SAND2021-14735PE

PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Spray Wall Interactions

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Annual Merit Review, 22 June 2021, 2:10 pm EDT, Project ACE144

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Gurpreet Singh, Program Manager

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Overview: spray wall interactions, films and soot formation

- **Timeline**
  - All projects started mid 2019 and are 46% complete (to 2023)

	Task	Description
experimental	S.E.4.1 Pickett	SNL, Free spray and wall film optical experiments Pickett, Manin, Karathanassis, White, Tagliante, Strickland
experimental	S.E.2 Manin	SNL, Soot and film combustion Manin, Pickett, Wan
experimental	A.E.4 Powell	ANL, Free spray and wall film x-ray experiments Powell, Sforzo, Tekawade, Moon
experimental	O.E.6.2 Wissink	ORNL, Spray impingement and wall film neutron scattering experiments; Wissink
modeling	S.M.4.2 Nguyen	SNL, Evaporative free spray and soot film combustion modeling; Nguyen, Tagliante, Strickland, Pickett, Chen
modeling	A.M.4 Torelli	ANL, GDI spray-wall interaction and engine spray modeling Torelli, Guo
	S.E.4.3 Pickett	SNL, Spray team coordination, data sharing, ECN lead Pickett, Maes, White, Prisbrey, Nguyen, Tagliante

ACE144 Pickett: Review spray wall interactions and films IN CHAMBERS
ACE167 Torelli & Sjöberg: Spray wall interactions and flows IN ENGINES
ACE168 Manin: Soot formation, including outcome of film combustion
ACE143 Powell: Free sprays IN CHAMBERS

Funded tasks are divided between different AMR presentations. See total budgets highlighted in Appendix

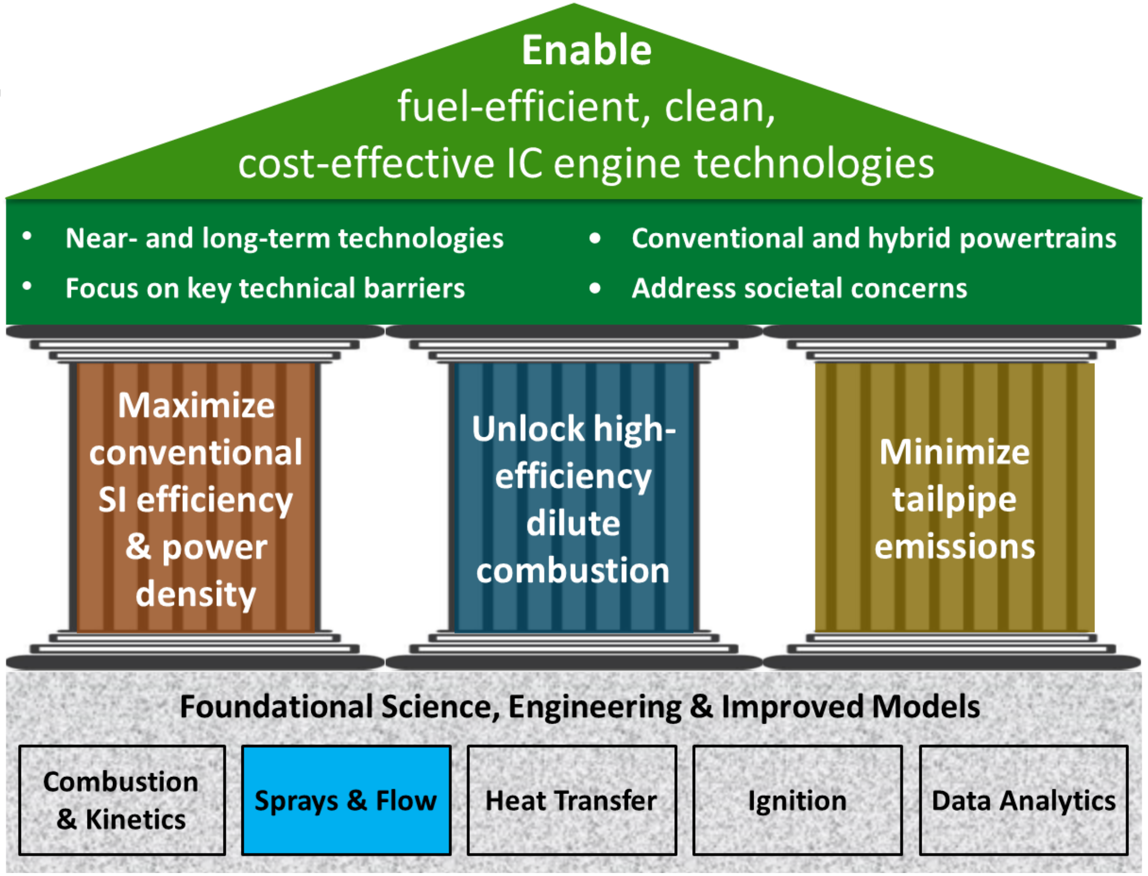
- **Addresses all major PACE outcomes/goals**
  - Minimizing emissions at all operating conditions, including cold-start with potential film combustion
  - Predicting free-spray and wall-impinging sprays, ultimately producing combustible mixtures at the spark plug for efficient (including dilute) combustion
  - Avoiding liner and piston liquid impingement, with implications on knock and premixed ignition
  - CFD spray and film combustion model improvement for engine design/optimization
  - Addressed barriers are guided directly by ACEC tech team

- **Partners**
  - 15 Industry partners in the AEC MOU
  - PACE sprays team coordinates tasks and sets direction
  - PACE linkages to cold-start, combustion, surrogates,..
  - Engine Combustion Network, Spray G (20+ partners)
  - Convergent Science Inc. software
  - + Many more discussed in slides

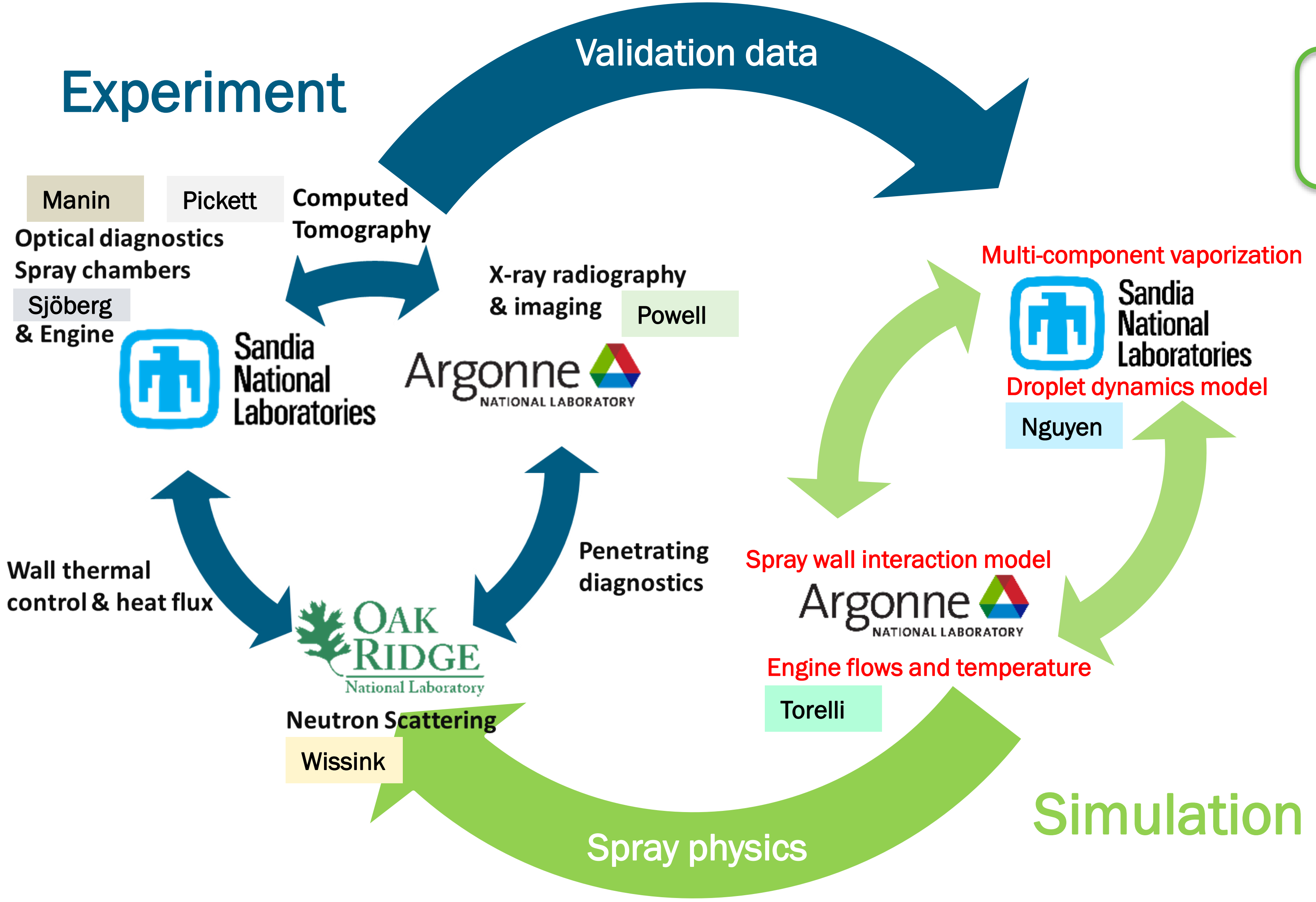
Relevance: Major Outcomes of PACE and the Role of the Sprays Team

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?



Overall approach: co-beneficial modeling tied to experiments



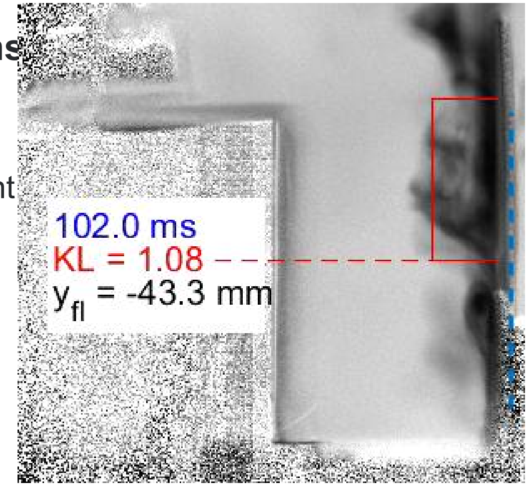
PACE Sprays Team meets biweekly to coordinate over 90 current tasks:

- Focusing on gasoline free spray and impingement phenomena
- Simulations at target conditions (guided from engine results), with different modeling assumptions, compared to unique validation data
- Identify key weaknesses in spray and film models and take action to fix these weaknesses

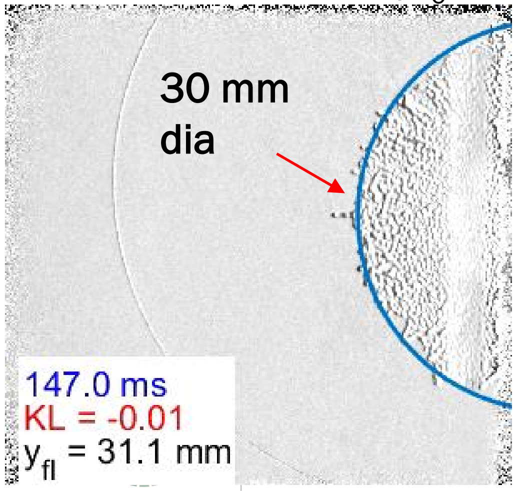
SNL experiments in combustion vessel (see 2020 AMR ACE144)

Predicting and then mitigating film formation is essential to minimize PM formation, particularly during cold-start

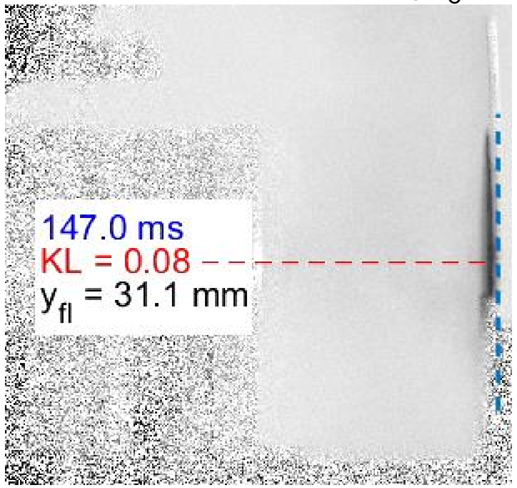
- **Liquid from single, axial plume impinges upon wall at z = 50 mm and forms a terminating film**
  - With particular backlighting, fuel film has “texture” indicating non-uniform thickness
  - Terminating film is about 30 mm diameter, or 10 mm larger than jet width at impingement
  - Asymmetry in film growth expected if spray hits wall at angle
  - Significant liquid remains in ambient as a wall jet and does not form wall film
  - Film persists on wall and soot forms SLOWLY after flame passes
- **Needs from experiments and simulations**
  - Accurate prediction/understanding of free spray (LVF, droplet velocity and size)
  - Ability to measure time resolved film thickness in midst of “background” free or wall jet
  - Measurement of film species composition (for multi-component gasolines)
  - Prediction of wall jet structure and penetration
  - Prediction of film center, offset of free spray plume direction, with multiple injections
  - Measurement of wall temperature, heat flux, and film vaporization rate

