M.05.02 (Ameen)
Spray and Combustion Models in Nek5000

- **Spectral element method (SEM) implemented in the Nek5000 code.** (Patera, 1984; Maday & Patera, 1989)
  - N^{th} order tensor-product Lagrange polynomials at GLL points.
    $G = E(N+1)^d$, G: grid points, E: elements
  - Exponential convergence with N → High accuracy at low cost.
  - Very low numerical dissipation.
  - Demonstrated scalability on more than 10^6 processors
  - Low-Mach formulation for weakly compressible flows.
- **Eulerian-Lagrangian approach to model fuel sprays using a stochastic parcels-based method.** (Reitz & Diwakar, 1987)
  - Spectral interpolation of gas properties is done at parcel locations.
  - Particle properties and source terms are projected on the Eulerian grid using a Gaussian projection filter.
- **The approach allowed for grid-independent results for sprays under non-evaporative conditions.**
  - Colmenares F. J., Ameen, M., Patel, S. (2020) 73rd Annual Meeting of the APS Division of Fluid Dynamics.

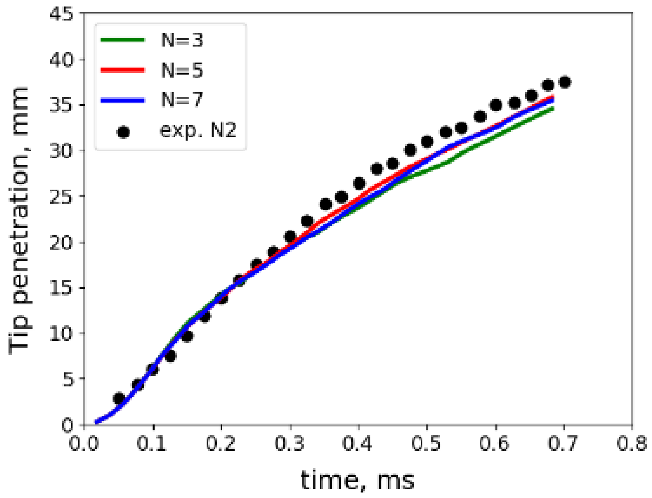


2D basis function, N=10

$$u_N(x) = \sum_{k=0}^{N} u_k h_k(x)$$

Physical models	
Evaporation model	Abramzon & Sirignano
Breakup model	KH-RT
Droplet distortion	TAB

Breakup model parameters	Value
B_0	0.61
B_1	80
C_{RT}	0.4



Nozzle Diameter	140 μm
Injection pressure	80 MPa
Ambient pressure	2 MPa
Ambient gas	Nitrogen
Fuel	Diesel

Liquid penetration for a spray under non-evaporative conditions with varying polynomial order, *N*. (AMR 2020, ACE146). Experimental data from Margot et al. (2008).

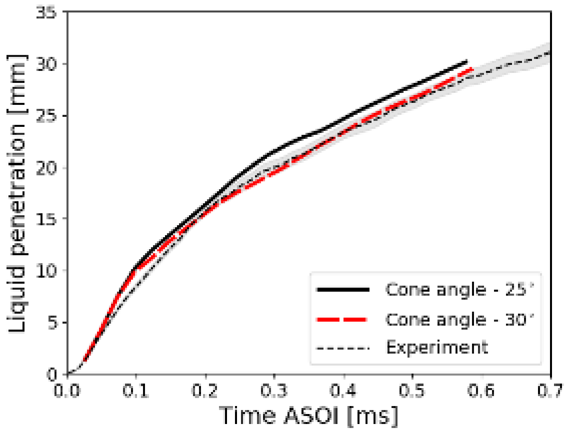
Technical Accomplishments: A.M.05.02 (Ameen)
Spray and Combustion Models in Nek5000

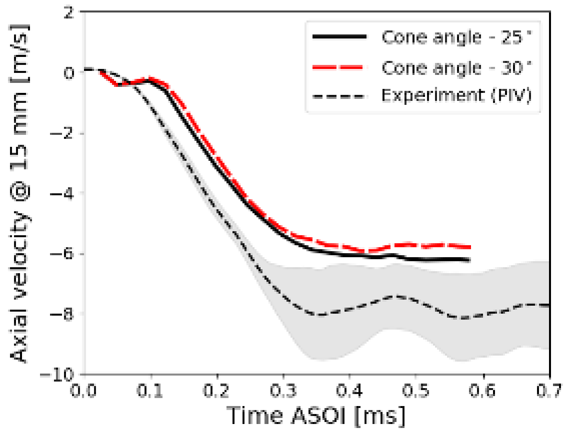
- **Performed high-resolution LES of sprays under G1 conditions.**
- **Spray parameters were tuned to match experimental liquid penetration.**
  - **Colmenares F., J, Ameen, M., Patel, S. (2021) ASME ICEF.**
- **Spray morphology is in good agreement with experiments.**
- **Axial recirculation was under-predicted, but the general trend was well captured.**
- **Simulations will be extended to include detailed nozzle geometry and flow past EOI.**
- **Numerical results will be evaluated against merit function. (Tagliante, S.M.04.02)**

Nozzle Diameter	165 μm
Injection pressure	20 MPa
Ambient density	3.5 kg/m^3
Ambient gas	Nitrogen
Ambient temperature	573 K
Fuel	Iso-octane
Injection time	0.76 ms
Plume cone angle, Θ	**25°, 30°**
Plume direction	**33°**
Area contraction, C_a	**0.65**

Order	N = 5
Minimum Δx @ axis [mm]	0.033
# elements	270 k
# unique grid points	33.9 M

PLV=0.2e-3 contours.





Responses to Last Year's Reviewer Comments

- **"The experiments are testing old hardware, it will be helpful to have a plan for upgrading the experimental hardware"**
- **"There is a lack of fuel system design and manufacturing expertise in the project… there should be a strong link to the injector design. The team should articulate how the spray physics could be mapped back to the technology and design requirements."**
  - New injectors will be acquired from Bosch with the support of Ford
  - Argonne and new Sandia experiments capture 3D info on the spray plumes, and these can be tied to the internal nozzle geometry
  - New injectors will be radically different than Spray G: side-mount vs symmetric, smoother surface finish, higher pressure. The new hardware will impose stringent tests on the models validated using the older geometries
- **"Capturing cycle-to-cycle variation should be incorporated. Not just be RMS levels but getting to the root of the variance and the occurrence of rare events"**
  - ACE146 will discuss CCV
  - Several future tasks will address this

Collaboration and Coordination with Other Institutions

- Collaboration within the sprays team and across PACE
- Collaboration with the Engine Combustion Network on target conditions
- 15 Industry partners in the AEC MOU for direction and feedback