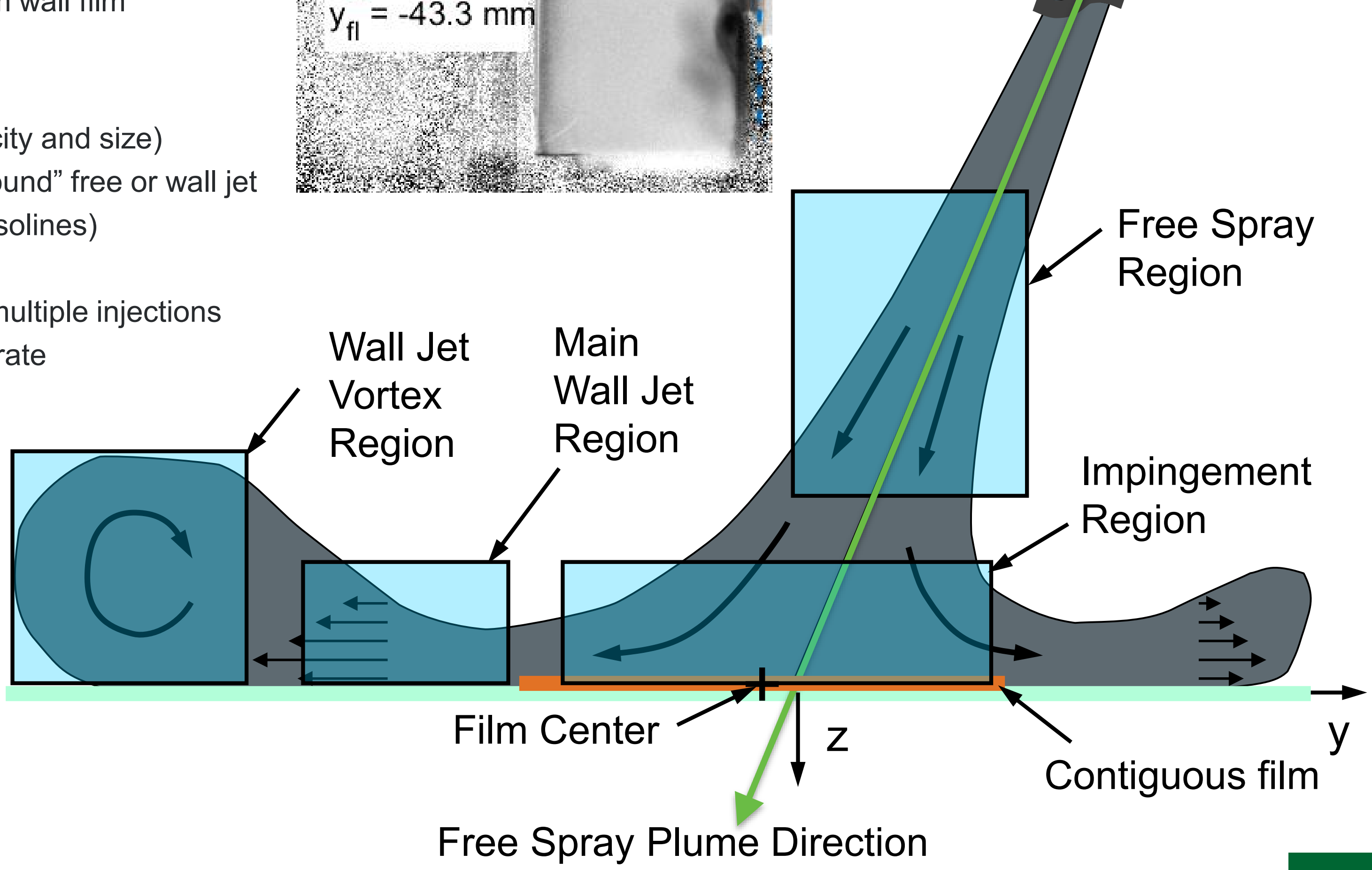


wall-view extinction I/I_0



side-view extinction I/I_0





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

__Importance of operating conditions__ (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**

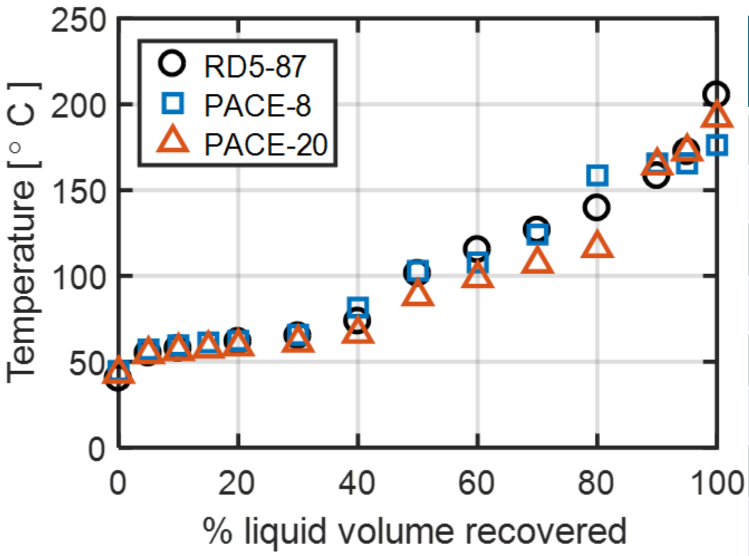
G3: intake injection at 1 bar

- **standard patternator and other SAE J2715 data available**

double injection and cold fuel are applicable to cold start

Overview

- **Injector: ECN Spray G, 8-hole unit provided by Delphi**
- **Fuels: iso-octane / E00 (3-component) / PACE-20 (9-component)**
- **Ambient: 100% N2**
- **Experiments designed to analyze free-spray at positions of potential wall impingement**
  - Is liquid volume fraction at z = 40 mm lower for iso-octane or



9-component PACE-20

Component	Boil Pt. [°C]	liq. vol. %
ethanol	78	0.0955
n-pentane	36	0.1395
cyclopentane	49	0.1050
1-hexene	63	0.0541
n-heptane	98	0.1153
iso-octane	99	0.2505
toluene	111	0.0919
1,2,4-trimethylbenzene	170	0.1187
tetralin	207	0.0295

PACE target conditions for spray-wall research in chambers

- **Sjöberg (Sandia) optical engine experiments and injection schedules guide initial selection of specific wall-target operating conditions (see ACE167 Torelli 2021 AMR presentation)**
  - First selections focus on cold-start, catalyst heating mode, with multiple injections (for Spray G)
  - Cold-start skip-firing (2 fired, 8 motored) yields colder cylinder walls
  - Wall positions defined correspond to distances in the engine at time of injection
  - Other conditions defined for lean-dilute and high-load knock

Condition Name	Ambient T (K)	Ambient P (kPa)	Fuel T (K)	Fuel P (MPa)	Fuel Mass (mg/inj)	Fuel	Wall Position	Wall T (K)
W1-C-Cycle10	293	50	293	20	11+11 = 20	PACE-20	40 mm	298
W1-C-Cycle1	293	50	293	20	15+15 = 30	PACE-20	40 mm	298 (TBD)
W2-2080-Cycle1	305 (TBD)	50	305 (TBD)	20	11+11 = 20	PACE-20	40 mm	323 (TBD)
W2-2080-Cycle1-W60	305 (TBD)	50	305 (TBD)	20	11+11 = 20	PACE-20	60 mm	323 (TBD)

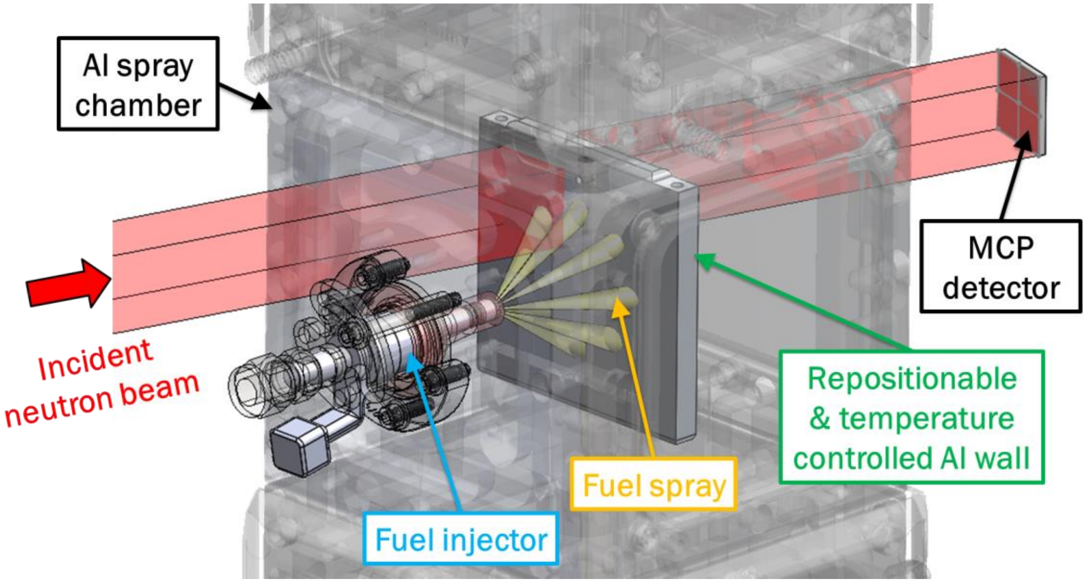
  - COVID-19 delayed experiments in spray chambers at all facilities, but new CFD simulations have been performed at W1-C-Cycle10 conditions
  - Previous wall experiments have been used to develop metrics and tools for experiment and CFD comparison, and to validate/improve new Spray-Wall Interaction models

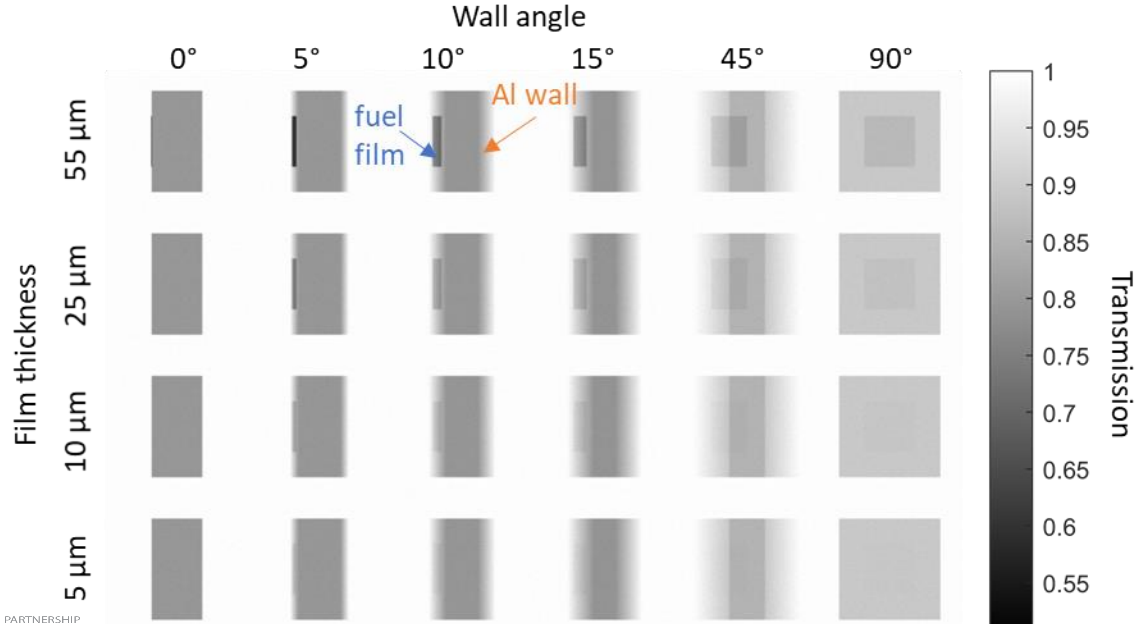
Milestones

Project	Month/ Year	Description	Status
S.E.4.1 Pickett	Nov 2020 Feb 2021	Design and acquire surface temperature and heat-flux probe mounted inside temperature-controlled chamber Measurements of free-spray 3D liquid volume fraction for PACE-20 fuel at wall impingement targets / positions	complete complete
S.E.2 Manin	Sept 2021	Quantify wall film thickness, near-wall temperature distribution and soot concentration to understand film-based soot formation processes	on track
A.E.4 Powell	Mar 2021 Jun 2021	Measurements quantifying the fuel distribution of GDI Spray G impacting a wall Dataset of measurement results including free-spray and wall-film measurements will be archived online	complete 70% complete
O.E.6.2 Wissink	Mar 2021	Perform high-speed neutron imaging of wall film evolution at prioritized PACE condition	Delayed due to COVID-19
S.M.4.2 Nguyen	Mar 2021	Wall impingement simulation for Spray G and single-hole injector, incorporating improved free-spray modeling	complete
A.M.4 Torelli	Aug 2020	Implementation of spray-wall interaction model against x-ray measurements under GDI cold-start conditions	complete
S.E.4.3 Pickett	July 2020	Release of iso-octane and E00 datasets to ECN archive in conjunction with ECN7	complete