Task	Description
A.E.04 Powell	• Internal collaboration with Argonne X-ray Sciences Division • Lead for ECN GDI Internal Flow studies
O.E.04.01 Wissink	• Ford has approved reproduction of 2.3L spray targeting • Bosch to produce new 500 bar HDEV 5.2 injectors
S.M.04.01-02 Nguyen/Tagliante	• Cold start PACE 20 spray simulations (Edwards, ORNL) • Engine Combustion Network accuracy test guidelines
S.E.04.01 Pickett	• PACE: fuel surrogate selection & blending (Wagnon), cold-start condition sprays and heat-transfer (Edwards); Engine Combustion Network • Co-Optima GDI fuel effects, experiments (Sjoberg) and simulation (Torelli)
A.M.05.02 Ameen	• Exascale Computing Project Center for Efficient Exascale Discretizations (CEED) team: Porting the simulations to NekRS, the GPU version of Nek5000 • Exascale Computing Project Co-Design Center for Particle Applications (CoPA) team: GPU porting of the spray models in NekRS

Remaining Challenges and Barriers

- **PACE-wide barriers are discussed in ACE138**
- **Experiments**
  - Current experiments are still testing relatively old hardware. New injection hardware and experiments will be in place next year.
  - Limited data on shot-to-shot variability
  - Limited data on the effects of gas flows
  - Limited data on droplet size
  - Limited data on multi-component fuels
- **Simulations**
  - Uncertainty in plume cone width, liquid volume fraction. These need to become predictive
  - Simulations are underpredicting vaporization
  - Multi-component fuels are still a challenge
  - The effects of gas flows are a challenge

Proposed Future Research

- **A.E.04: Free Spray and Wall-Film X-ray Experiments (Powell)**
  - Measurements with multi-component fuels
  - Measurements of sprays in cross-flows
- **O.E.04.01: New Injector Procurement and Characterization (Wissink)**
  - Expand characterization matrix to multiple injections, effects of dwell time and duration, or different temperature/pressure conditions as prioritized by Sprays Team
- **S.M.04.01-02: Spray accuracy toolkit development and multi-component vaporization (Tagliante/Nguyen)**
  - Free spray in both liquid and vapor phase
  - Multi-component vaporization with non-ideal mixtures
  - Extend accuracy toolkit to wall film validation: film center, height and other criteria to be defined
- **S.E.04.01: Free Spray and Wall-Film Optical Experiments (Pickett)**
  - Quantify liquid spray distribution for PACE-relevant injectors (Sjoberg and EcoBoost 2.3 L) & conditions
- **A.M.05.02: High-Fidelity Spray and Combustion Models in Nek5000 (Ameen)**
  - Implement corrected distortion and multi-component evaporation models.
  - Implement one-way coupling injection method using maps from internal-nozzle flow simulations

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

Summary

- **A.E.04: Free Spray and Wall-Film X-ray Experiments(Powell)**
  - PACE engine injectors have been measured to quantify their geometry and enable simulations
- **O.E.04.01: New Injector Procurement and Characterization (Wissink)**
  - Using a matched and characterized set of injectors will ensure alignment between various experimental and modeling efforts within PACE. Transition to 500 bar capability will be representative of modern injector hardware.
  - Expected FY21Q4 delivery of new injectors is compatible with timeline for PACE engine installations
- **S.M.04.01: Free Spray Modeling (Nguyen)**
  - Importance of tip geometry and near-field plume emergence clarified
- **S.M.04.02: Spray accuracy toolkit development (Tagliante)**
  - A merit function evaluating the performance of the liquid spray (CFD) has been developed
- **S.E.04.01: Free Spray and Wall-Film Optical Experiments(Pickett)**
  - Tool to quantify 3D plume-plume variations applied to wide range of conditions
- **A.M.05.02: High-Fidelity Spray and Combustion Models in Nek5000 (Ameen)**
  - High-resolution LES of free sprays show the need for improved Lagrangian spray submodels.