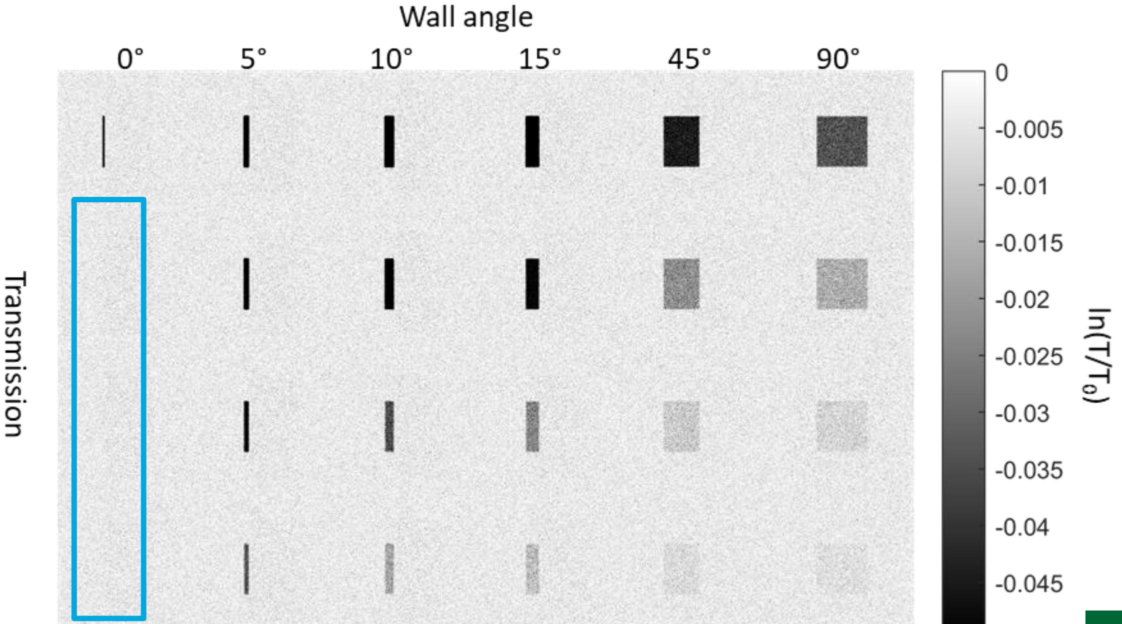
Evaluating potential for quantitative neutron imaging of fuel films through metal substrates at PACE conditions

- **Neutron imaging simulations show potential for resolving fuel films <5 μm thick through metal substrate**
  - Rotate wall relative to beam to increase path length through film
  - Al wall 10 mm thick, 60 s exposure, Poisson noise, Gaussian blur
- **Experiments will be a high-speed ensemble movie**
  - 60 s exposure per frame = 3M injection events to achieve 50,000 fps
  - Record from multiple angles to reconstruct film thickness distribution
  - 7 days of beam time awarded at HFIR CG1D in 2020, but experiments have been on hold due to COVID-19
  - Expect first wall film experiments Summer 2021, pending scheduling





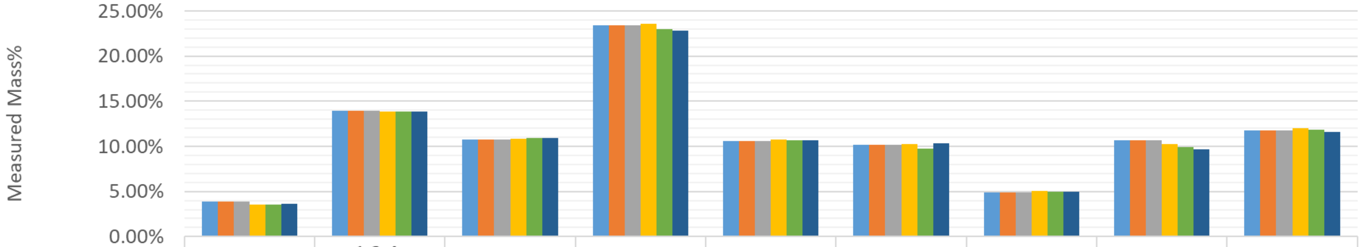
Transmission images



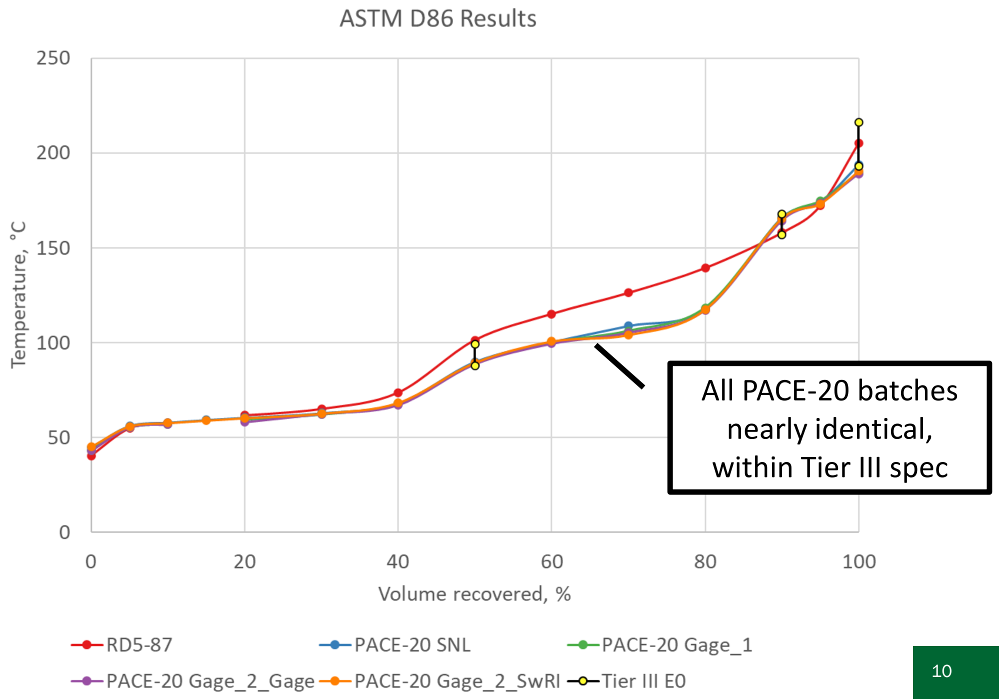
Normalized images

Facilitated bulk order of PACE-20 surrogate

- **Need for bulk order of PACE-20 surrogate for engine and spray experiments**
  - Single-origin blending reduces chance of batch-to-batch variation and duplication of effort
  - Experiments consume large amount of fuel, costly to hand blend
- **Worked with Gage Products to develop order**
  - Reduced cost from ~$900/gal hand blend to ~$50/gal group order
  - Performed extensive trial batch testing at multiple laboratories to ensure purity
  - Total of 15 drums PACE-20 and 2 drums PACE-20 BOB between ORNL, SNL, ANL

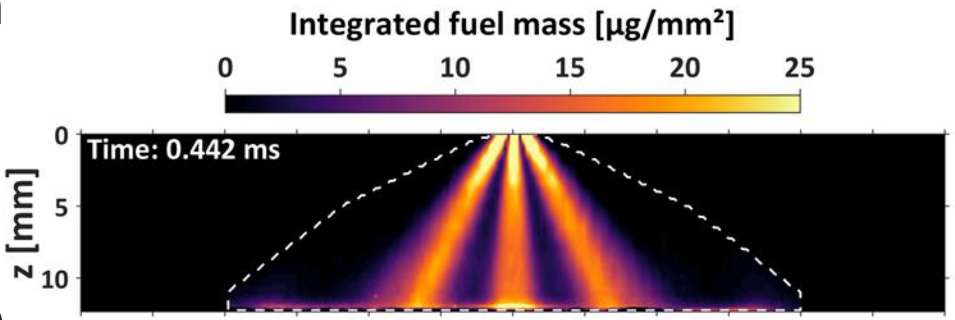


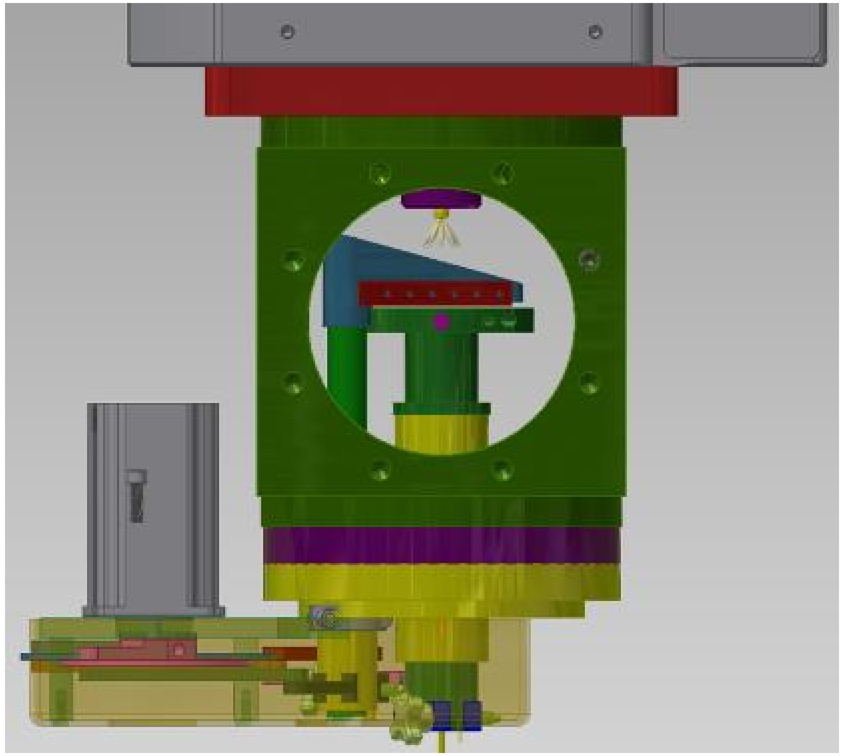
		tetralin	1,2,4-trimethylbenzene	toluene	iso-octane	n-heptane	ethanol	1-hexene	cyclo-pentane	n-pentane
Scale	PACE-20-A	3.85%	13.97%	10.73%	23.38%	10.62%	10.14%	4.90%	10.66%	11.75%
Scale	PACE-20-B	3.84%	13.98%	10.73%	23.38%	10.62%	10.14%	4.90%	10.65%	11.75%
Scale	PACE-20-C	3.84%	13.98%	10.73%	23.38%	10.62%	10.14%	4.90%	10.65%	11.75%
Scale	Gage2	3.55%	13.85%	10.81%	23.56%	10.73%	10.22%	5.07%	10.22%	11.99%
DHA	Gage2 GageDHA	3.55%	13.89%	10.95%	23.01%	10.69%	9.73%	4.94%	9.91%	11.85%
DHA	Gage2 SwRIDHA	3.63%	13.81%	10.89%	22.84%	10.67%	10.31%	4.94%	9.70%	11.57%