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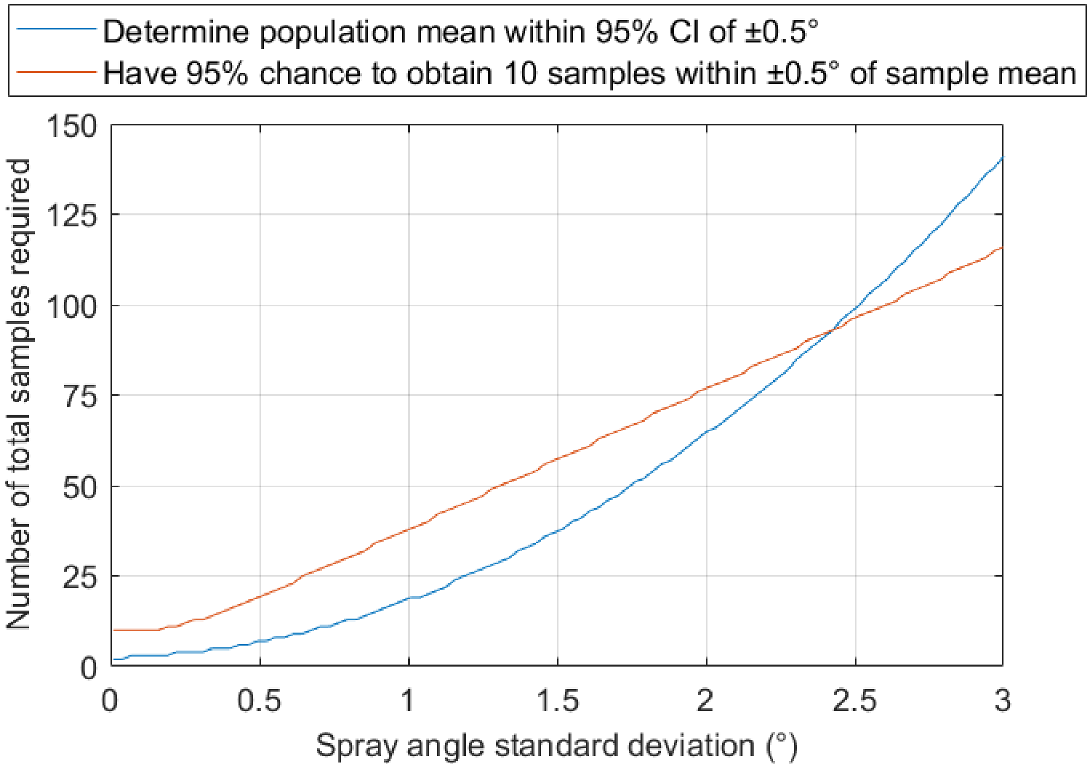
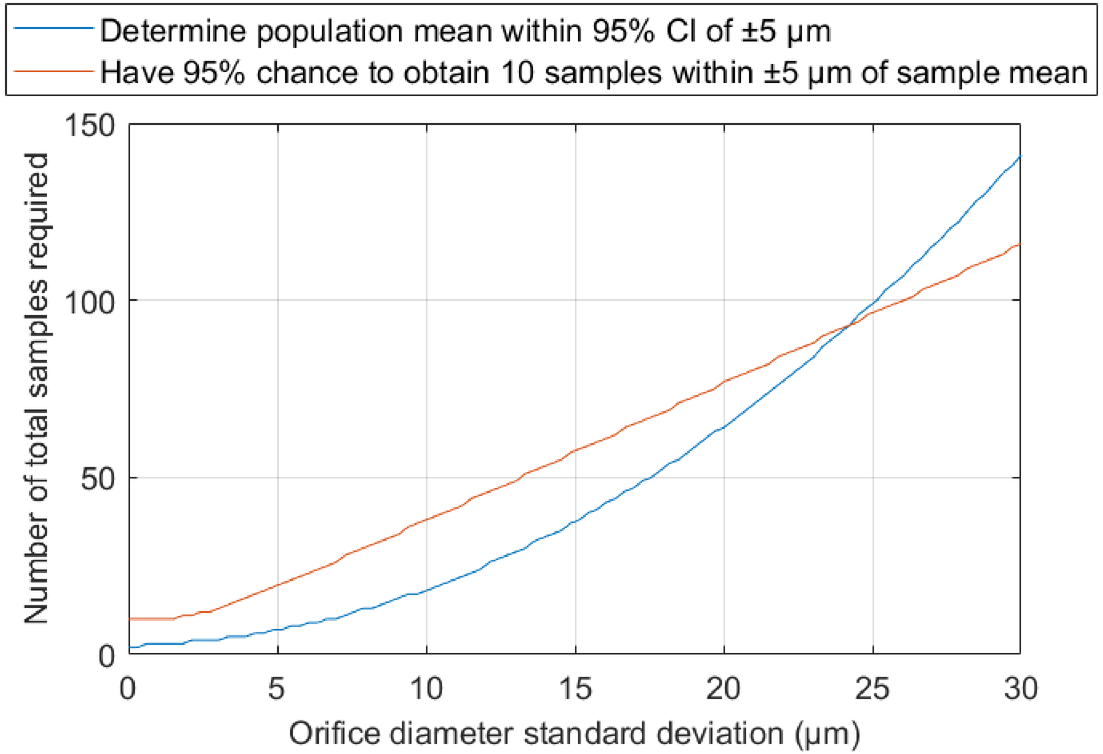
Technical Backup Slides

O.E.04.01: Injector Characterization & Distribution (Wissink)

How many samples are required? Two driving goals:

- Determine nominal geometric property $\bar{X}$ within a given confidence interval $\pm E$
- Obtain a set of N injectors which are within $\pm E$ of $\bar{X}$