Approach and Accomplishment: X-ray Studies of Spray/Wall Interaction

- **Near the wall, drop density and optical thickness are high**
  - X-rays can quantify the density distribution in this region
  - Can capture rollup vortex formation, extensible to 3D
  - Shows plume impact, drop recoil, film development and wall flow
- **Last year, tests with existing spray chamber were used to quantify free spray and wall impingement**
  - Uncertainties with wall angle, but still actively used for model validation
- **Design of purpose-built spray/wall chamber is nearly complete**
  - New large FOV windows have passed pressure tests
  - Measurements will focus on spray impinging on clean wall
    - ⇒ Vacuum wiper mechanism to clear wall between sprays
  - Temperature-controlled wall, 0 to 100 °C
  - Allows "plan view" through the wall to map the wetted region





Torelli, ANL

CFD predictions with new spray-wall interaction model appear more consistent with x-ray experiments

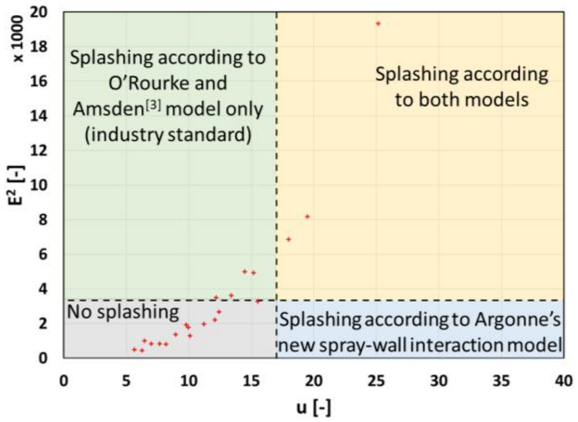
Powell, ANL

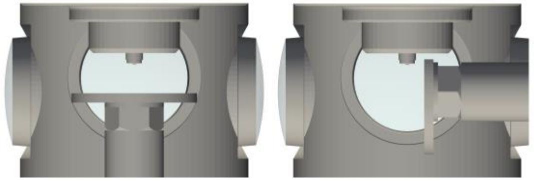
ACCOMPLISHMENTS (4/9)

Argonne's new spray-wall interaction (SWI) model's splashing criterion[1] accounts for multi-droplet impingement dynamics by estimating the impingement frequency for Lagrangian spray parcels:

[2] $$u = \frac{U_0}{\left(\frac{\sigma}{\rho_l}\right)^{1/4} \nu_l^{1/8} f^{3/8}} > 16-18$$

[1] $$f_{imp}(x,y)\Big|_{A_d} = \frac{3}{4}\frac{r_d^2}{r_c^3}\frac{U N_d}{\cos(\theta)}$$



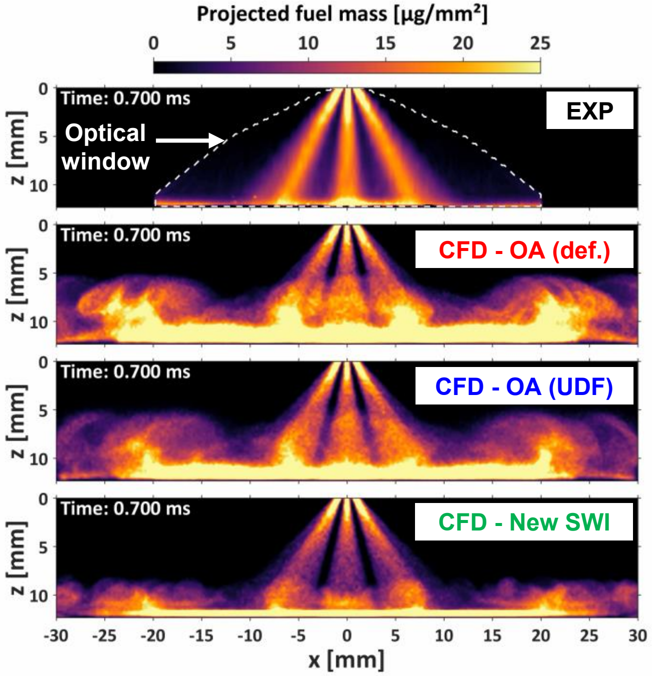


Model tested against two X-ray datasets:

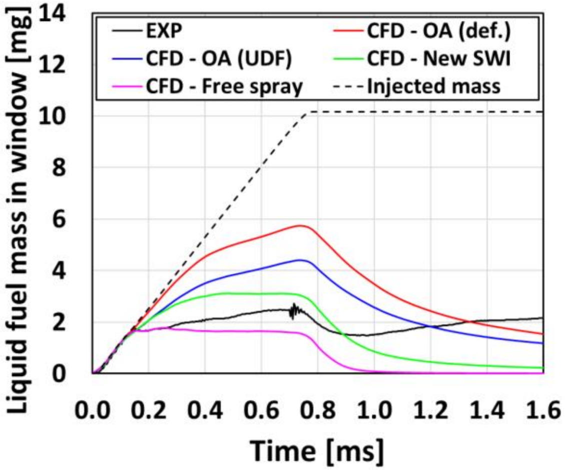
- front wall (**12.3 mm from injector tip**)
- side wall (7.0 mm from injector axis)*

- Created user-defined function (UDF) of new SWI model in CONVERGE 3.0
- Proposed additional revised version of O'Rourke and Amsden (OA) SWI model[3] to reflect original OA theory more closely (also in UDF format)
- Shared plug-and-play executable of new SWI and revised OA models with PACE team members, including Edwards (ORNL) and Nguyen (SNL)
- Successfully applied new model to simulations of SWI in SANDIA's GM SG2 optical engine* with both RANS and LES turbulence models

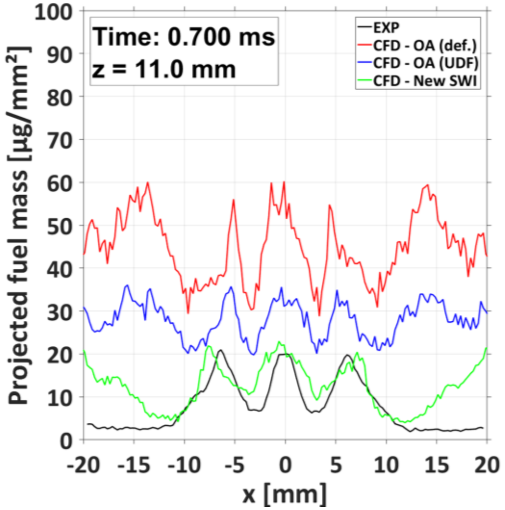
The use of the new model results in reduced fuel splashing and increased film formation, consistent with the observations from x-ray experiments



Validation performed for ECN Spray G G3-cold conditions (T=298 K, p=100 kPa)



Near-wall fuel mass distributions predicted with the new SWI model are also improved implying achievement of a more accurate split between splashed and film masses



[1] **Torelli et al, IJER, 2020** [2] Yarin and Weiss, J. of Fluid Mech., 1995 [3] O'Rourke and Amsden, SAE 961961, 1996

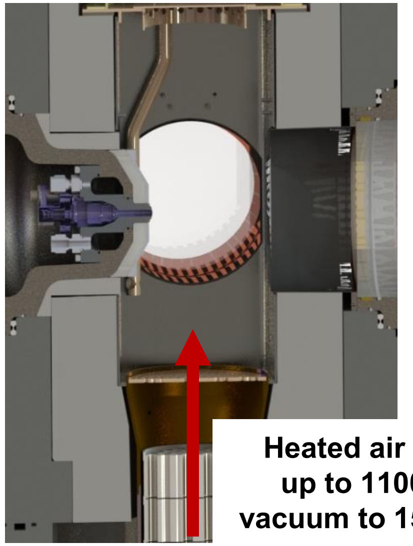
* More details reported in ACE-167

Pickett, SNL

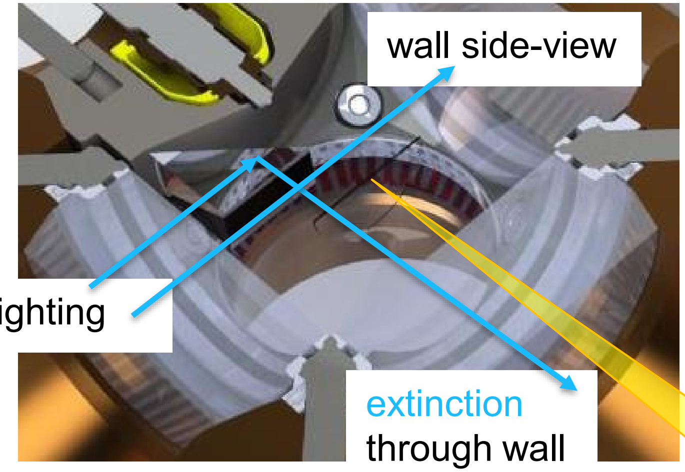
Sandia spray-wall impingement and film combustion experiment in different chambers

Manin, SNL

Continous-flow vessel (spray, film, non-reacting)

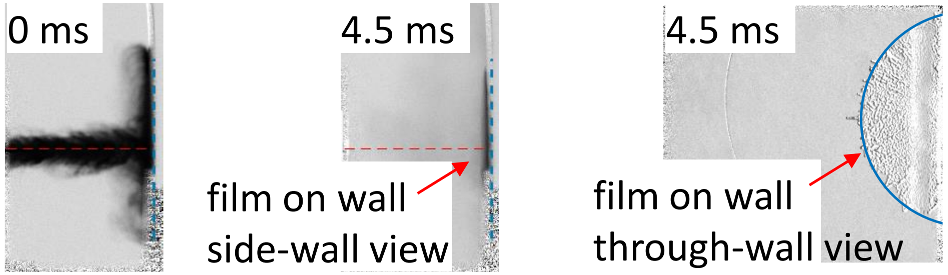


Constant-volume chamber (spray, film, combustion)



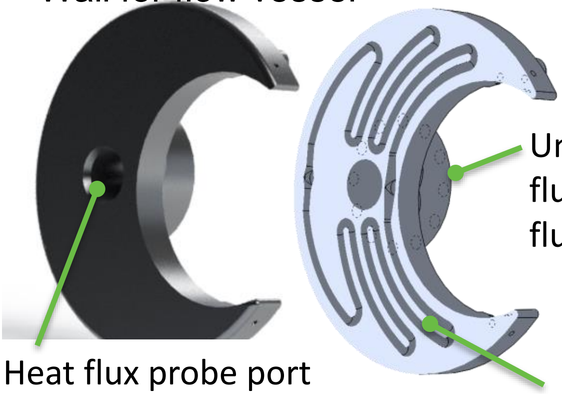
Steps of film combustion experiment:

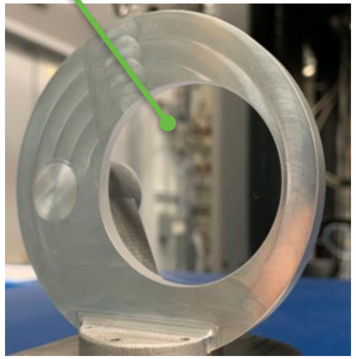
1. Prepare chamber with stoichiometric reactants in chamber
2. Spark ignite at two locations at top of chamber
3. Inject fuel spray to form film on flat wall



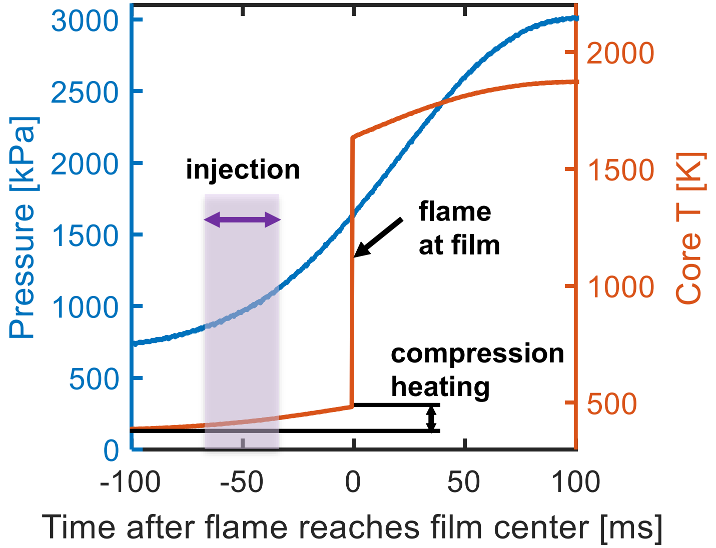
4. Observe flame passing over film, in analog to engine combustion with fuel films on surfaces

Wall with optical section and circulated fluid for temperature control





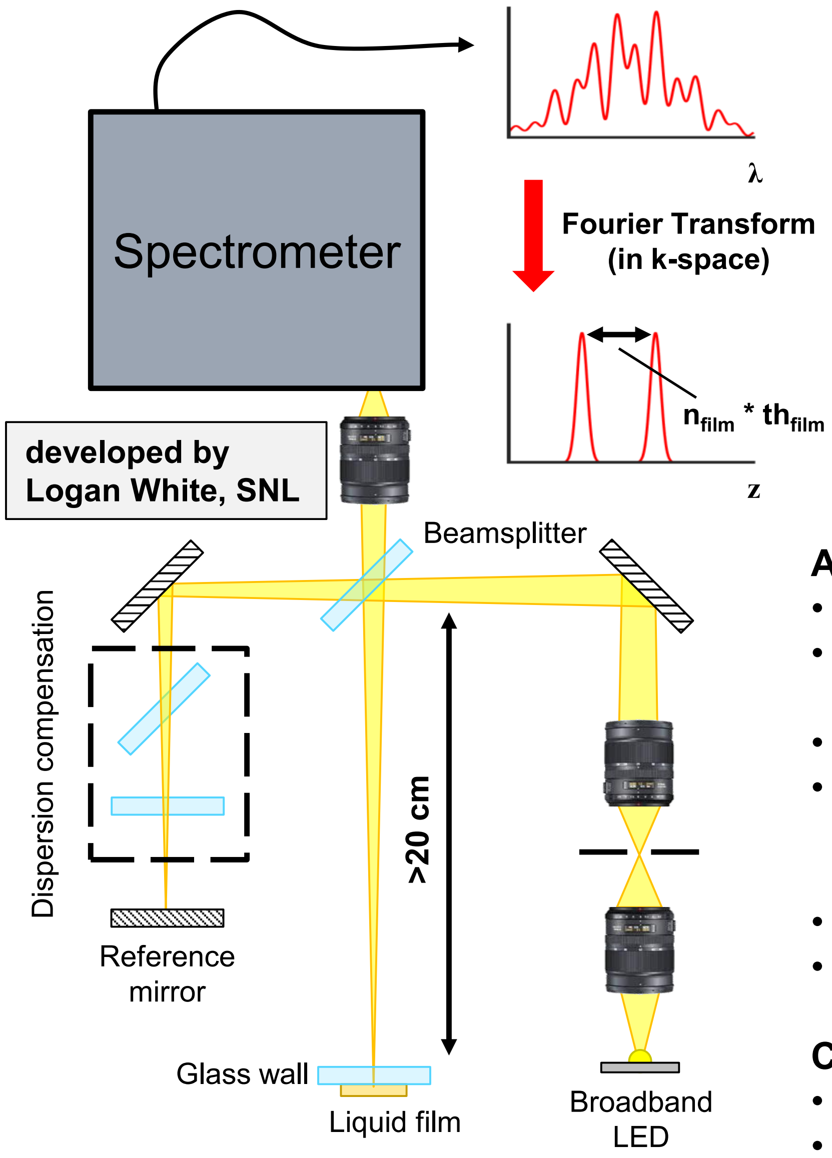
- CV chamber initial T & P and injection timing determine conditions at the time of (1) spray impingement and (2) film combustion
- (1) & (2) may have different objectives



Pickett, SNL

Diagnostic developed to measure dynamic film thickness using Low-Coherence Interferometry

Manin, SNL



developed by Logan White, SNL

Low-Coherence Interferometry (LCI)

- A **broadband** light source (pulsed white LED) illuminates a **Michelson interferometer**
  - Sample leg → **fuel film**
  - Reference leg → broadband mirror
- Broadband source has a **low coherence length**
  - Interference only present when reference leg distance is close to a surface in sample leg
- Spectral detection allows a stationary reference mirror and **high-speed measurements**

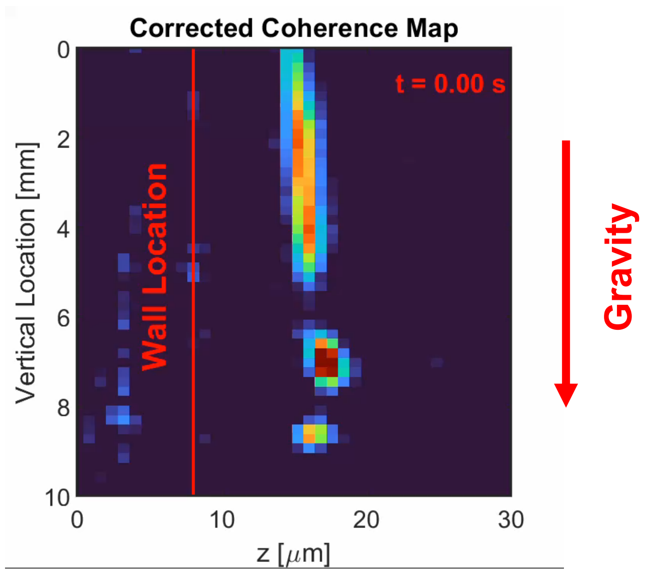
Advantages:

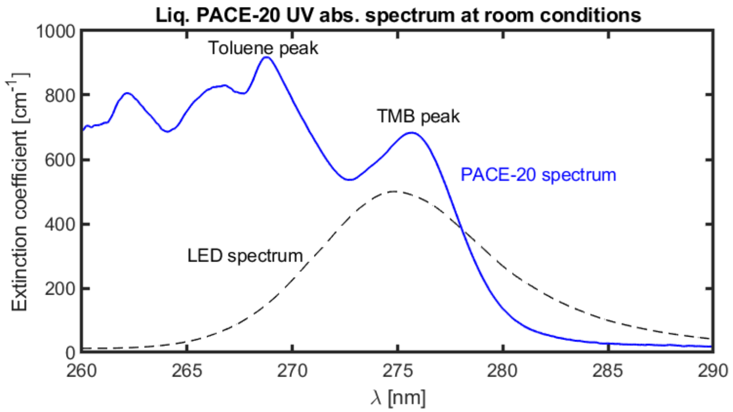
- High speed with **micron-scale** thickness resolution
- **Unaffected by ambient conditions above film**
  - → **Can distinguish film from background droplets**
- Calibration free
- Avoids roughened surfaces
  - a criticism for Refractive Index Matching techniques
- Mostly **insensitive to film composition**
- Can be performed on opaque surfaces (front illumination)

Challenges:

- Film corrugation can disrupt detection
- Can only image along one spatial direction at a time

Benchtop measurements: Iso-octane film on glass slide





→ **Combine LCI with absorption-based measurement to provide composition of film**

Manin, SNL

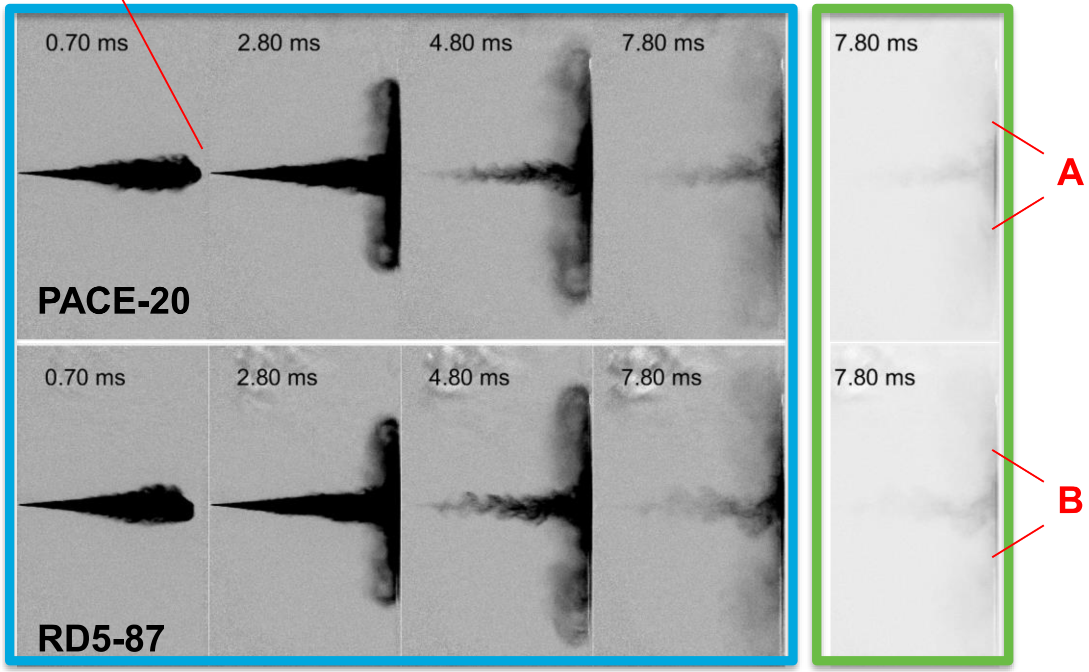
First measurement of PACE-20 spray impingement and film combustion performed in constant-vol. chamber

Pickett, SNL

- **High-speed side-view extinction imaging of PACE-20 spray wall impingement, but in a simplified configuration**
  - Single-hole axial nozzle, rather than Spray G
  - Wall and chamber initially at 13-bar, 90 °C rather than 0.5 bar, 25 °C PACE cold-start target
  - Focus here is on films that persist during compression and are present at the time of flame arrival
- **Comparison of PACE-20 and RD5-87 impingement and film formation shows remarkable similarity**
  - Similar jet structure and roll-up wall jet vortex
  - Significant liquid (by high-contrast extinction) in wall jet region
  - Liquid cloud present near wall even 5 ms after end of injection
  - Films on wall are visible from the side and persistent as liquid vaporizes in gas away from the wall
  - No discernible difference between the film footprint for PACE-20 (**A**) and RD5-87 (**B**), shown in full-range contrast images
  - Detailed measurements through the wall are needed to provide more quantitative details on the film
  - Need to quantify film mass and shape before flame arrives to understand the outcome of film combustion

Injector conditions		Wall & gas conditions	
Inj Pressure	200 bar	Axial distance	32 mm
Inj Duration	3.1 ms	**Wall Initial T**	**90 °C**
Inj Mass	~3.3 mg	Gas Initial T	90 °C
Injector nozzle	single-axial	Gas Initial P	12.8 bar
Nozzle diam.	0.094 mm	**Gas T @ Inj**	**105 °C**
		Gas P @ Inj	15.0 bar

Normalization to initial intensity I_0 – no evidence of wall or film prior to impingement



High contrast I/I_0 [0.8 1.1]

Full range I/I_0 [0 1.1]

Nguyen, SNL

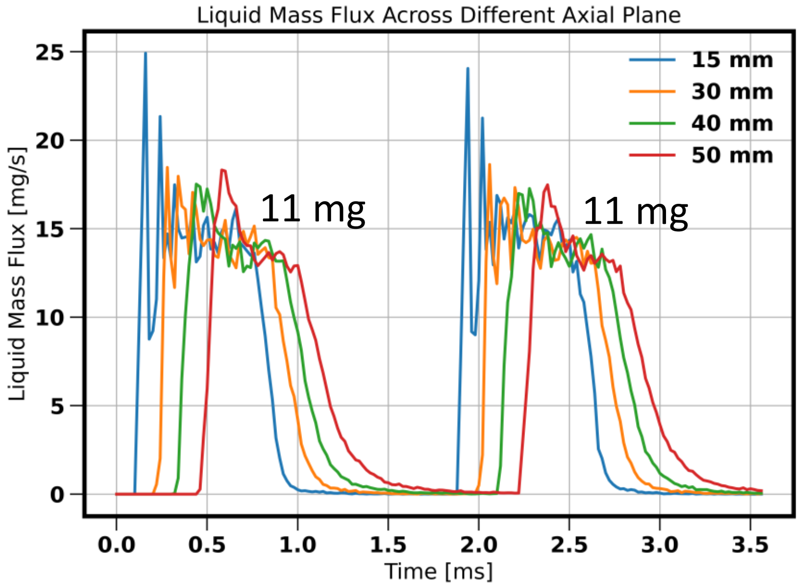
Free-spray modeling at wall position using corrected distortion model, compared to experiment

- **ECN G2 cold condition with PACE 20**
  - P_{amb} = 0.5 bar, T_{amb} = 293 K, T_f = 293 K
  - 0.78 ms / 1 ms dwell / 0.78 ms

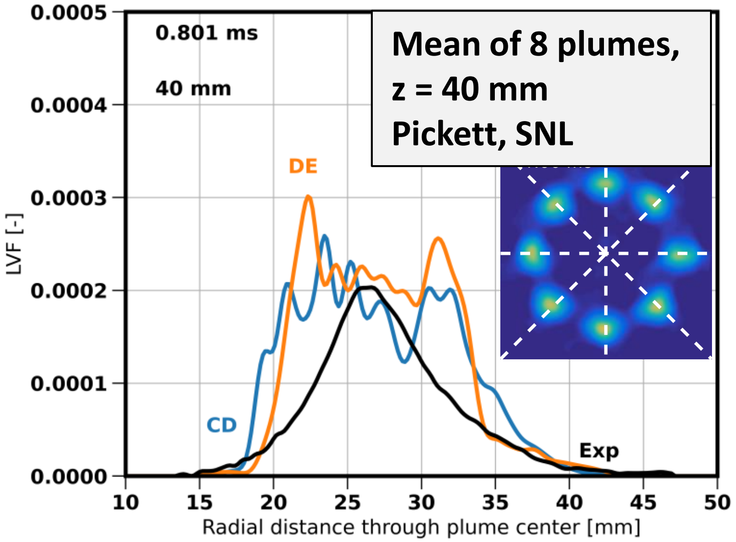
Total liquid mass & component mass fraction across a z plane formulation

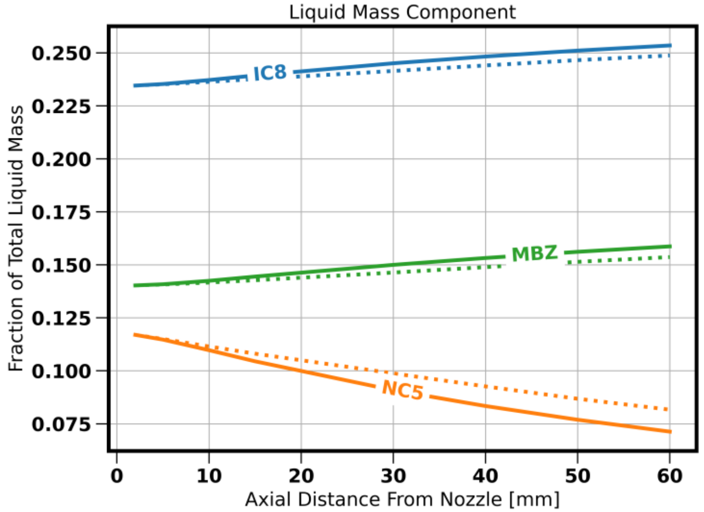
$$norm_{mass}\Big|_{z=z_a} = \frac{\iint \rho_p(x,y)U_p(x,y)\,|_{z=z\_a}\,dA\,dt}{mass_{inject}}$$

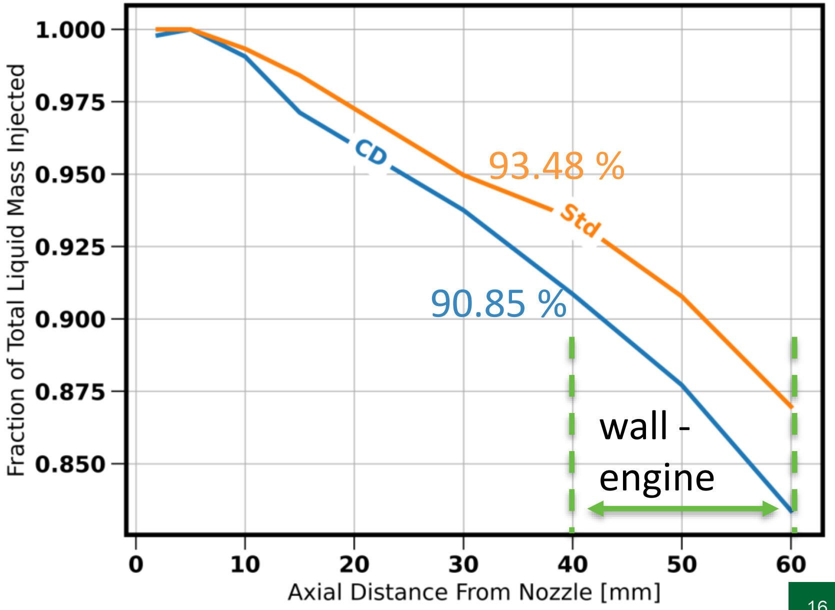
$$Y_k\Big|_{z=z_a} = \frac{\iint \rho_p(x,y)U_p(x,y)Y_k(x,y)\,|_{z=z\_a}\,dA\,dt}{\iint \rho_p(x,y)U_p(x,y)\,|_{z=z\_a}\,dA\,dt}$$



- **More than 85% of the injected liquid reaches the engine wall region**
  - Both models overpredict the width of liquid, while CD model has lower LVF & mass
- **PACE 20 fuel impinging on the wall contains heavier component-> higher surface tension -> lower Weber number -> more propensity to stick**



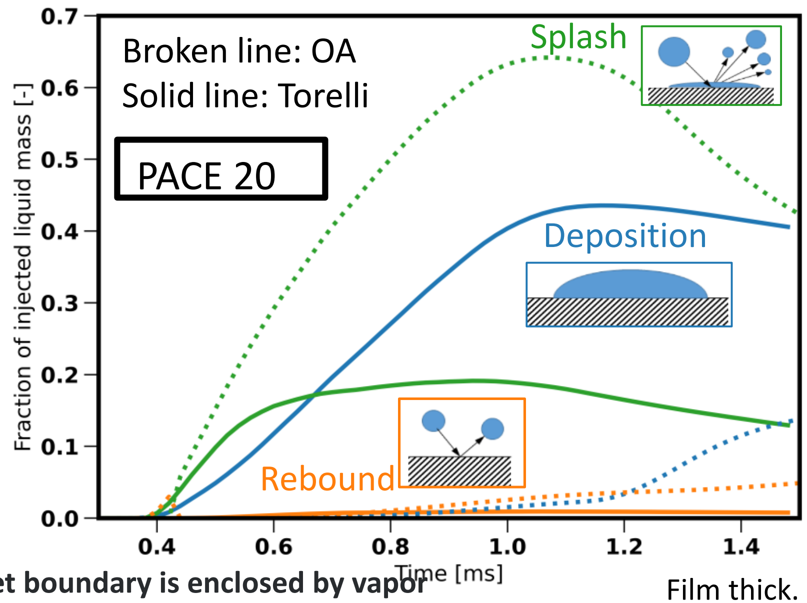


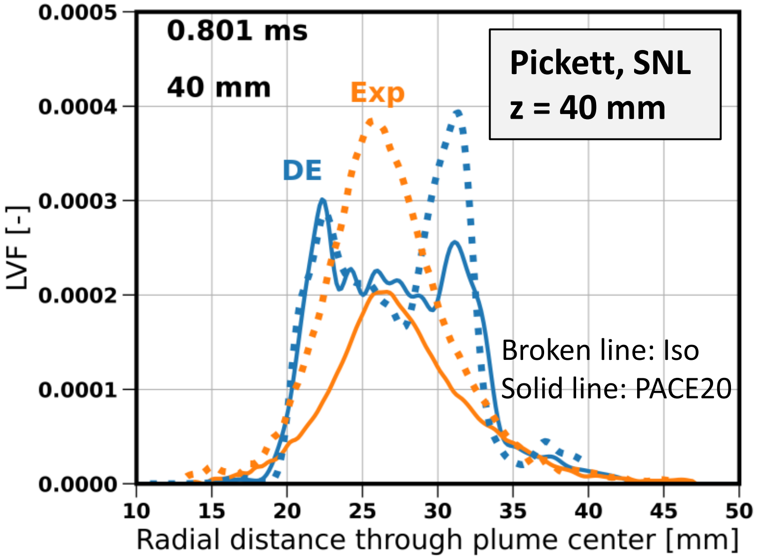


Nguyen, SNL

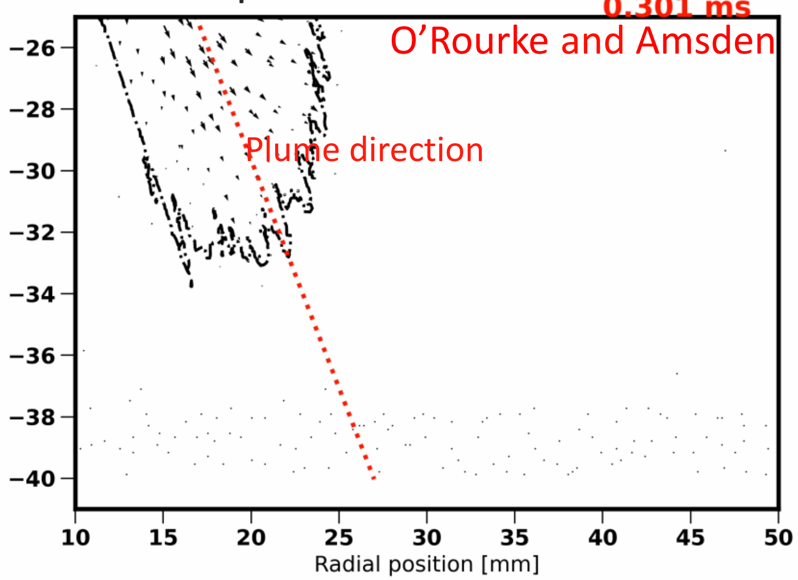
Spray wall interaction model comparison between the O'Rourke and Amsden (OA) and Torelli (ANL) models

- **Maximum LVF predicted by free-spray simulations are in good qualitative agreement with measurements for both Iso-octane and PACE 20**
- **But plume widths are larger than measurements, which likely leads to different wetted area**
- **Film center does not coincide with plume direction angle**
- **There is less splashing predicted by the Torelli model compared to the OA model, which leads to MUCH HIGHER film deposition and thicker film**
- **Wall jet penetration is slower for Torelli model, perhaps because parcel momentum is lost to the wall film**

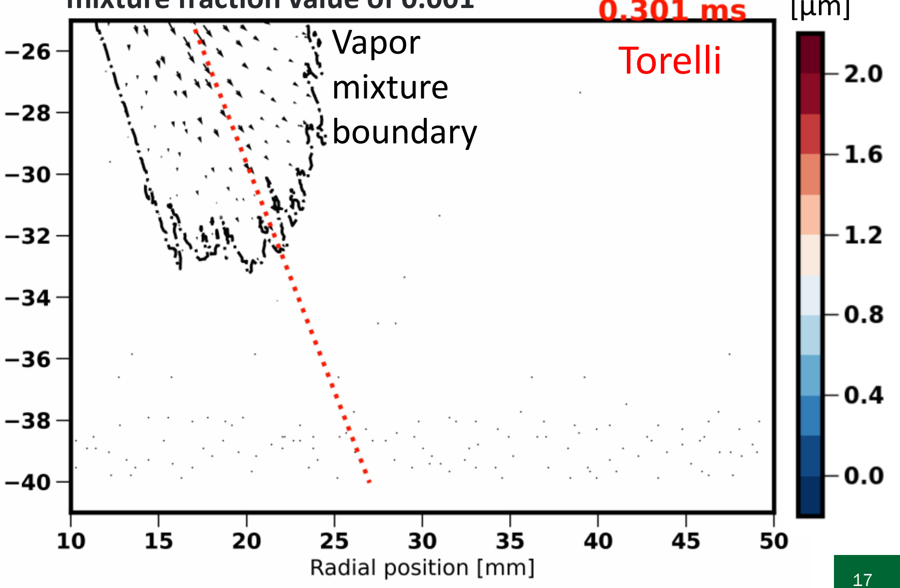




Wall jet in OA model penetrates further radially compared to Torelli model

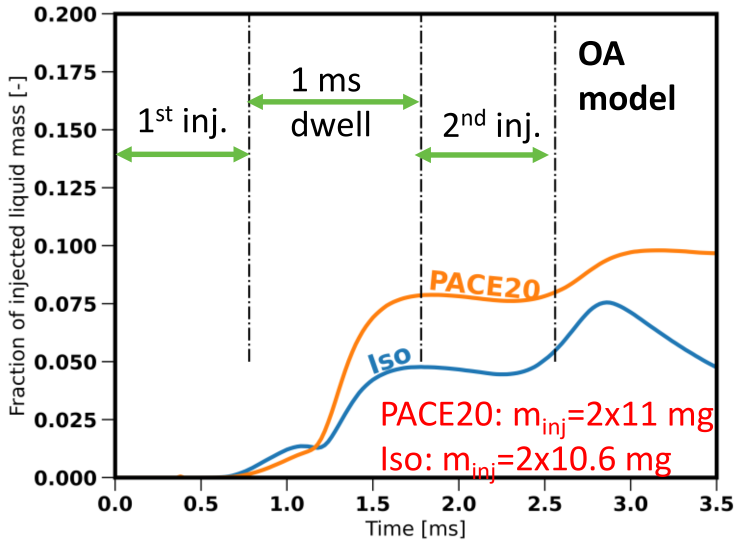


Jet boundary is enclosed by vapor mixture fraction value of 0.001



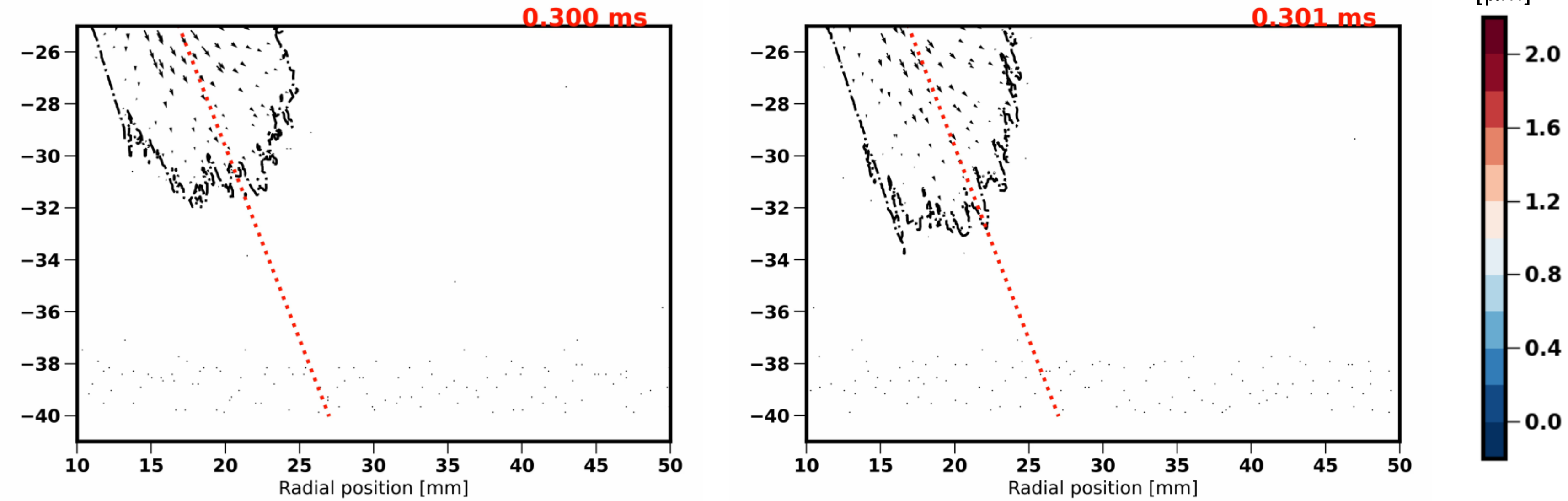
Double injection and fuel effect

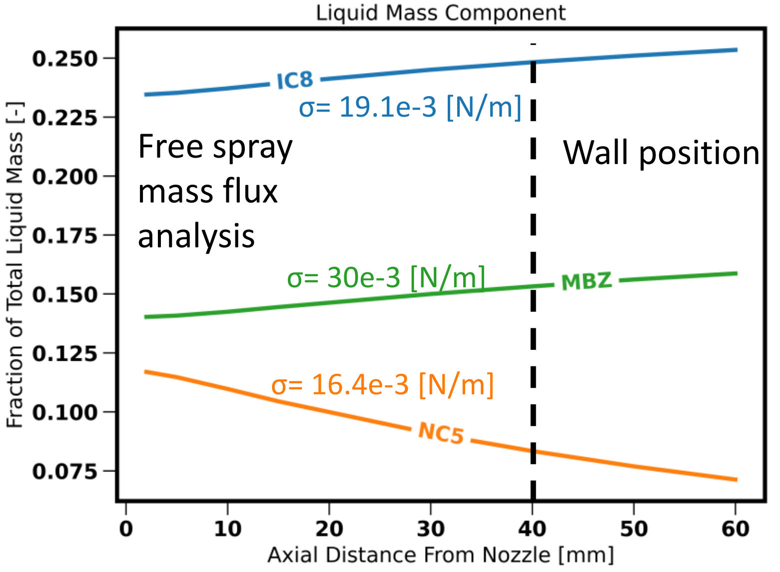
- More film deposition INITIALLY for pure iso-octane compared to PACE20 during the first injection but the trend reverses at later dwell before 2nd injection
- Liquid PACE-20 hitting the wall consists of less-volatile components with higher surface tension, but also more volatile components – ultimately the former dominates the film as the wall jet spreads and dilution increases
- There is more film deposition by the first injection compared to the second injection, but more persistence for PACE-20 compared to iso-octane
- CFD results for <u>specific quantities identified here</u> will be validated with experimental measurements by PACE Sprays team in the remainder of FY21 and FY22



Iso-Octane

PACE 20





Responses to Last Year's Reviewer Comments

- **Reviews were overall positive, garnering a high score**
- **"It is very difficult to ask questions on the technical attributes with a menagerie of content from all the collaborators" (8 contributors represented last year)**
  - Two new AMR presentation slots opened this year (ACE167 Torelli, ACE168 Manin)
- **"The shortcomings of the CFD models, like the over-prediction of the rebound, are being identified and provide areas where the models have to be improved"**
  - This type of detail was used to confirm the modeling approach taken by Torelli, with new simulations applied to spray chambers as well as engines.
- **"The influence of ambient air temperature and wall temperature should be studied independently as well as in unison"**
  - Care has been taken to prepare chambers with careful control for wall and gas temperature, and to provide critical experimental data on temperature and heat flux

Collaboration and coordination with other institutions

- **PACE Sprays & Films team meets monthly to coordinate more than 90 different tracked tasks**
  - Decisions about target conditions, including CFD and experimental boundary conditions, are coordinated in advance
  - Data and analysis tools are shared/combined to reach physical conclusions about current models
  - Work is foundational to other PACE objectives in a DOE-funded consortium of 5 National Laboratories working towards a common goal (ACE138)
  - All team members participate in the Engine Combustion Network, an international collaboration with 20+ members and 10+ institutions who have specifically chosen Spray G wall films and combustion as a special topic
  - ECN7 workshop was held in June 2020 (online web meetings)

Remaining challenges and barriers

- **Free-spray simulations need to be improved to provide quality predictions at the wall**
  - Free-spray simulations to date show higher LVF and wider footprint than experiments
    - Closer LVF at cold-start conditions than hot, vaporizing conditions (refer to merit function in ACE143)
  - Simulations show high sensitivity to assumptions, not predictions, for plume cone angle
  - Methodology for preferential evaporation with multi-component fuels needs to be verified
- **Validating spray-wall interaction models with isolation of different mechanisms**
  - Comprehensive understanding of film deposition as well as wall-jet dynamics
  - Roles of temperature gradients and heat exchange at the wall
- **Experiments need to provide improved accuracy in wall & liquid/vapor regions**
  - Optical experiments are highly sensitive to droplet size—sizing measurements are needed at all timings and positions
  - X-ray experiments are difficult at low fuel concentration and need to address vapor fuel and temperature gradients, in addition to liquid fuel
  - Throughput with neutron imaging is inherently limited by flux and time constraints and needs to be coordinated with other tasks to prioritize cases of maximum value

Future work

- **Execution of wall-impingement experiments with new capabilities**
  - Precise wall orientation and temperature control at PACE-selected non-reacting/reacting conditions
  - Beam paths move through wall and along wall (optical, x-ray, neutron)
  - Techniques for absorption (x-ray, neutron, and optical) and scatter or interferometry combined to assemble comprehensive datasets revealing the physics of impingement
- **Experiments to quantify thickness and composition of film, for PACE-20 surrogate**
- **Free-spray and wall-jet experiments using EcoBoost HDEV5.2 injector with injection pressure range to 500 bar**
  - Use in both engine and spray chamber experiments, applying similar diagnostics and target conditions
- **Simulations matched to experiments for validation over the range of conditions**
  - Distinct quantities already identified for comparison, subject to a SWI "merit function" test
- **Modeling capability added for VOF and vaporization to inform engineering models in complicated wall region**
- **ALL model advancements passed to PACE team to meet major outcomes**

Summary

- Combined and complementary optical, x-ray, and neutron experiments offer the potential to advance understanding and CFD of free-spray and wall-impingement physics
- New models and better boundary conditions affecting multi-component (PACE-20) free-sprays and spray-wall interaction have been developed and released to the PACE team
- These model improvements are important to PACE major outcomes in mixture preparation for cold-start, lean and dilute combustion, and knock avoidance

Acknowledgements

- The experimental and modeling work supporting Sandia tasks was performed at the Combustion Research Facility, Sandia National Laboratories, Livermore, CA. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Technical Back-Up Slides

Collaboration and coordination with other institutions (detailed)

S.E.4.1 Pickett	• Coordination with PACE team to select and prioritize target operating conditions, develop temperature and heat flux probe, • PACE activities not reviewed here: fuel surrogate selection & blending (Wagnon), cold-start condition sprays (Edwards) • Co-Optima participants on GDI fuel effects: experiments with fuel blends suggested for ACI combustion with early- and late-injection
S.E.2 Manin	• Lead or co-lead on combustion and soot-related activities in the Engine Combustion Network and the International Energy Agency • Collaborating with nearly 10 institutions on problems related to sprays, wall-films and soot formation • Working with engine research groups at SNL (Sjöberg) and ORNL (Jatana) to study the effects of cold-start condition on soot processes
A.E.4 Powell	• Lead for ECN internal flow and near-nozzle behavior for Spray G • Internal collaboration with Argonne X-ray Sciences Division
O.E.6.2 Wissink	• Injector hardware provided by GM, Delphi, Bosch • Bulk PACE-20 surrogate order organized with Gage Products • Internal collaboration with ORNL Neutron Sciences Directorate to develop new detector hardware and improve quantitative data analysis techniques
S.M.4.2 Nguyen	• Shared corrected distortion model with PACE CFD users Torelli (ANL) and Edwards (ORNL), and led joint processing scripts and data exchange • Collaborated with Killingsworht/Kukkadapu (LLNL) on soot precursor chemical kinetics validation for soot wall film problem • Volunteer for ECN data exchange synthesis with Lucchini (PoliMi) for GDI topic
A.M.4 Torelli	• Implementation of new scripts for comparison with x-ray experiments and development of joint scripts with Nguyen to enable quick, uniform data analysis • Active feedback loop with x-ray team at Argonne to ensure insightful and consistent comparisons between experiments and simulations • Initiated exchange of plug-and-play executable of ANL's spray-wall interaction model with PACE CFD users (e.g., Dean Edwards (ORNL) and Sprays Team)
S.E.4.3 Pickett	• PACE Sprays Team lead and ECN lead; created online ECN archive for GDI; ECN has chosen wall and film combustion with 20+ volunteer researchers • Led ECN7 with over 100 attendees, including coordination on a new topic on Sray G film formation and combustion • Received new experimental Spray G datasets and posted these to the ECN website

Remaining challenges and barriers (detailed)

S.E.4.1 Pickett	• Proof that interferometry diagnostics work when installed in harsh conditions of chamber • UV lighting and high-speed imaging for extinction-based film thickness measurements
S.E.2 Manin	• Droplet size information is important for film formation but experimental data are missing • Experimental variability in film evaporation and soot formation may be linked to variability in film formation as a result of temperature distribution • Quantification of gas temperature and mixture concentration in proximity to wall and film • Liquid film temperature and evaporation rate
A.E.4 Powell	• Measurements involving long pathways next to surfaces, or in dilute (and evaporative) zones far from the injector where signal-to-noise ratio suffers • Distinguishing between wall film and atomized sections of film/wall jet sprays, when film thickness may be < 5 μm
O.E.6.2 Wissink	• Simulations suggest that neutron imaging should be able to resolve fuel films < 5 μm, but this remains to be experimentally verified • Throughput with neutron imaging is inherently limited and needs to be coordinated with other tasks to prioritize cases of maximum value
S.M.4.2 Nguyen	• Predictive multi-component evaporative spray and film models, especially under cold-start-relevant conditions • Long computational time due to viscous timescale limitation in the wall film region
A.M.4 Torelli	• Liquid fuel reaching the wall is overestimated. Need for more accurate predictions of free-spray evaporation. This is very relevant for multi-component fuels as well (i.e., PACE-20) due to non-linearities of physical properties. • Performance of spray-wall interaction model with multicomponent PACE-20 fuel is currently unknown. Effect of non-linear properties and evaporation behavior will likely apply to film formation and evaporation as well.
S.E.4.3 Pickett	• Development of workflow and database sharing such that all team members process/benefit from experiments and simulations, accelerating model development

Future work (detailed)

S.E.4.1 Pickett	• Apply low-coherence interferometry to film thickness measurements in flow chamber over a wide range of conditions • Development of diagnostics for film thickness and speciation within multi-component films • Spray and film experiments using PACE-partner fuel injection equipment (Sjoberg, Edwards, EcoBoost HDEV5.2)
S.E.2 Manin	• Experiments with Spray G injector and temperature-controlled wall to match PACE set targets • Measure film thickness in presence of flame with low-coherence interferometry (temperature insensitive) and/or UV absorption diagnostic (2-D) • Develop diagnostic to measure film temperature and assess evaporation rate
A.E.4 Powell	• Finalize design and fabricate new purpose-built spray/wall chamber for X-ray diagnostics. First measurements in FY22. • X-ray measurements with PACE-20 fuel: needle lift, near-nozzle spray density • Measurements of GDI sprays in crossflow for validation of engine spray simulations
O.E.6.2 Wissink	• Perform high-speed neutron imaging of wall wetting and film evolution from multiple viewing angles to obtain quantitative measure of film dynamics on metal substrate at a condition prioritized by PACE and Spray Team partners • Extend range of experiments to other pressure/temperature conditions, multiple injections
S.M.4.2 Nguyen	• Solve problems with slow computational time for multi-component fuels • Development of preferential evaporation model for PACE-20, including operation specific to flash-boiling conditions • Development of CFD accuracy test and merit function for key quantities, such as transient film thickness with multiple injections
A.M.4 Torelli	• Complete conjugate heat transfer model of GM SG2 engine and perform wall temperature predictions (ongoing) • Perform validation of new spray-wall interaction model with PACE-20 and, if needed, improve the model to ensure predictivity with multi-component fuels • Assess cross-flow effect on free-spray and spray-wall interaction development in both vessel and Sandia's GM SG2 engine • Test new CONVERGE capability for transition from Discrete Particle Model to Eulerian wall film and assess film evolution predictions
S.E.4.3 Pickett	• Coordinate with ECN to select wall-impingement conditions and datasets, including use of PACE-20 • Provide/require experimental uncertainties for all free and wall-jet experimental datasets • Create searchable/shareable archive for simulations as well as experiments

Any proposed work is subject to change based upon funding levels

Summary (detailed)

S.E.4.1 Pickett	• Free spray experiments with multiple injections provide downstream 3D liquid volume fraction to understand likelihood of wall wetting • Measurements show the strong effect of multi-component fuels representative of gasoline, affecting plume interactions and final vaporization
S.E.2 Manin	• Experiments show good agreement between RD5-87 target fuel and PACE-20 surrogates regarding film formation and evaporation • Extinction measurements enable extracting information about film evaporation and evaporation rate • Comparison to past data indicate that film formation and volume/thickness appear to be strongly related to injection mass flow rate and spray morphology
A.E.4 Powell	• Proof of concept experiments have shown that x-ray diagnostics can generate unique, quantitative measurements of spray/wall interactions
O.E.6.2 Wissink	• Design and construction of a spray chamber specifically for quantitative neutron imaging of fuel films through metal substrates has been completed • Simulations show potential for resolving film thickness <5 μm • Plans going forward are to perform quantitative measurements of film evolution on metal substrates at PACE conditions
S.M.4.2 Nguyen	• The new Torelli model shows substantially greater film thickness and slower wall jet penetration compared to the standard O'Rourke and Amsden model, emphasizing the need for validation data on these quantities • Multi-component PACE 20 shows a higher film deposition rate compared to iso-octane, while the second injection deposits less liquid fuel on the wall compared to the first injection • The new Corrected Distortion model, now released to all PACE CFD users, predicts higher vaporization as free jet before impingement
A.M.4 Torelli	• The validation of Argonne's new spray-wall interaction (SWI) model against X-ray experiments shows clear improvements in the predictions of spray mass distribution in the near-wall region • The new SWI model has been made available to PACE CFD users as a "plug-and-play" executable for further testing under engine cold-start conditions and with multi-component fuels
S.E.4.3 Pickett	• The combination and availability of detailed free and wall jet data, aligned with uniform CFD post-processing metrics, provides a unique opportunity to substantially improve free and spray wall interaction modeling processes • These model improvements are important to major outcomes in mixture preparation for cold-start, lean and dilute combustion, and knock avoidance

Complete PACE Budget FY21

Code and Work Flow Development

		Lab	PI	FY20	FY21
A.M.05.01	Spray and Combustion model implementation	ANL	Ameen	350k	340k
A.M.05.02	Gridding, validation, and workflow development	ANL	Ameen	350k	300k
A.M.05.04	MO1 Integration	ANL	Som		75k
A.M.05.05	MO5 Integration	ANL	Scarcelli		75k
L.M.05.01	Accelerated multi-species transport in engine simulations	LLNL	Whitesides	275k	250k
L.M.05.02	Improved chemistry solver performance with machine learning	LLNL	Whitesides		250k
L.M.05.04	Scalable performance and CFD integration of ZERO-RK	LLNL	Whitesides	275k	75k
L.M.05.06	Mechanism Reduction	LLNL	Whitesides		75k
L.M.05.07	Accelerate Mechanism Reduction Tools	LLNL	Whitesides		75k

Cold Start

		Lab	PI	FY20	FY21
O.E.07	Multi-cyl Cold Start & surrogate testing	ORNL	Curran	350k	350k
S.E.07	Engine experiments characterizing wall films & PM formation	SNL	Sjoberg	270k	270k

Combustion and Emissions

		Lab	PI	FY20	FY21
O.E.02	Effectiveness of EGR to mitigate knock throughout PT domain	ORNL	Szybist	220k	175k
S.E.02	Experiments supporting particulate modeling -- wall film & pyrolysis	SNL	Manin	500k	400k
L.M.01	Improved Kinetics for Ignition Applications	LLNL	Pitz	150k	
S.M.02.01	DNS and modeling of turbulent flame propagation & end gas ignition	SNL	Chen	50k	50k
S.M.02.02	Flame wall interactions	SNL	Nguyen	150k	50k
S.M.02.03	Engineering PAH Model Development	SNL	Hansen		100k

Data Analytics

		Lab	PI	FY20	FY21
O.E.08	Machine Learning and Nonlinear Dynamics	ORNL	Kaul	200k	200k

Flows and Heat Transfer

		Lab	PI	FY20	FY21
O.E.06.01	Neutron diffraction for in situ measurements in an operating engine	ORNL	Wissink	100k	100k
O.E.06.02	Neutron Imaging of Advanced Combustion Technologies	ORNL	Wissink	200k	200k
O.M.06	Conjugate heat transfer	ORNL	Edwards	350k	350k
LA.M.06.01	Heat Transfer through Engine Metal - - -	LANL	Carrington	200k	
LA.M.06.02	Heat Mass Transfer in Liquid Species - - -	LANL	Carrington	200k	

Flows and Heat Transfer

		Lab	PI	FY20	FY21
O.E.06.01	Neutron diffraction for in situ measurements in an operating engine	ORNL	Wissink	100k	100k
O.E.06.02	Neutron Imaging of Advanced Combustion Technologies	ORNL	Wissink	200k	200k
O.M.06	Conjugate heat transfer	ORNL	Edwards	350k	350k
LA.M.06.01	Heat Transfer through Engine Metal - - -	LANL	Carrington	200k	
LA.M.06.02	Heat Mass Transfer in Liquid Species - - -	LANL	Carrington	200k	

Fuel Kinetics and Surrogates

		Lab	PI	FY20	FY21
A.E.01	Measurements of autoignition fundamentals at dilute gasoline conditions	ANL	Goldsborough	280k	252k
L.M.01	Surrogates and Kinetic Models	LLNL	Pitz	500k	425k
L.M.01.02	Models for improved prediction of PAH/soot	LLNL	Kukkadapu	200k	200k

Ignition

		Lab	PI	FY20	FY21
A.M.03	Advanced Ignition Modeling Tools	ANL	Scarcelli	400k	370k
N.M.03	ML based LES ignition model	NREL	Yellapantula	275k	275k
S.M.03.01	DNS of early ignition kernel development	SNL	Chen	100k	100k
S.M.03.02	Physics based flame-kernel LES modeling	SNL	Nguyen	100k	100k
A.E.03	Fundamental Ignition Experiments	ANL	Rockstroh	380k	342k
S.E.03.01	Advanced Ignition to Enable Alternative Combustion Modes	SNL	Ekoto	420k	420k
S.E.03.02	Fundamental ignition experiments	SNL	Ekoto	420k	420k

LSPI

		Lab	PI	FY20	FY21
O.E.09.01	Fuel spray wall wetting and oil dilution impact	ORNL	Splitter	220k	220k

Sprays

		Lab	PI	FY20	FY21
A.E.04	X-Ray Studies of Fuel Injection and Sprays	ANL	Powell	490k	441k
O.E.04.01	Injector Characterization & Distribution	ORNL	Wissink		125k
S.E.04	Spray Experiments	SNL	Pickett	380k	380k
S.E.04.03	GDI sprays leadership & data sharing	SNL	Pickett	140k	140k
A.M.04	Towards Predictive Simulations of Sprays in Engines	ANL	Torelli	300k	220k
A.M.04.01	Improved free spray and spray-wall interaction modeling	ANL	Torelli		125k
LA.M.04.01	Simulate free sprays in chamber and engines - - -	LANL	Carrington	200k	
S.M.04.01	Free spray modeling	SNL	Nguyen	50k	50k
S.M.04.02	Free spray modeling addition	SNL	Tagliante		125k

Reviewer-Only Slides

Publications and Presentations

D.01.05 Pickett	Karathanassis et al. "Comparative Investigation of Gasoline-like Surrogate Fuels using 3D Computed Tomography" ICLASS 2021 Hwang et al. "Spatio-temporal identification of plume dynamics by 3D computed tomography using engine combustion network spray G injector and various fuels," Fuel 280:118359, 2020
D.01.01 Powell	"X-Ray Characterization of Real Fuel Sprays for Gasoline Direct Injection", Sforzo et al., ASME-ICE Fall Technical Conference, https://doi.org/10.1115/ICEF2020-2974, December 2020. "Effects of detailed geometry and real fluid thermodynamics on Spray G atomization", Marco Arienti, Everett A.Wenzel, Brandon A. Sforzo Christopher F. Powell. Proceedings of the Combustion Institute 38, Issue 2, 2021, pp. 3277-3285, September 2020. “Synchrotron X-ray Tomography for Non-Destructive Metrology of Micro-Orifices in Automotive Fuel Injectors”, A. Tekawade, B. A. Sforzo, A. L. Kastengren, C. F. Powell. Proc. SPIE 11382, Smart Structures and NDE for Industry 4.0, Smart Cities, and Energy Systems, 1138207, April 2020 “X-ray Diagnostics for the Validation of Nozzle Flow and Spray Simulations”, Converge User Conference, September 2020.
D.01.02 Wissink	Wissink, “Update on Neutron Diagnostic Tasks”, presented at Advanced Engine Combustion Program Review Meeting, Aug 2020, virtual
S.M.4.2 Nguyen	Nguyen, T et al., “Toward Predictive Free Spray Simulation of PACE Gasoline Surrogate”, Advanced Engine Combustion Program Review Meeting, Feb 2, 2021 (Virtual Meeting)
D.02.01 Torelli	Torelli, R., “Recent Developments in CFD Modeling of Spray-Wall interaction for GDI Sprays,” 2020 Summer AEC presentation (virtually held) Torelli, R., “Development and Validation of Spray-Wall Interaction Models for GDI Applications,” 2020 USA CONVERGE User Conference (virtually held) Torelli, R., “Preliminary Evaluation of a New Spray-Wall Interaction model in a DISI Optical Engine under Motored Operating Conditions,” 2020 Winter AEC presentation (virtually held) Torelli, R., Kim, N., Sjoberg, M., Som, S., “Large Eddy Simulations of Spray-Wall Interaction in a Direct-Injection Optical Engine,” Large-Eddy Simulation for Energy Conversion in electric and combustion Engines (LES4ECE) Conference June 17-18, 2021, (submitted). Torelli, R., Sforzo, B.A., Bautista Rodriguez, A., Tekawade, A., Powell, C.F., and Som, S., “Development and Validation of Spray-Wall Interaction Models for GDI Applications,” (under preparation), 2021.

Critical Assumptions and Issues

S.E.4.1 Pickett	We assume that free spray simulations can be improved to the level that spray-wall interaction effects are not confounded by uncertainties with droplet size, velocity, liquid volume fraction, and so forth at the wall
S.E.2 Manin	Temperature gradients with flame and film at wall are very steep, particular at pressure. We assume that these gradients will not prevent quantitative measurements due to beam steering. We also assume that the temperature gradient may be measured
A.E.4 Powell	
O.E.6.2 Wissink	COVID-19 access restrictions are relaxed and HFIR continues to remain operational at planned capacity. Previous experimental timelines have been impacted by unscheduled reactor shutdowns, which are rare but impossible to predict.
S.M.4.2 Nguyen	
A.M.4 Torelli	
S.E.4.3 Pickett	