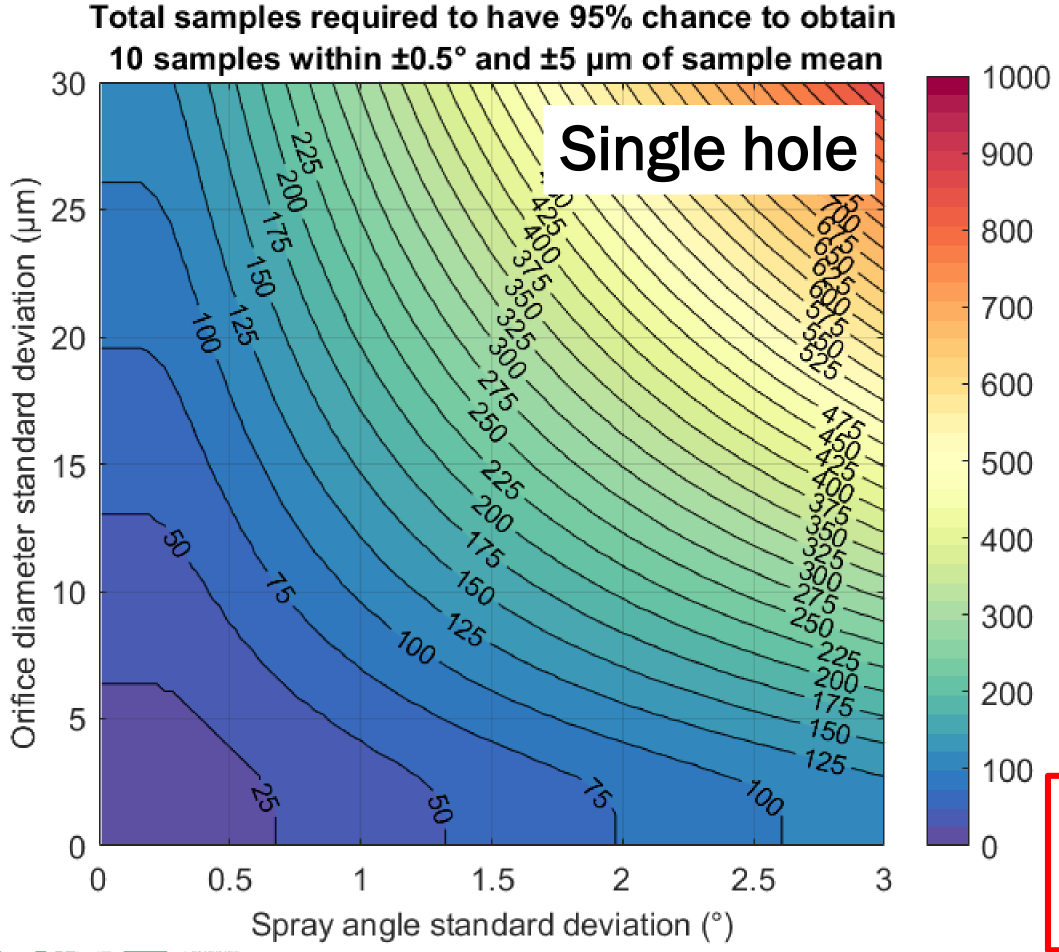


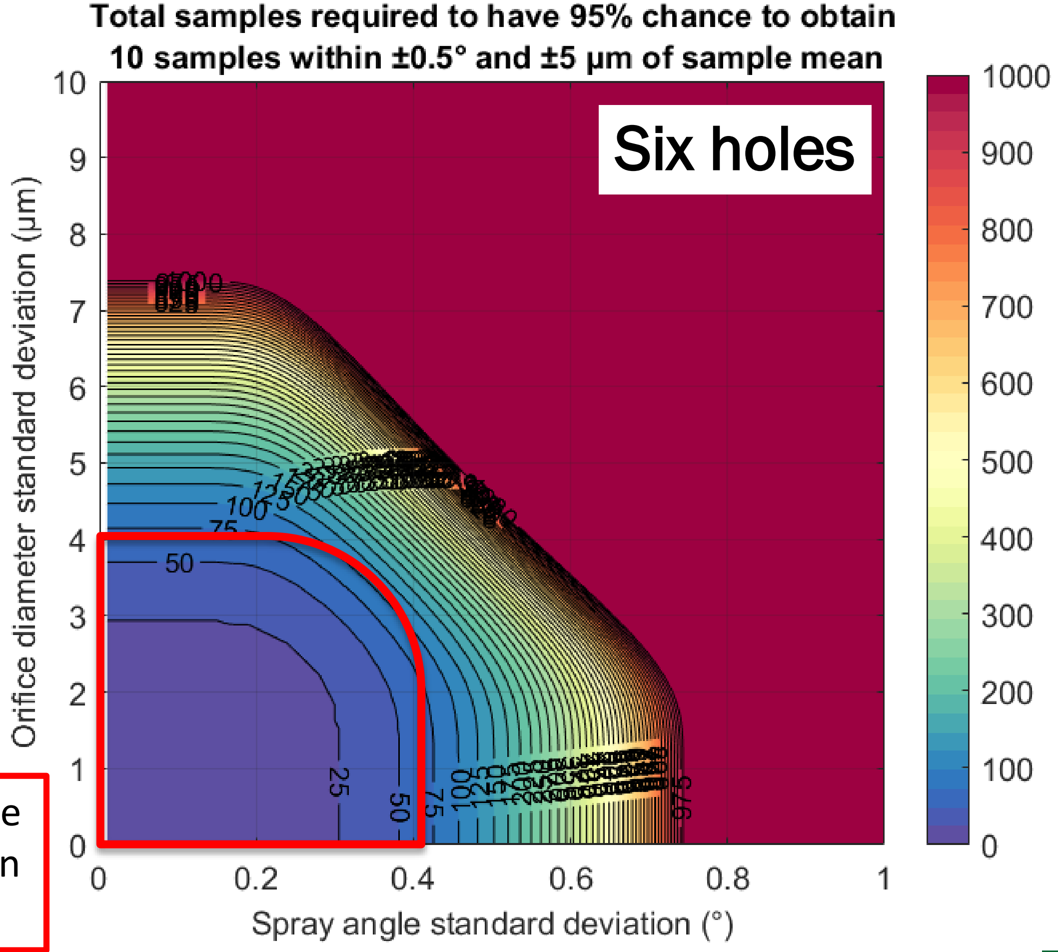


O.E.04.01: Injector Characterization & Distribution (Wissink)

Joint probability of having correct spray angle and hole size

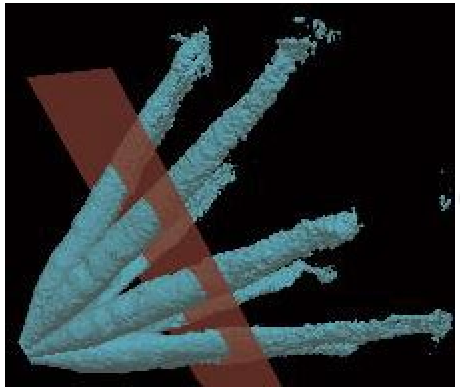
- Assuming all parameters independent across all holes
- Sample pool required blows up quickly for 6 holes
- Can we estimate population parameters, required tolerances, and injectors required for "matched" set?

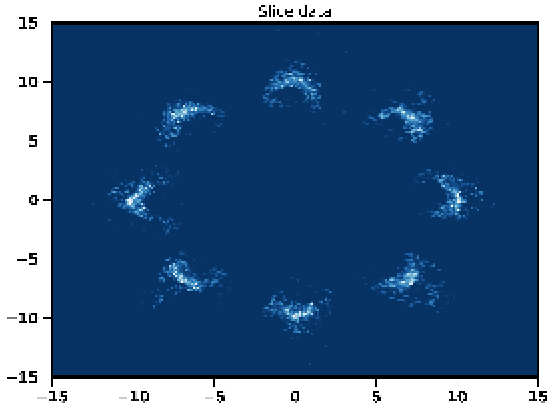


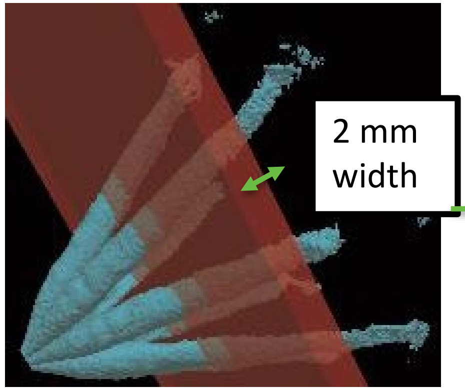


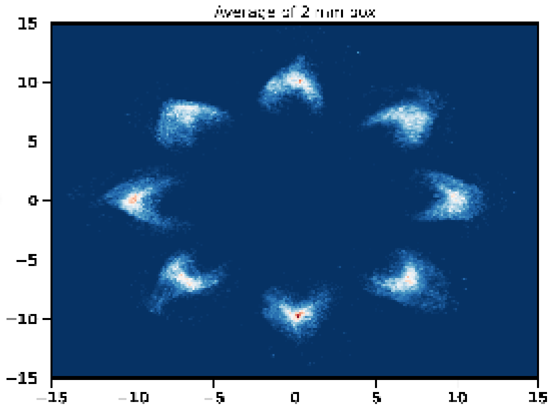
Must assume we are in this region to have success

Merit Function: Radial distribution of liquid throughout plume post-processing methodology

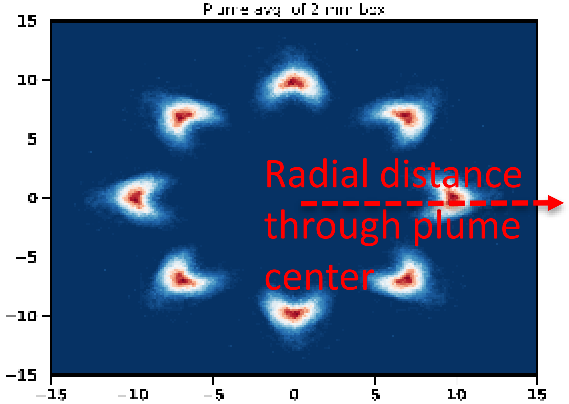


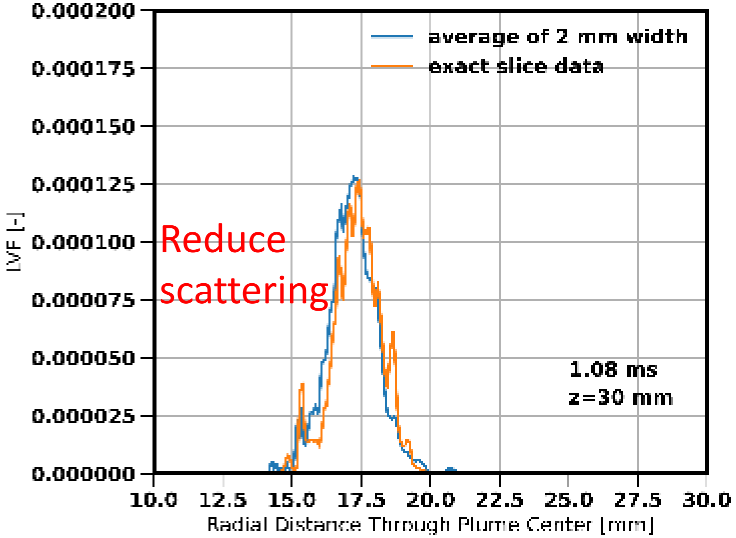


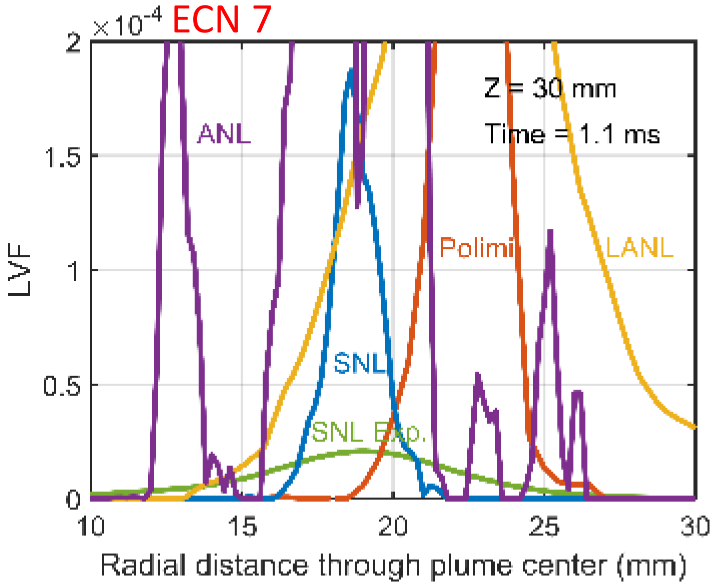




mean of all 8 plumes
at an axial cut plane



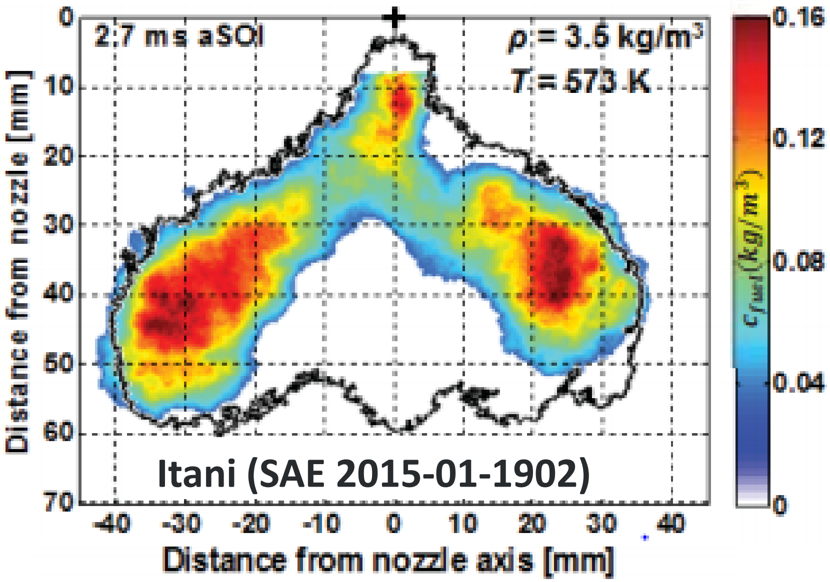


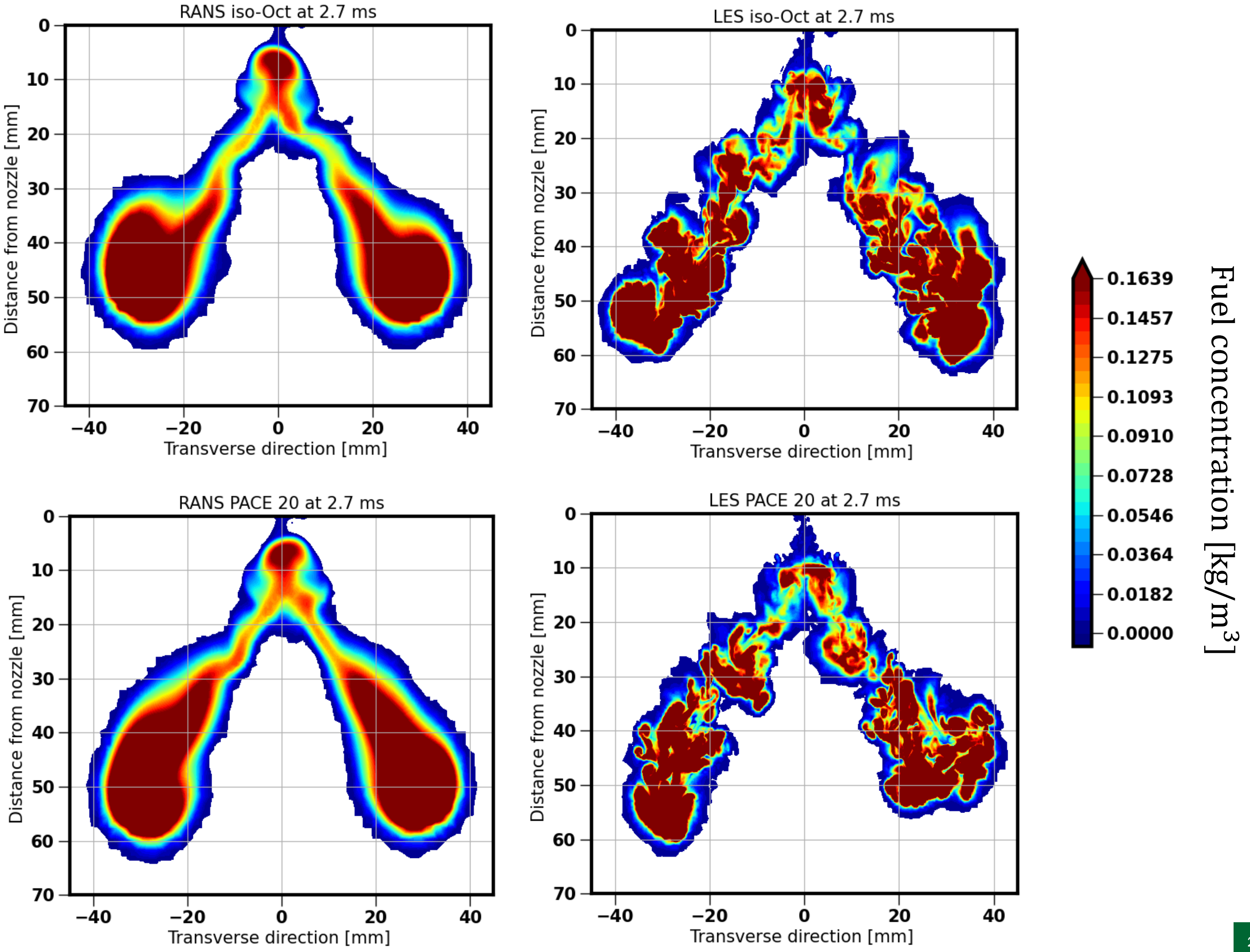


- **Because the random nature of Lagrangian parcel distribution, slicing through the plume cannot quantitatively capture the correct plume shape and movement.**
- **Slicing through the plumes using a 2-mm finite width enhances plume resolution while reducing the scattering around edges of the plume**

PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

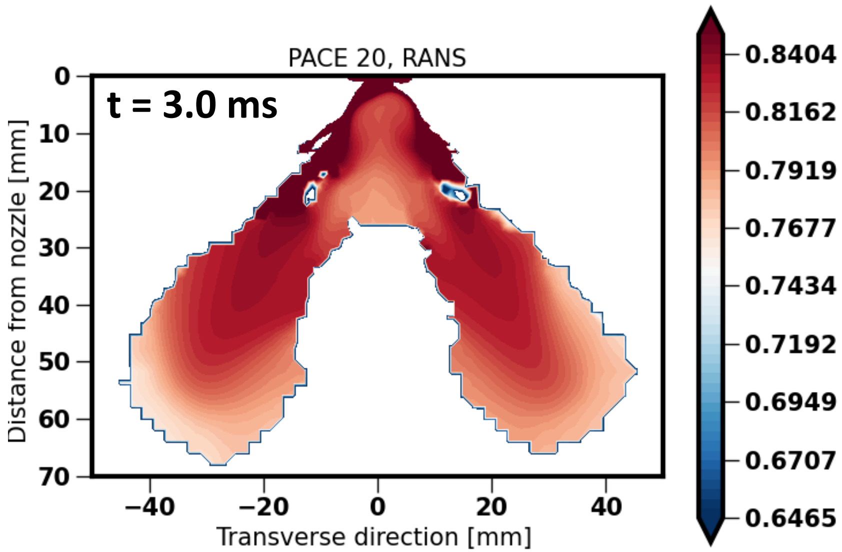
Preferential Evaporation: Comparing Mixture Formation Between iso-Octane and PACE-20

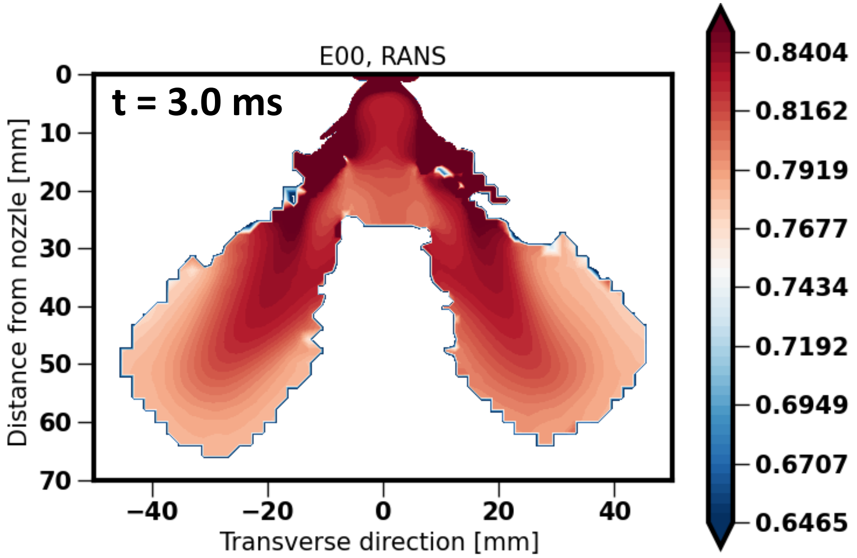


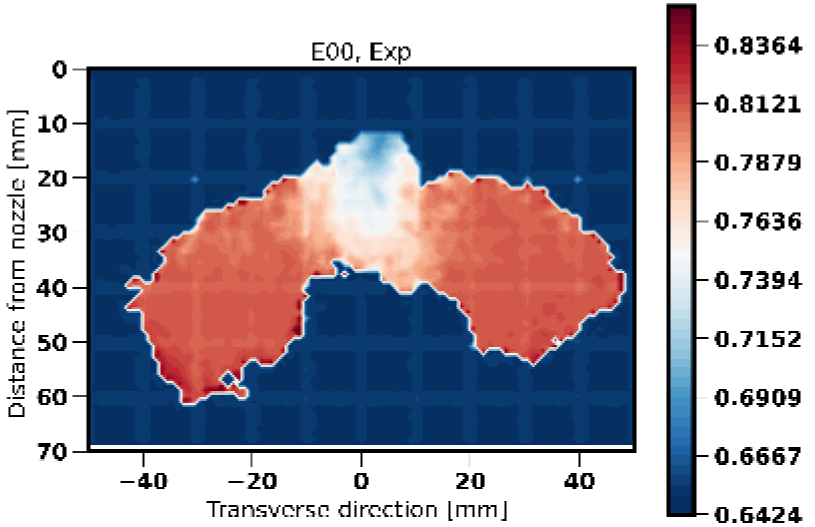


Comparison of preferential evaporation RANS

- **Comparison between IFPen cut plane mixing measurement of high volatility component ($y_{i-C_8H_{18}} + y_{n-C_5H_{12}}$).**
- **Region with lower value indicate strong preferential evaporation**
- **Preferential evaporation is qualitatively the same for both CFD calculation**







Reproduced from Cordier et al. (2019 IJER, IFPen)

E00 Composition			
Species	$i\text{-}C_8H_{18}$	$n\text{-}C_5H_{12}$	$n\text{-}C_{11}H_{24}$
Mass fraction	0.47	0.33	0.2

$$m_{high} = \frac{m_{i-C_8H_{18}} + m_{n-C_5H_{12}}}{m_{n-C_{11}H_{24}} + m_{i-C_8H_{18}} + m_{n-C_5H_{12}}}$$

PACE20 Composition									
Species	C6H12-1	C7H8	CPT	$i\text{-}C_8H_{18}$	$n\text{-}C_5H_{12}$	$n\text{-}C_7H_{16}$	T124 MBZ	TETRA	ETHA
Mass fraction	0.05	0.11	0.11	0.23	0.12	0.11	0.14	0.04	0.10

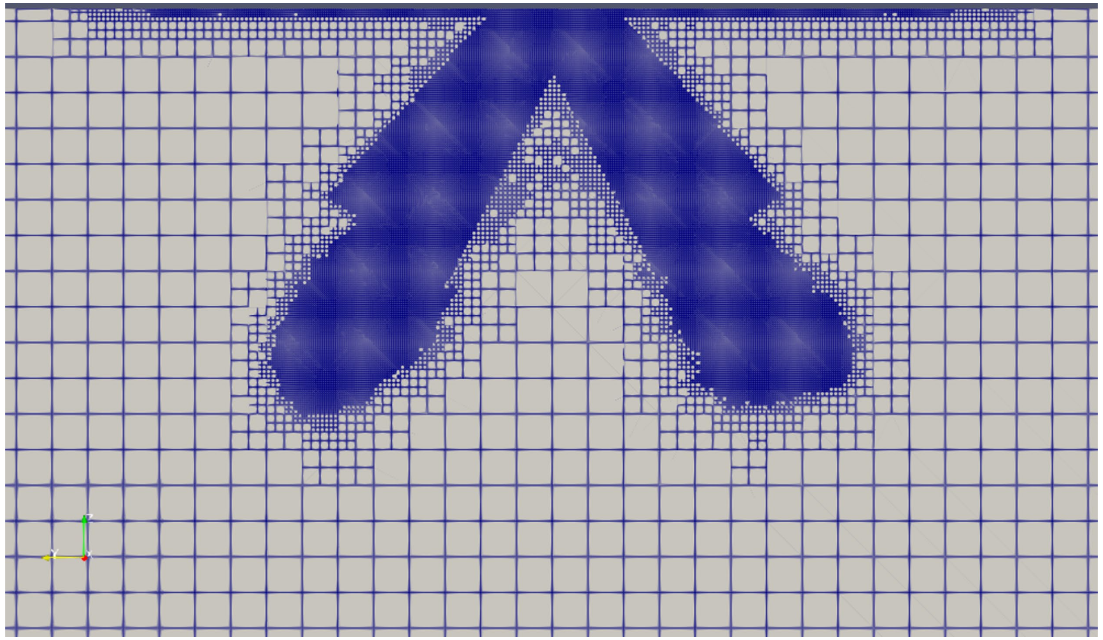
$$m_{high} = \frac{m_{i-C6H12} + m_{i-C7H8} + m_{i-CPT} + m_{i-C8H18} + m_{i-C5H12} + m_{i-C7H16}}{m_{i-C6H12} + m_{i-C7H8} + m_{i-CPT} + m_{i-C8H18} + m_{i-C5H12} + m_{i-C7H16} + m_{i-T124MBZ} + m_{i-TETRA}}$$

PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Case and simulation parameters

Numerical setup	
CFD code	*CONVERGE* V3.0
Type grid	AMR and fixed embedding
Base grid [mm]	2
Embedding level for AMR and fixed embedding	4
Maximum grid resolution [mm]	0.125
Turbulence	RANS $k{-}\varepsilon$ STD
Spray model	Lagrangian parcel
Cone distribution	distribute injected parcels evenly throughout the cone
Injection distribution	BLOB
Breakup model	KH-RT
KH breakup time constant (B1)	5
Vaporization	Frössling + CD [1]
Droplet collision	No time counter (NTC)
Droplet drag	Dynamic sphere + CD [1]
Droplet dispersion	O'Rourke
Number of parcel injected	560,000
Plume cone angle	30°
Plume direction angle	34°

Numerical setup	
Standard	G1
Ambient Temperature [K]	573
Injector hole radius [um]	165
Ambient Pressure [bar]	60
Ambient density [kg/m3]	3.5
Initial turbulent kinetic energy [m^2/s^2]	6.4e-3
Initial TKE dissipation rate [m^2/s^3]	5.08e-1



[1]: Nguyen et al., *International Journal of Heat and Mass Transfer (2021)*, Submitted

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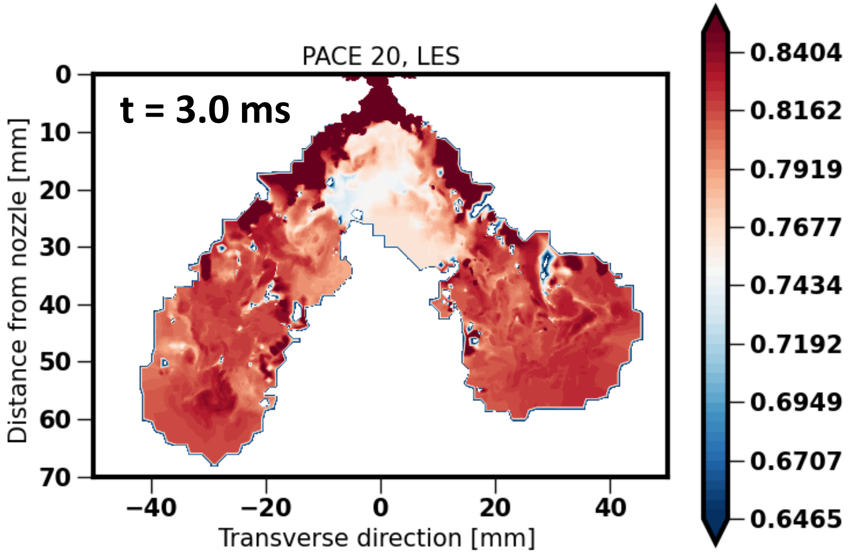

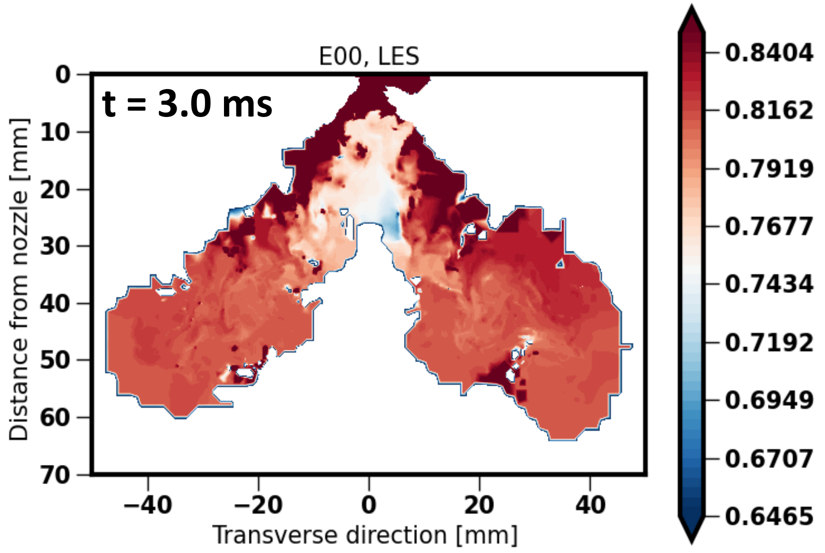

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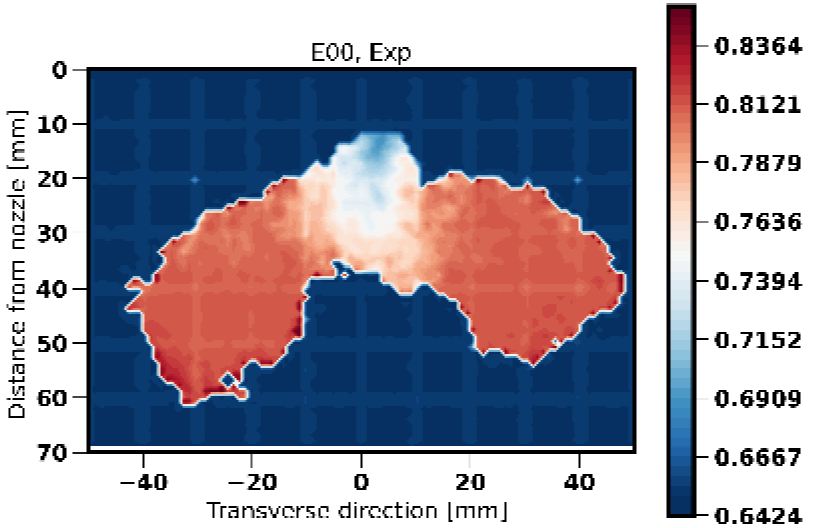
PACE20 Composition									
Species	C6H1 2-1	C7H8	CPT	$i-C_8H_{18}$	$n-C_5H_{12}$	$n-C_7H_{16}$	T124 MBZ	TETRA	ETHA
Mass fraction	0.05	0.11	0.11	0.23	0.12	0.11	0.14	0.04	0.10

$$m_{high} = \frac{m_{i-C6H12} + m_{i-C7H8} + m_{i-CPT} + m_{i-C8H18} + m_{i-C5H12} + m_{i-C7H16}}{m_{i-C6H12} + m_{i-C7H8} + m_{i-CPT} + m_{i-C8H18} + m_{i-C5H12} + m_{i-C7H16} + m_{i-T124MBZ} + m_{i-TETRA}}$$



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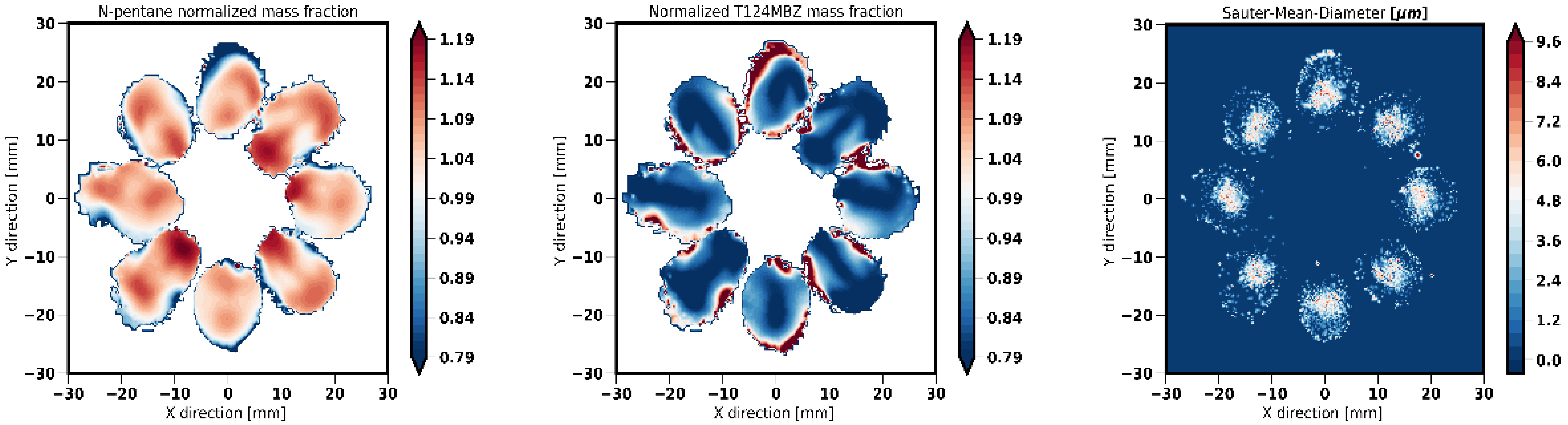
Assessment of Mixture under Preferential Evaporation



- **Heavy-end component tends to preferentially evaporate around plume periphery**
- **Lighter-end component tends to vaporize more inside the plume and near the center.**

$$Y_{\{norm,k\}} = \frac{1}{Y_k^0} \frac{Y_k}{(\sum_{i=1}^{n} Y_i)}$$

PACE20 Mass Composition									
Species	C6H12-1	C7H8	CPT	i-C_8H_{18}	n-C_5H_{12}	n-C_7H_{16}	T124MBZ	TETRA	Ethanol
Mass fraction	0.05	0.11	0.11	0.23	0.12	0.11	0.14	0.04	0.10

PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES