Spray Combustion and Soot Formation: Cross-Cut Engine Research

Lyle M. Pickett, Scott A. Skeen

Sandia National Laboratories

FY 2019 DOE Vehicle Technologies Program Annual Merit Review
11:00 AM, Tue. 11 June 2019

Project ID# ACE005

Sponsor: **DOE Vehicle Technologies Program**
Program Managers: **Gurpreet Singh and Michael Weismiller**

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

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. SAND2019-4745 PE

Overview

Timeline

- Project provides fundamental research that supports DOE/ industry advanced engine development projects.
- Project directions and continuation are evaluated annually.

Budget

- Project funded by DOE/VT:
  - FY18 $845K (spray)
  - FY19 $720K (spray) $770K (soot)
- Project lead: Sandia
  - PIs
    - Lyle Pickett
    - Scott Skeen

Barriers

Engine efficiency and emissions

- Understanding direct-injection sprays
- Lack of quantitative databases
- CFD† model improvement for engine design/optimization

Partners

- 15 Industry partners in MOU: Advanced Engine Combustion
- Engine Combustion Network (ECN)
  - >20 experimental + >20 modeling
  - >100 participants attended ECN6
- International Energy Agency
  - CONVERGE Working Group

†Computational Fluid Dynamics

Engine efficiency gains require fuel delivery optimization—Direct Injection (DI) Spray

- Objectives toward enhanced efficiency and reduced emissions for diesel and gasoline combustion strategies (cross-cut)
  - Enhance understanding of fuel spray fundamentals including internal and near nozzle flows and rate of injection; provide data driving development of improved spray and mixing models
  - Apply advanced diagnostics tools to expand availability of qualitative and quantitative engine relevant data, lead international efforts through ECN, make data available on ECN database
  - Improve understanding of wall interactions for mixing controlled compression ignition (MCCI) and gasoline direct injection (GDI) applications

Project Objectives

Major objective: experimentation at engine-relevant spray conditions, allowing development of predictive computational tools used by industry

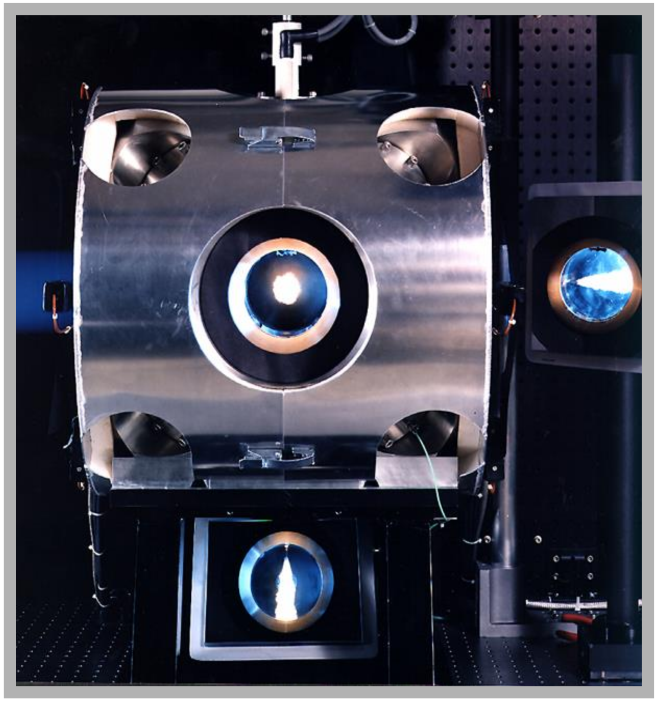
Engine efficiency gains require fuel (DI spray) delivery optimization

- Improved understanding of nozzle and sac initial conditions on rate of injection (ROI) ramp up and initial penetration behavior
  - Finite element analysis reveals effects of needle and nozzle elasticity
  - Nozzle temperature, gas in sac, greatly influence initial rate of injection (ROI) and mixing
- Understand potential for and consequences of supercritical conditions on spray mixing
- Provide quantitative soot data toward the improvement of models including wall interactions, multiple injections (literature survey shows SNL soot data heavily used)
- C/D Data summary, ECN data release
- Characterization of liquid penetration in GDI sprays to understand propensity for wall impingement (ECN G2 and G3 conditions)
- Simulations of wall-impinging GDI sprays to evaluate model performance

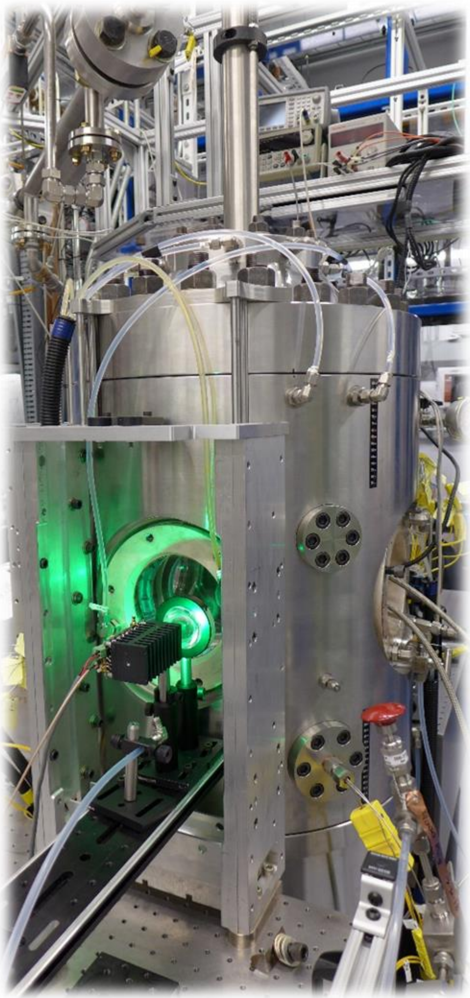
Experimental approach utilizes well-controlled conditions in constant-volume and constant pressure chambers

- Well-defined ambient conditions:
  - 300 to 1300 K (1100 K)
  - up to 350 bar (150 bar)
  - 0-21% O_2 EGR† (O_2/N_2)
- Injector
  - single- or multi-hole injectors
  - diesel or gasoline (cross-cut)
- Full optical access
  - 100 mm on a side
- Boundary condition control needed for CFD model development and validation
  - Better control than an engine
  - Easier to grid

Pre-burn spray chamber



High-throughput spray vessel



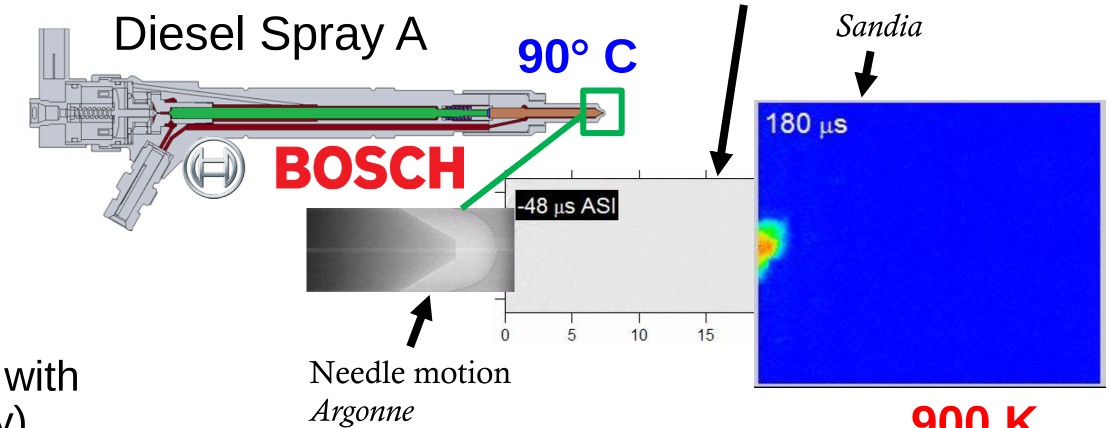
†Exhaust gas recirculation

Approach: Collaborative research through the Engine Combustion Network accelerates CFD model development

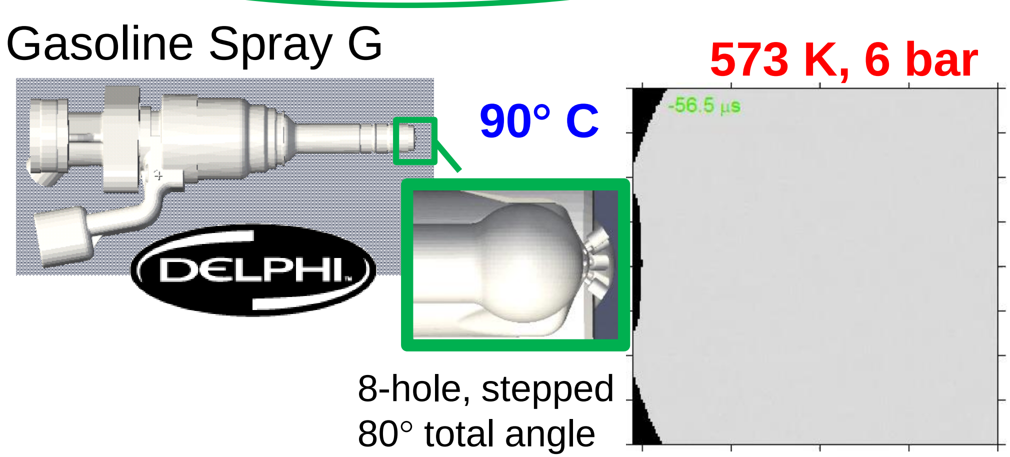
Approach
- Develop diesel and gasoline target conditions with emphasis on CFD modeling shortcomings
- Comprehensive experimental and modeling contributions
- Diesel Spray A, B, C, D
- Gasoline Spray G
- Results submitted to online archive with fields (like geometry and uncertainty) specifically tailored for CFD simulations

Impact
- Established in 2009, there are already 1500 citations of the ECN data archive
- Comprehensive Spray C/D, Spray G datasets added in FY18 (ECN6)
- ALL US automotive industry (light- and heavy-duty) use ECN archive to test their own CFD methods
- DENSO Corporation provides ECN with 8 piezo-driven injectors, 90 micrometer orifice, k-factor ~3

ECN formed by Sandia in 2009



>75 measurements/diagnostics contributed from >20 institutions

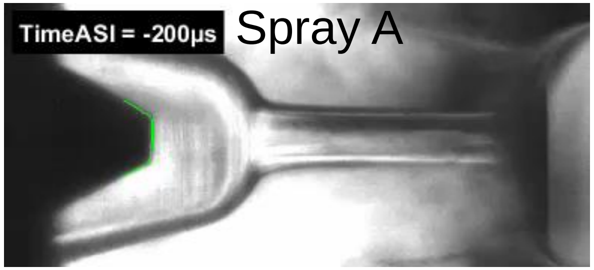


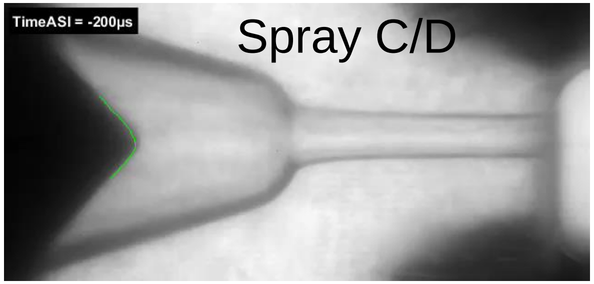
Approach - Milestones

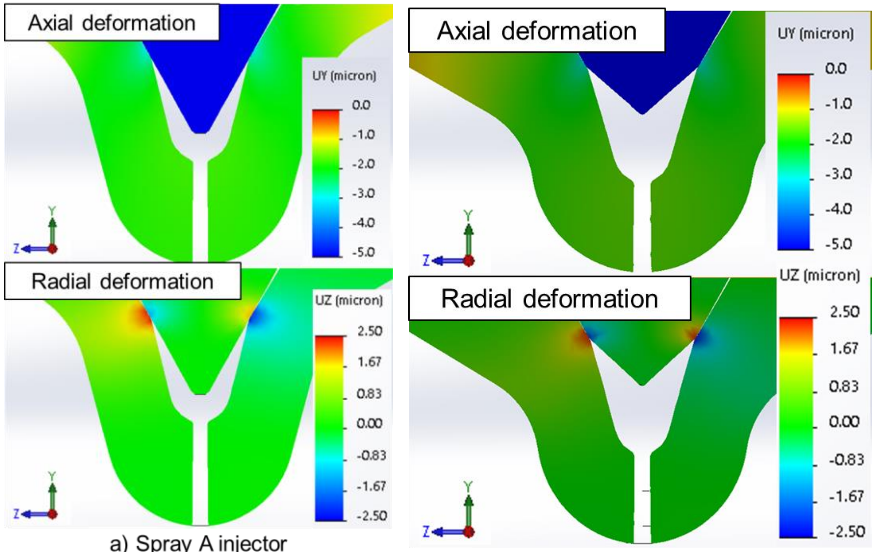
- ✓ **Mar 2018**
  Investigate effect of injector temperature on rate-of-injection in cavitating and non-cavitating injectors
- ✓ **May 2018**
  Quantitative soot measurements comparing free- and wall-impinging sprays with various multiple injection schedules
- ✓ **Jun 2018**
  Combustion and soot formation characteristics of three global diesel blends
- ✓ **Jul 2018**
  Long-distance microscopy of reacting drops demonstrating supercritical behavior
- ✓ **Oct 2018**
  Experimental and computational investigation of nozzle elasticity effects on spray rate of injection (ROI)
- ✓ **Dec 2018**
  GDI 3D liquid spray penetration measurements in high-throughput vessel
- ✓ **Feb 2019**
  GDI wall impingement simulations
- ✓ **FY 2019 (Planned)**
  Laser ignition of GDI sprays with quantitative soot measurements, quantitative GDI mixture fraction diagnostic – laser ignition source in preparation, dopants being evaluated

Improved understanding of nozzle and sac initial conditions on rate-of-injection (ROI) ramp up and initial penetration (1)

- X-ray measurements show needle lift >100µs before start of liquid
- Long distance microscopy of metal and acrylic nozzles confirm gas ingestion prior to liquid injection
- Finite Element Analysis (FEA) reveals effects of needle and nozzle elasticity

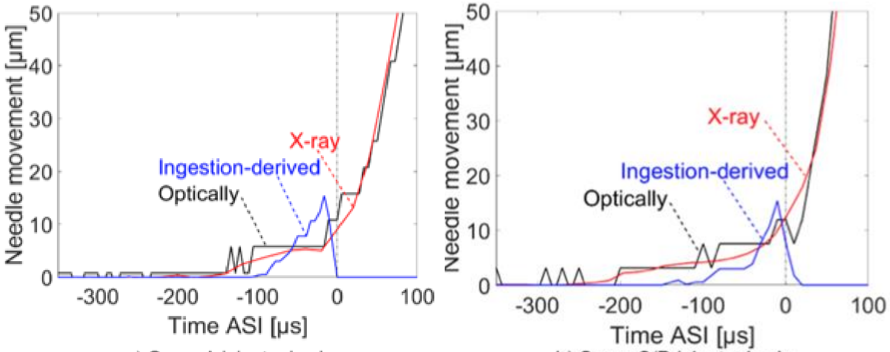






a) Spray A injector

b) Spray C/D injector



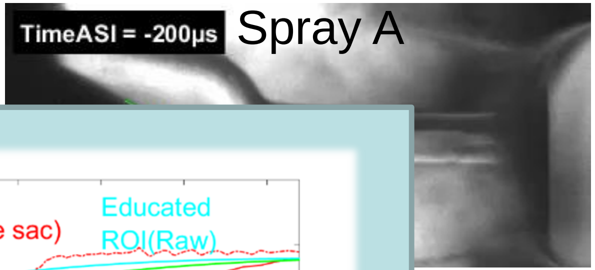
a) Spray A injector body

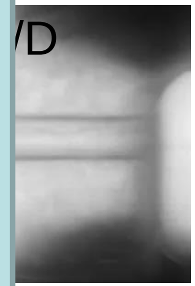
b) Spray C/D injector body

Yasutomi et al., SAE PFL, Sandia, 2019

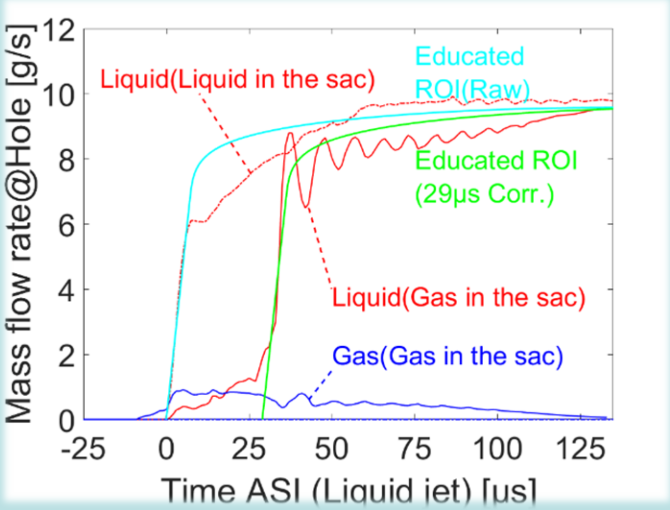
Improved understanding of nozzle and sac initial conditions on rate-of-injection (ROI) ramp up and initial penetration (1)

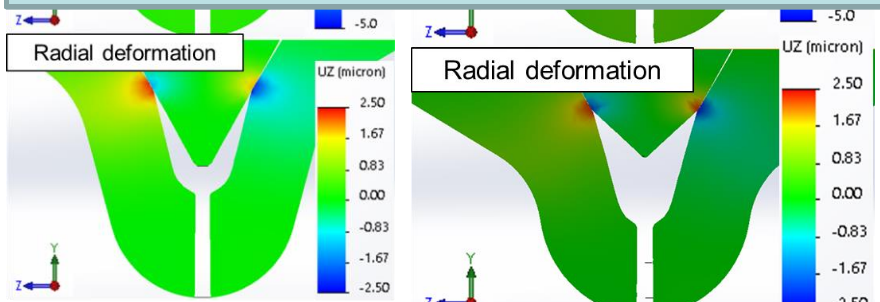
- X-ray measurements show needle lift >100µs before start of liquid





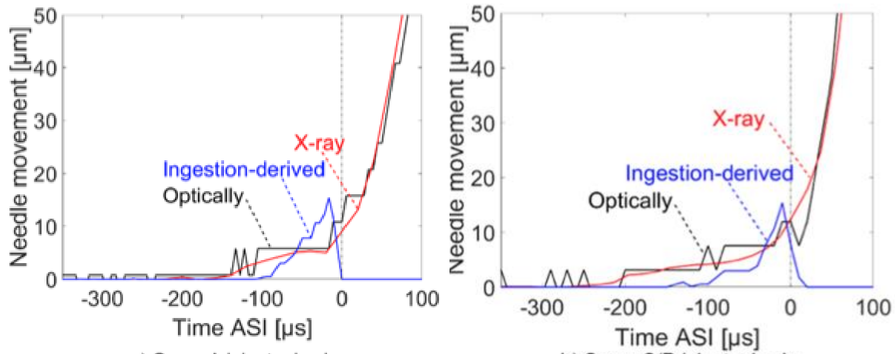
Injector deformation influences ROI at startup; models must implement correct ROI to capture early mixing field at ignition





a) Spray A injector

b) Spray C/D injector



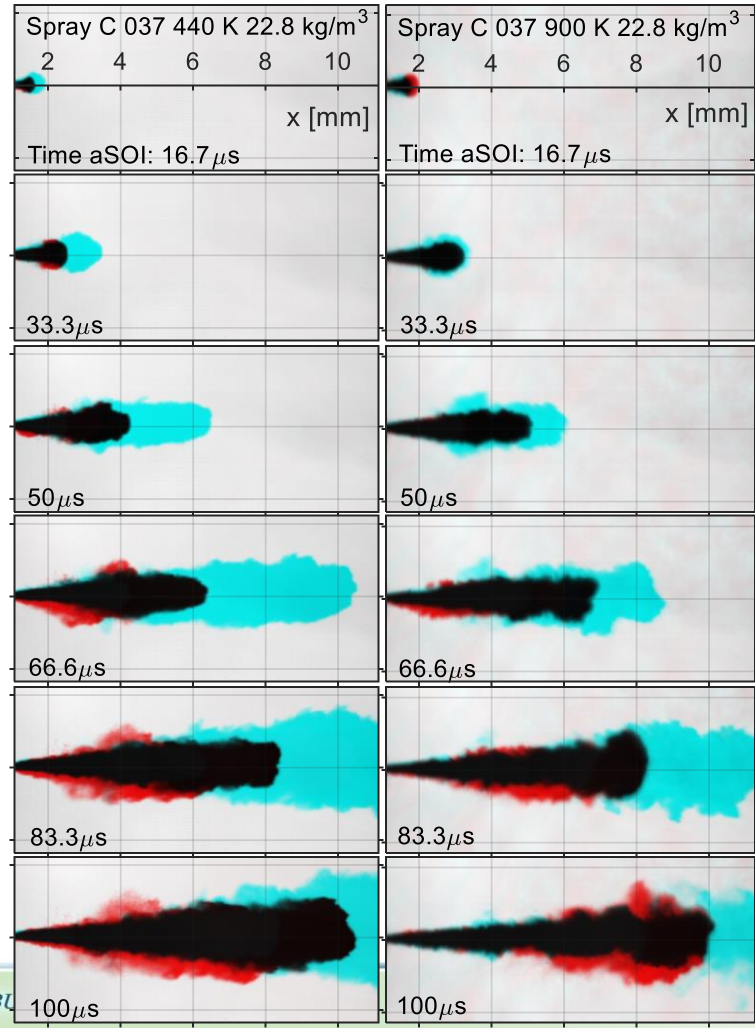
a) Spray A injector body

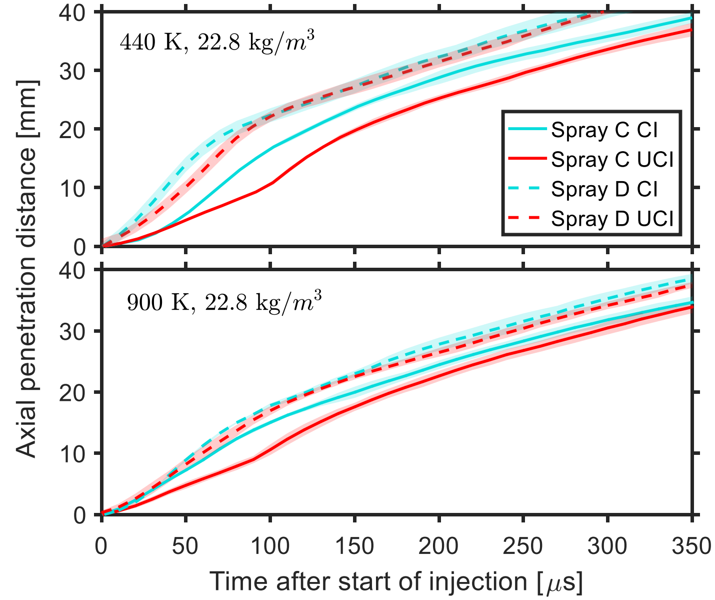
b) Spray C/D injector body

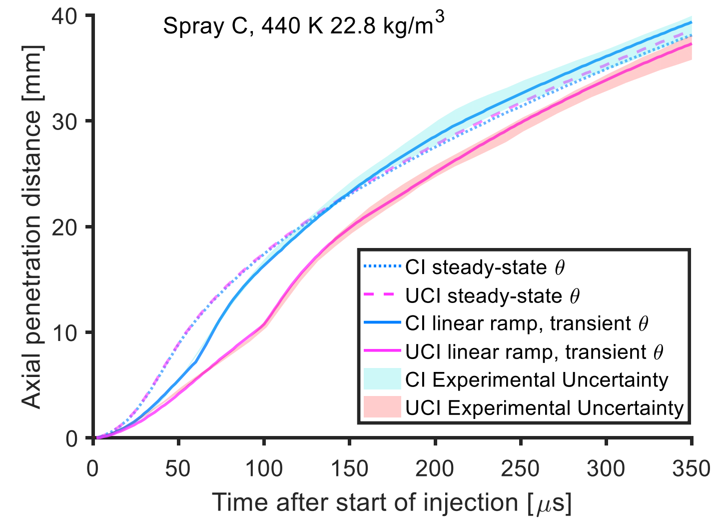
Yasutomi et al., SAE PFL, Sandia, 2019

Improved understanding of nozzle and sac initial conditions on rate-of-injection (ROI) ramp up and initial penetration (2)

- High-speed long distance microscopy and shadowgraphy imaging reveal impact of nozzle temperature on early penetration





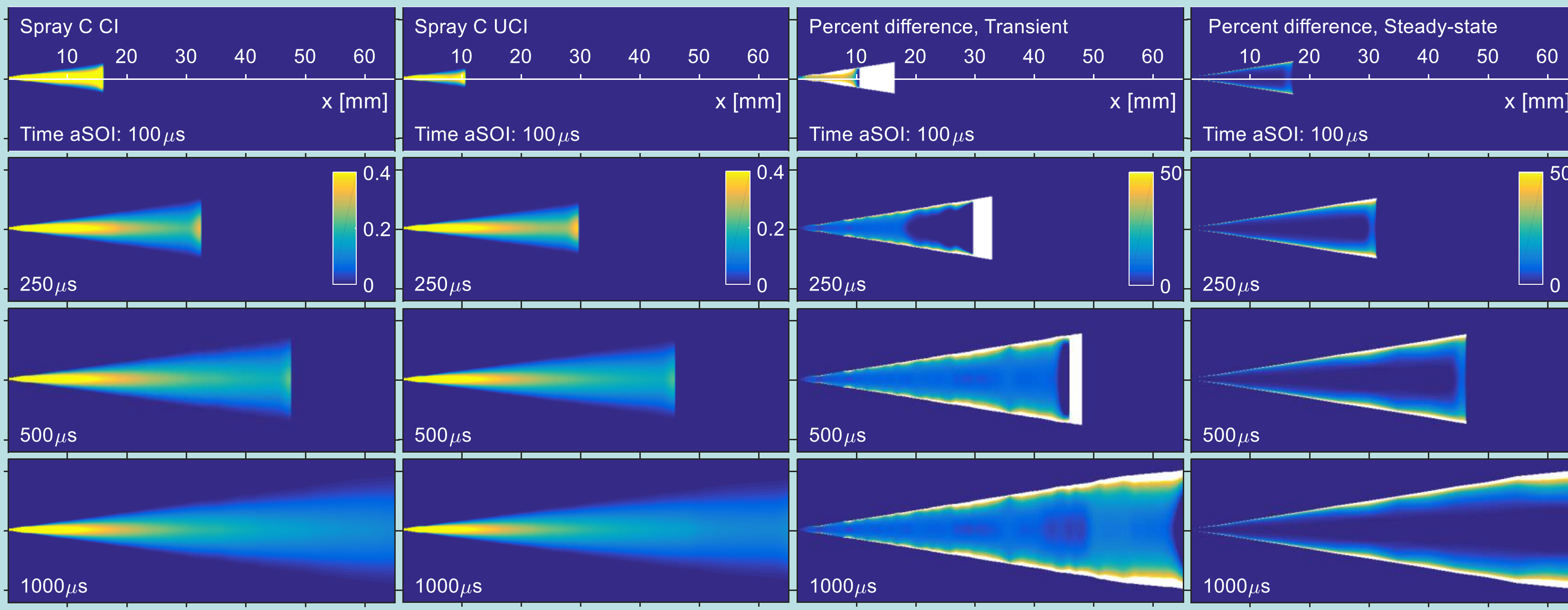


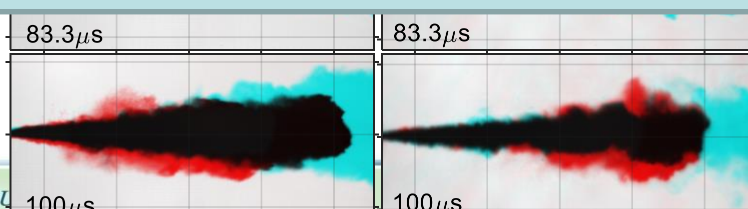
Daley et al., SAE, Sandia, 2018

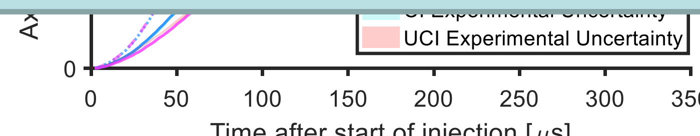
Improved understanding of nozzle and sac initial conditions on rate-of-injection (ROI) ramp up and initial penetration (2)

Nozzle temperature influences gas in sac, early penetration, spreading angle, and mixing at timings associated with ignition

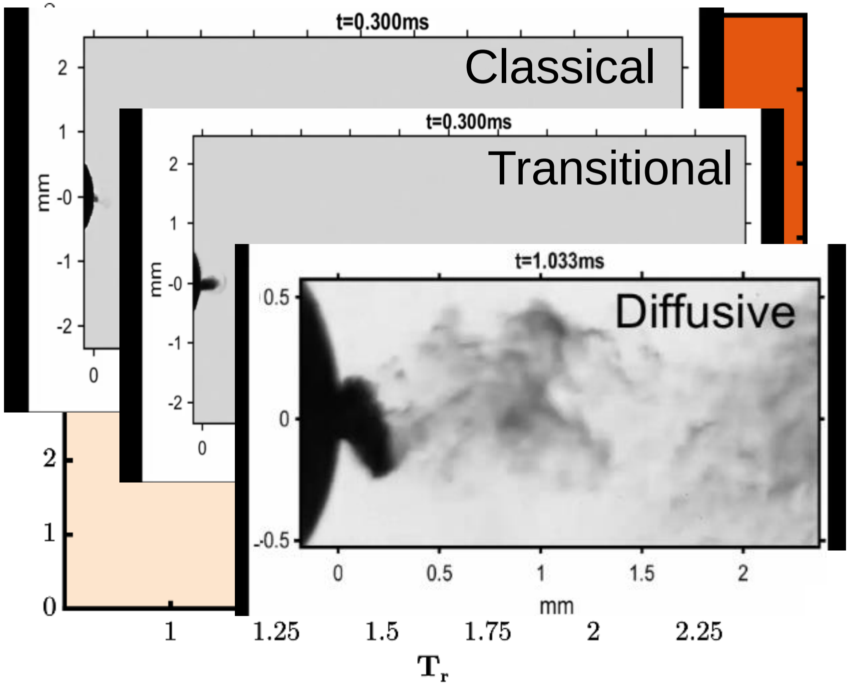
Models failing to capture correct ROI and early penetration may lead to erroneous calibration of kinetic mechanisms

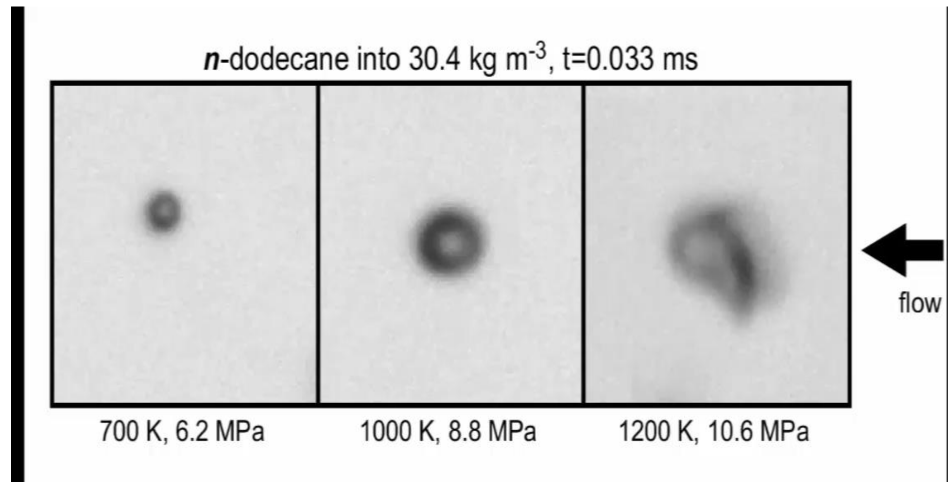


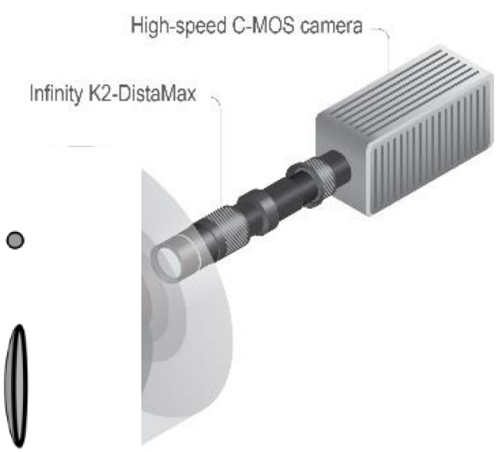


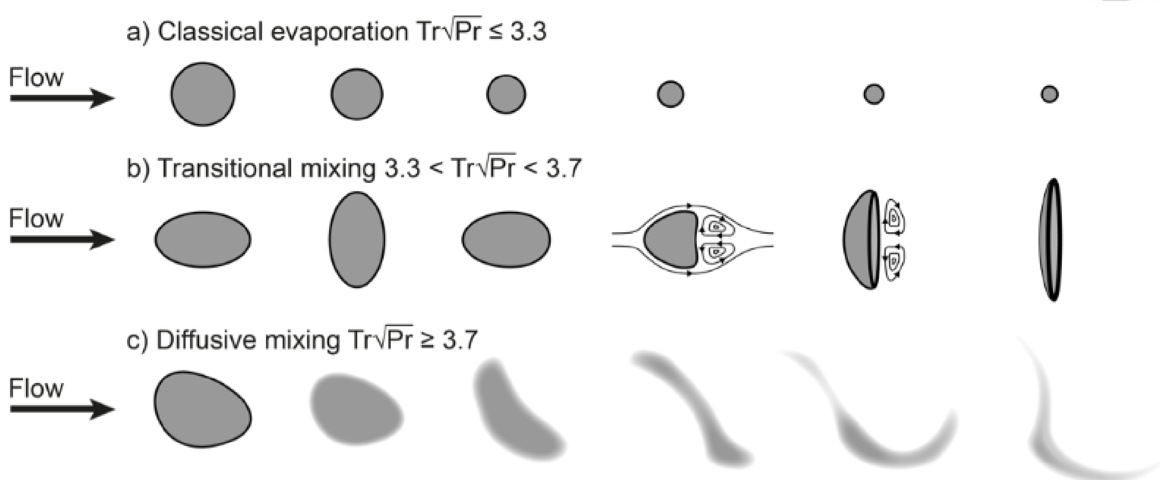


Demonstrate potential for non-equilibrium phase transition resulting in enhanced mixing due to local supercritical conditions

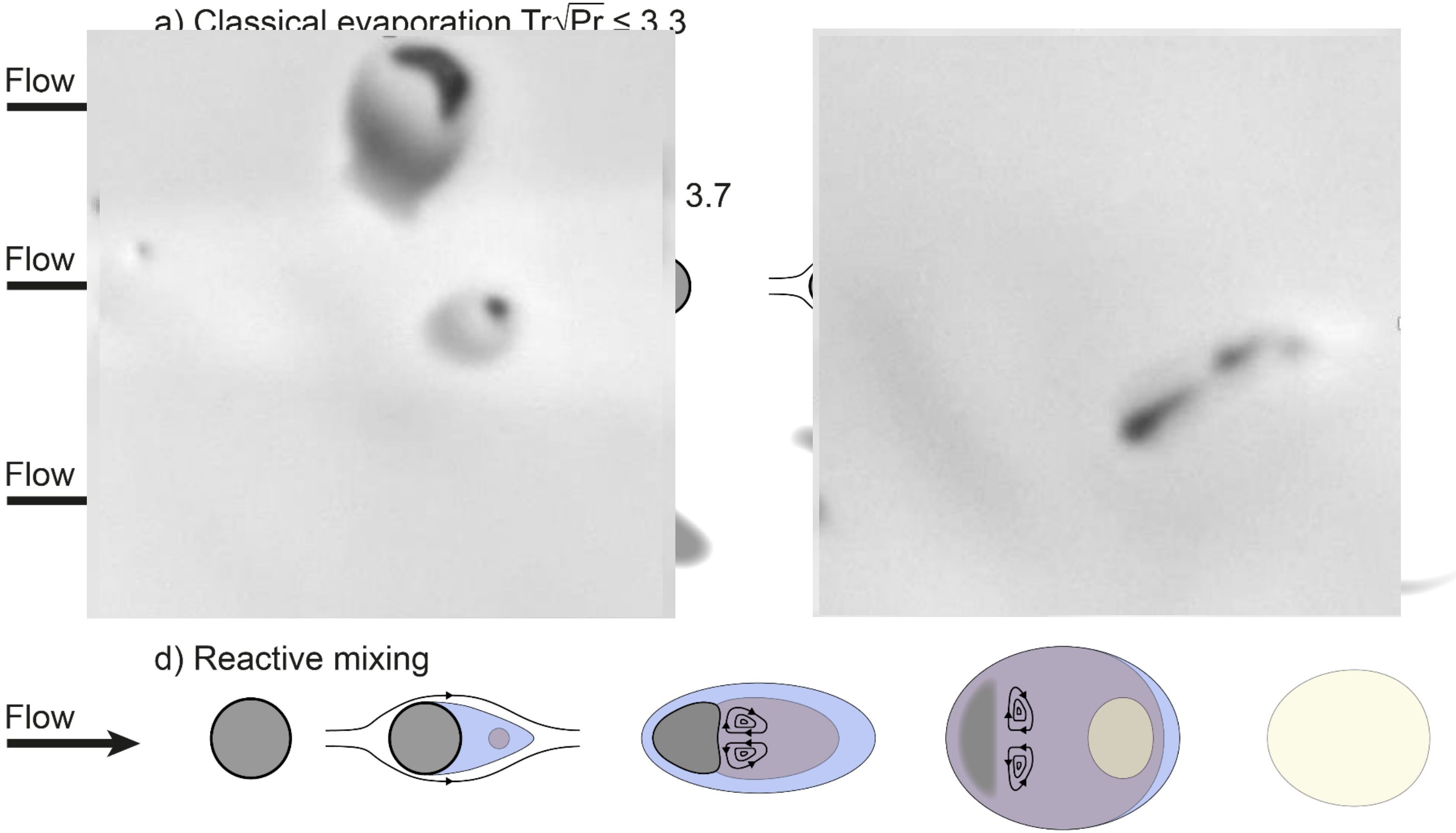








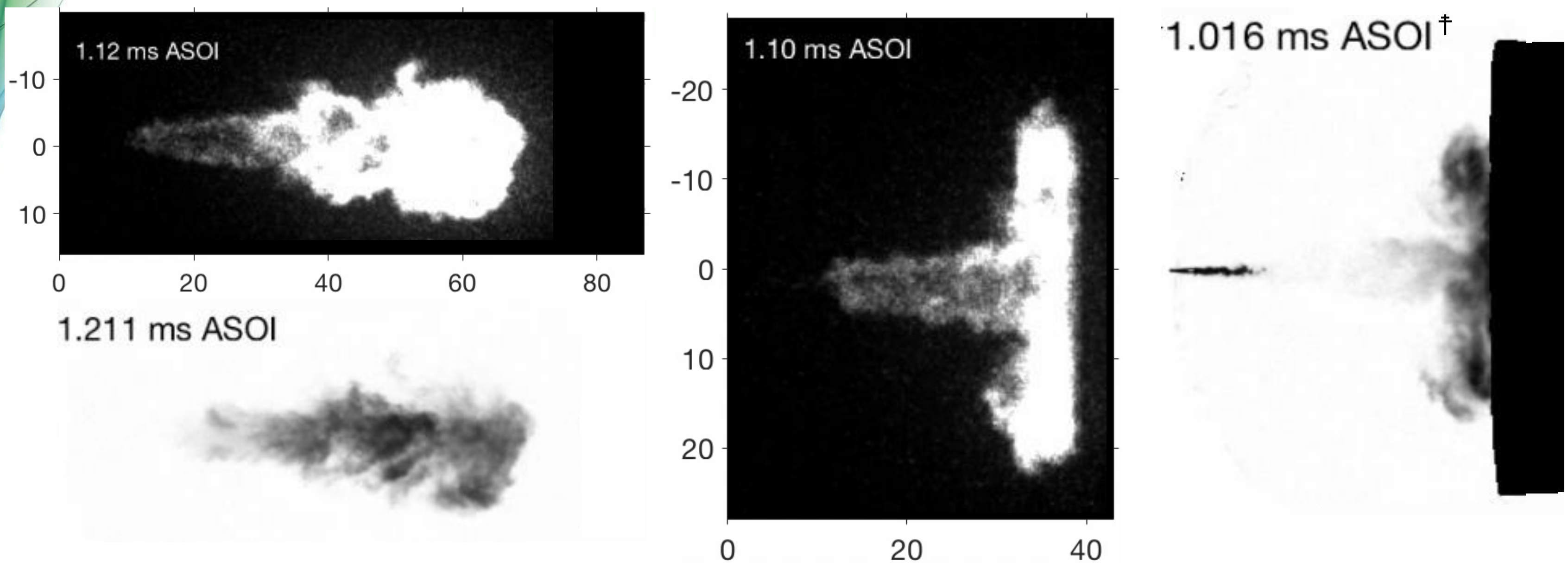
Demonstrate potential for non-equilibrium phase transition resulting in enhanced mixing due to local supercritical conditions



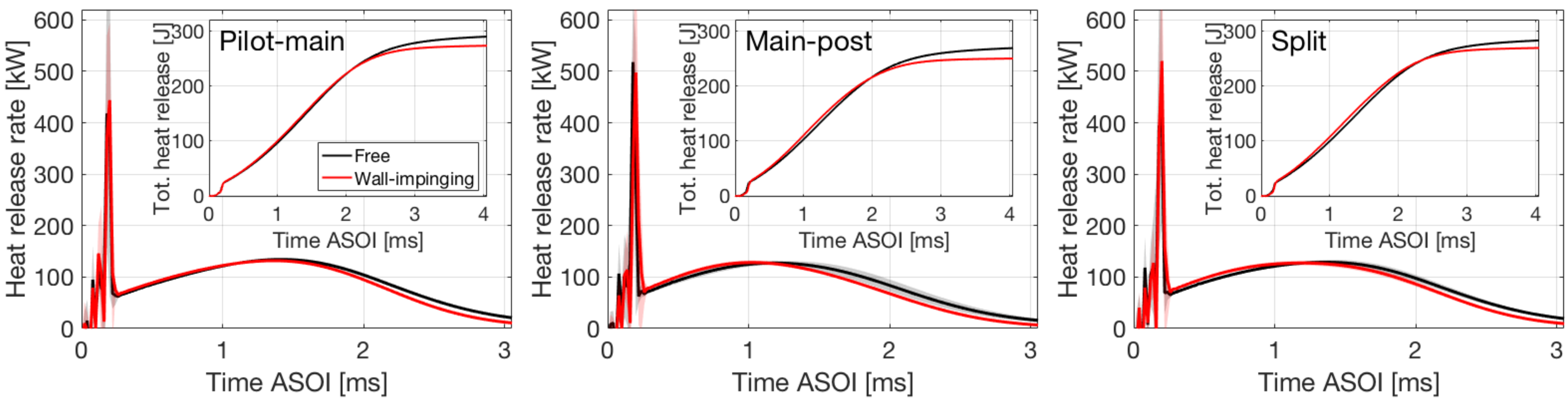
Steep temperature gradients in reacting spray promote supercritical behavior locally, leading to non-equilibrium phase transitions and enhanced mixing…even at Spray A conditions

Quantitative soot for wall-impinging sprays with various multiple injection schedules

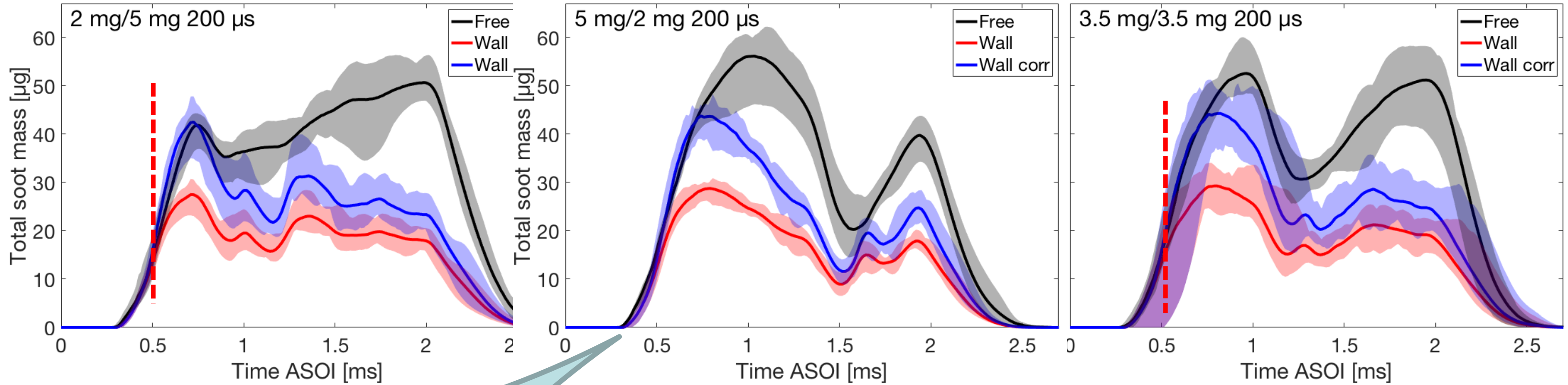
†ASOI-After Start of Injection

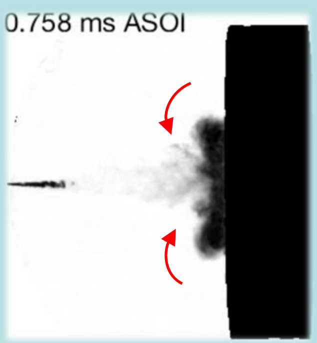


Wall heat flux quantified; wall enhances mixing leading to higher heat release rate



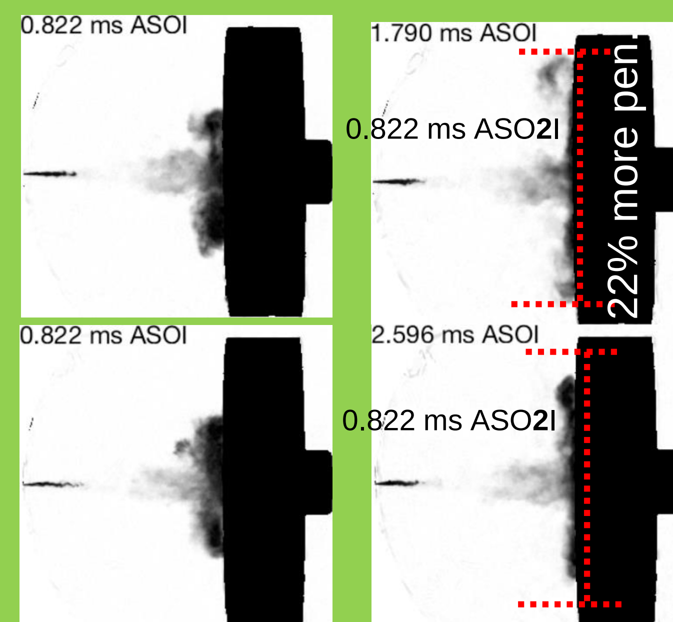
Soot reduction begins when wall jet radial penetration exceeds spray width, less enhancement of radial penetration for 2nd injection with longer dwell



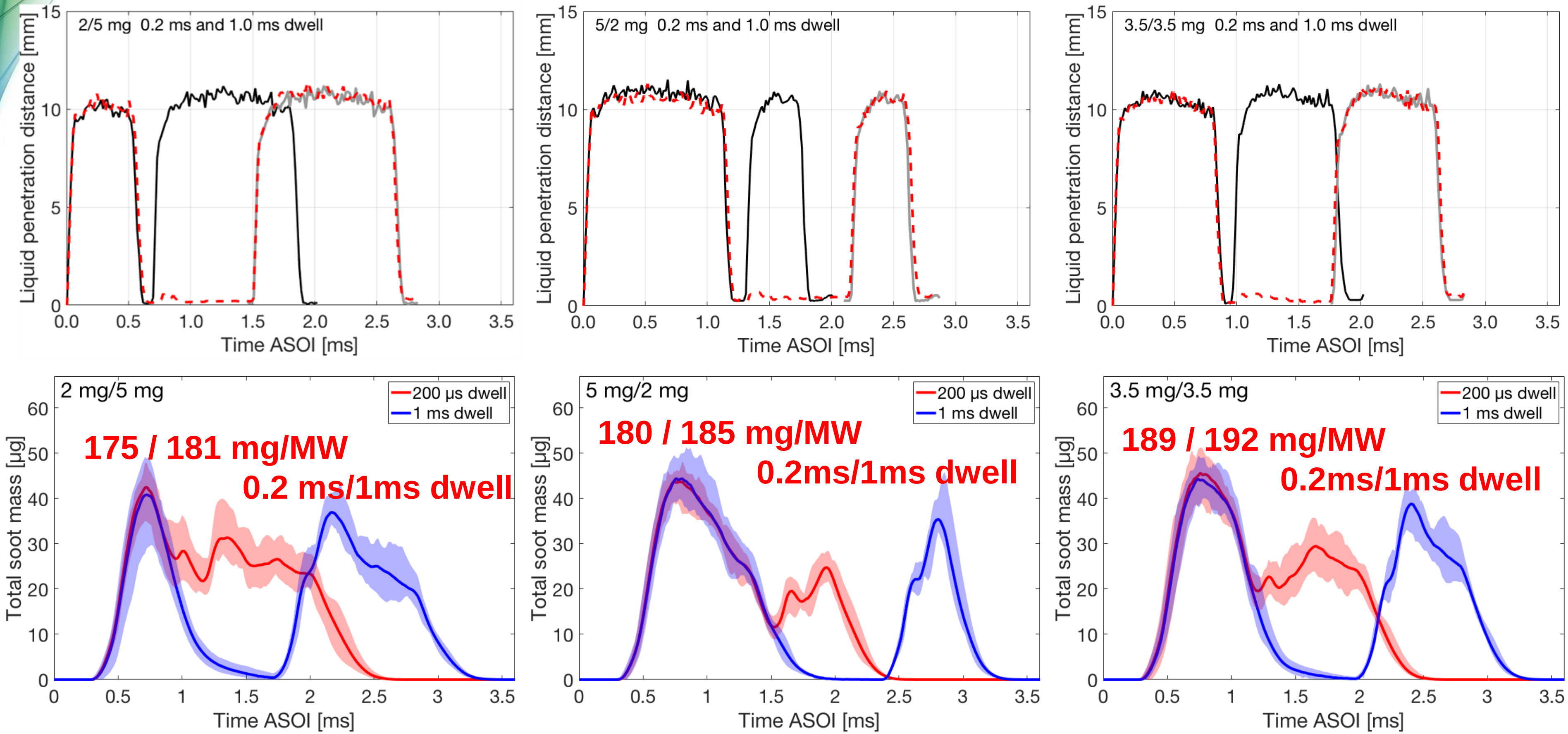


Soot reduction for 1st injection begins when wall jet radial penetration exceeds upstream spray width

Enhanced penetration of the 2nd injection due to the lower density and slipstream remaining from 1st injection is lessened with longer dwell



Subtle differences in normalized soot yield observed among injection schedules for wall-impinging sprays



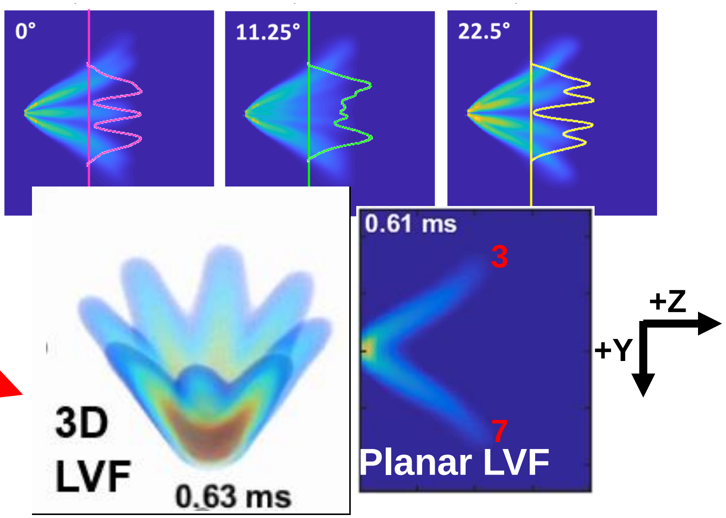
- Soot formation per unit (fuel) energy is minimized with pilot-main, short dwell injection schedule
- A short dwell always yields lower soot for the present conditions

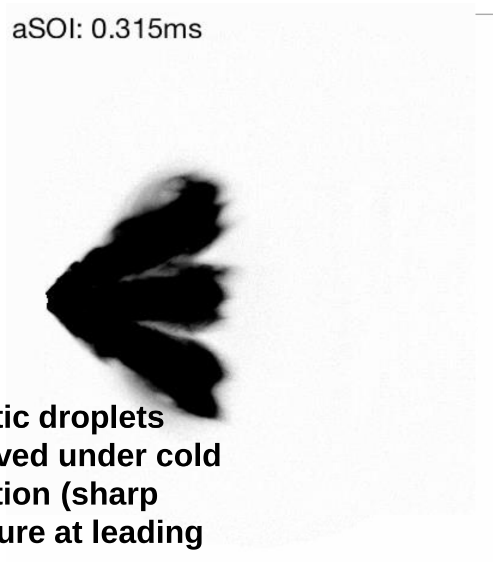
3D liquid volume fraction: Characterization of liquid penetration in GDI sprays quantifies propensity for wall impingement

ECN Spray G (300 repetitions)

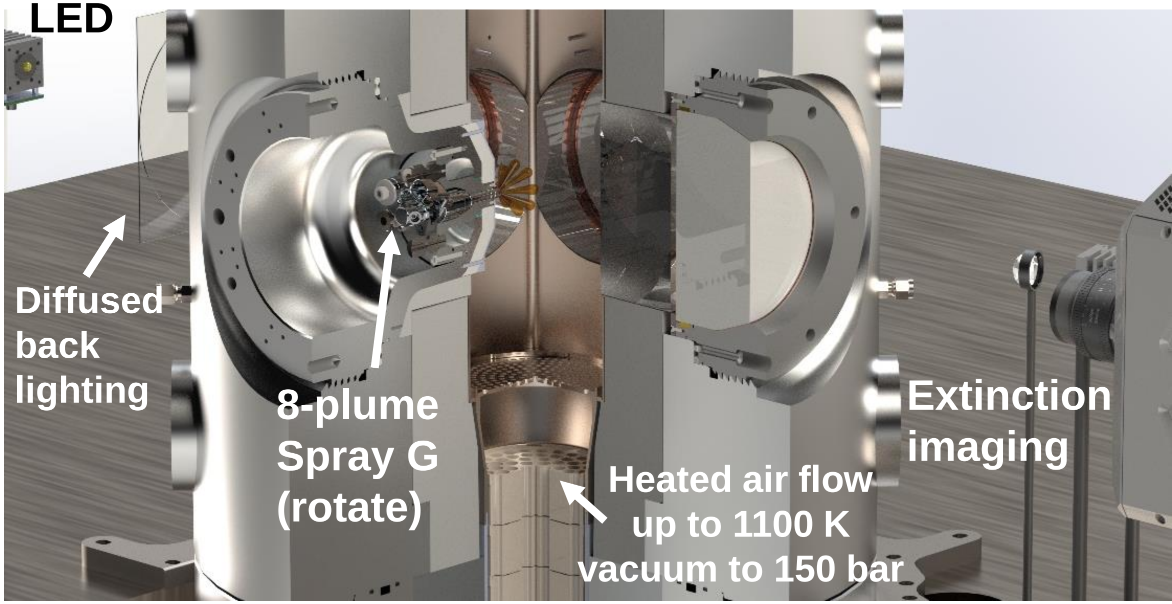
- Injector:
    - Delphi solenoid-activated,8-hole, stepped lip
- Injection (iso-octane)
    - *P*: 20 [MPa]
    - duration: 680 [µs] mass: 10 mg
- Ambient & Fuel T [°C]
    - Cold: 20 (both)
    - Warm: 60 amb. / 90 fuel
- Ambient *ρ* [kg/m^3]
    - G2: 0.5 (0.5 bar) G3: 1.12 (1 bar)

Tomographic reconstruction

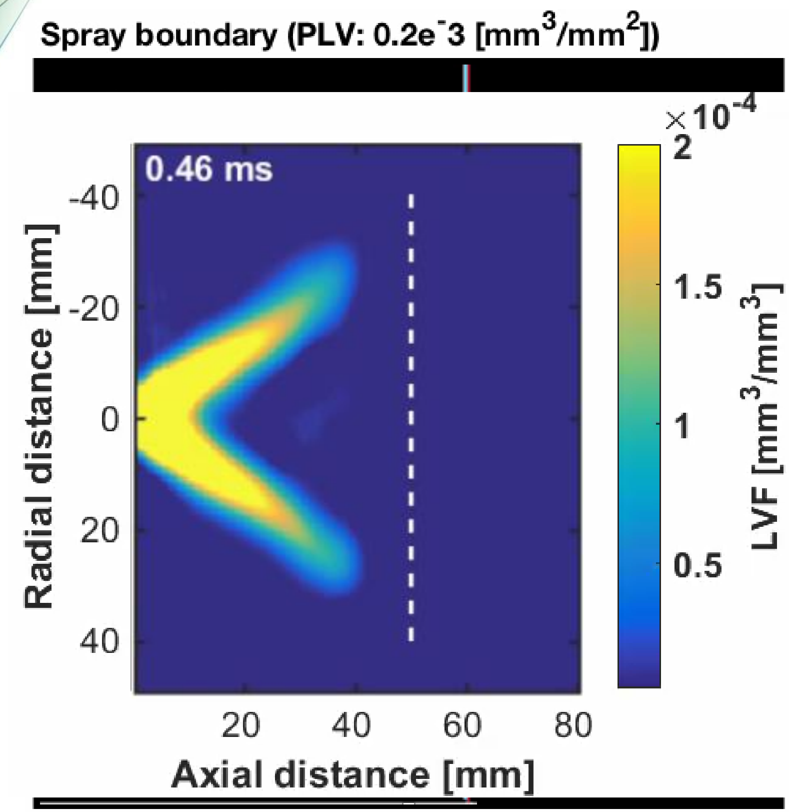


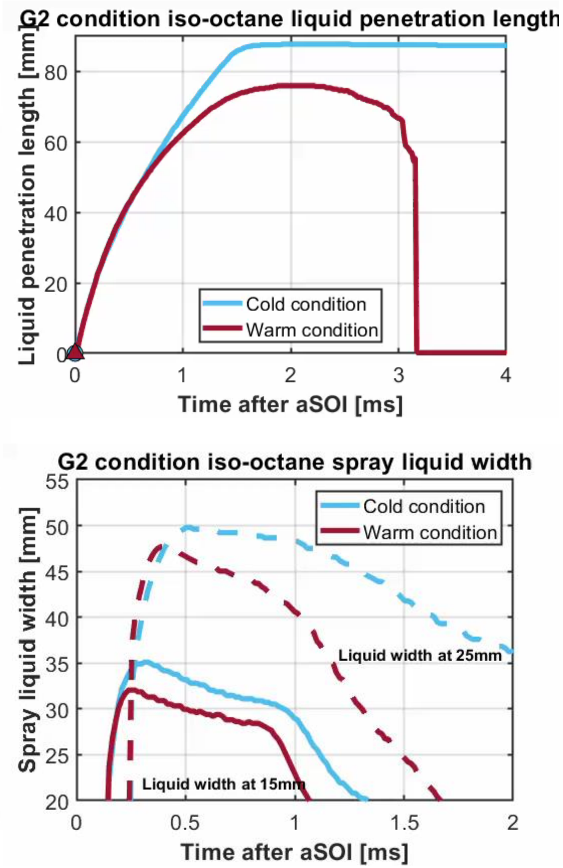


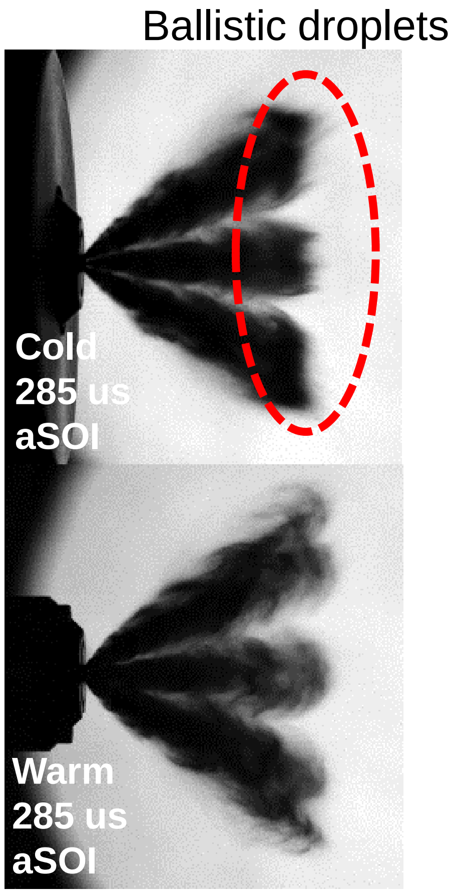
Ballistic droplets observed under cold condition (sharp structure at leading edge).



Cold vs. Hot fuel at Spray G (G2) Conditions

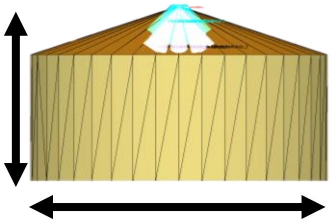






- Lower density and minor spray collapse under warm condition leads to slightly faster initial liquid penetration
- Slower evaporation → greater width under cold condition
- Liquid persists under cold condition

Simulations of wall-impinging GDI sprays to evaluate model performance



50mm

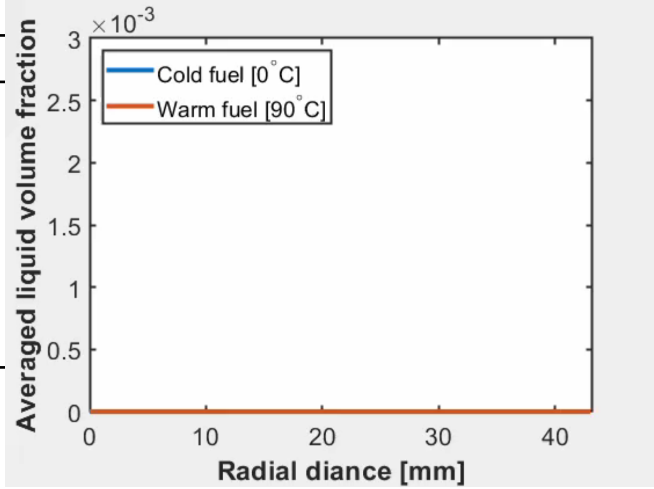
86mm

Fuel: iso-octane

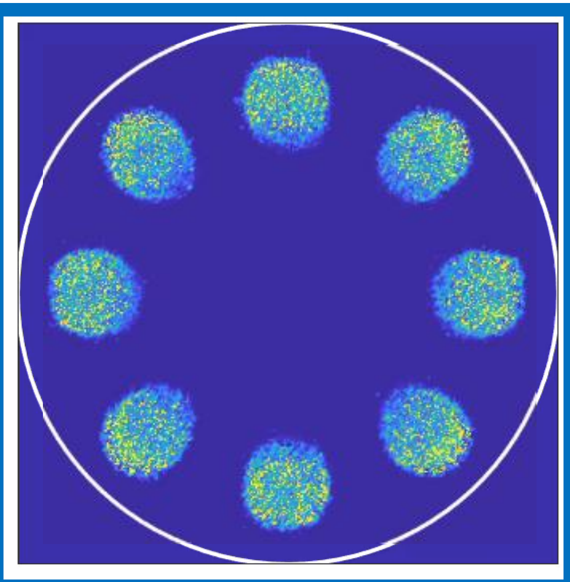
Boundaries: 353 K
Nitrogen: 333 K, 1bar
Cold fuel: 0°C
Warm fuel: 90°C

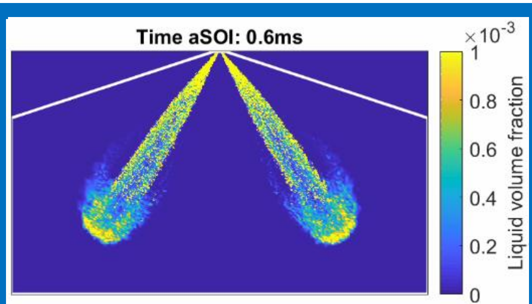
Item	Level
Total cell #	~401,000
Cell size [µm]	20 - 160
Turb. model	RANS* (Std k-ε)
Parcel #	70,000/plume
Sim. time	~5.5ms aSOI
Calc. time [h]	~16 / case

Liquid distribution through plume center @ 50mm

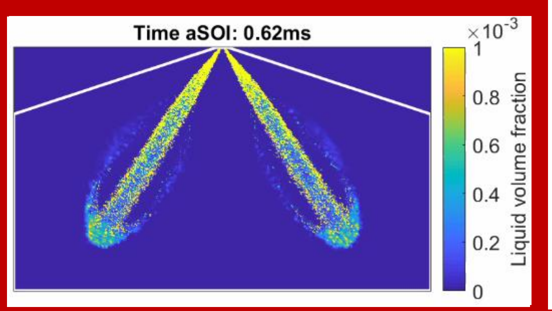


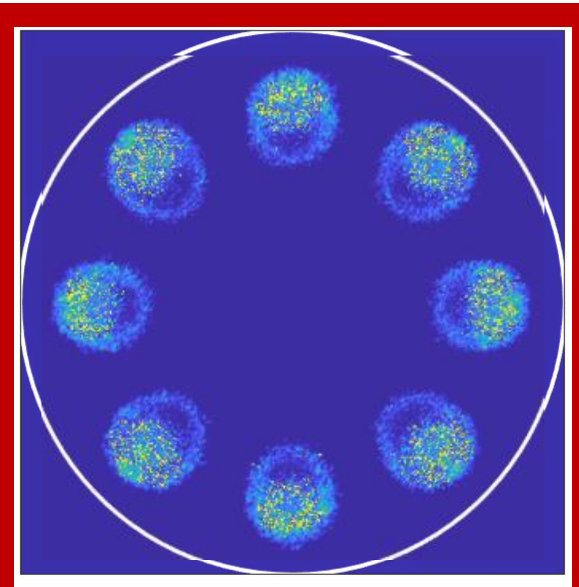
Cold fuel [0°C]





Warm fuel [90°C]





Responses to previous year reviewer comments

- Comment: The reviewer commented that it would perhaps be useful to incorporate some parallel CFD-based research to assist in interpreting and rounding out the information gathered in the experimental work, similar to the approach now being used in the optical engine research at the same laboratory.
- Response: In addition to ECN efforts and collaborations with other laboratories, in-house CFD efforts with CONVERGE are underway. Recently hired postdocs in both PIs groups are trained in experiments and simulations. Parallel CFD efforts are also implemented via the CONVERGE Working Group (International Energy Agency).
- Comment: For the quantitative mixing measurement, fullerene molecule used as a conductor (C70) seems to be a promising dopant, but the team needs a careful comparison for distillation matching.
- Response: C70 fullerene does not boil, rather, it sublimes just above 1100 K. The fullerene nanoparticles therefore remain in the solid phase at the temperatures experienced in our non-reacting mixing measurements. The assumption that the nanoparticles are distributed homogeneously within the solution and retain their local distribution after fuel vaporization occurs is a potential source of error. Our greatest concern with the use of fullerene nanoparticles is the potential for spray drying effects after fuel vaporization, which could lead to coagulation of fullerene particles into larger clusters. The larger clusters would impact the extinction coefficient as scattering may become significant.
- Comment: The reviewer noted, of course, it would be beneficial to the diesel OEMs to see more work done on the diesel side. Additionally, the reviewer noted that there are certainly plenty of problems to consider, particularly in the area of spray/soot relationships. In this context, a greater collaboration with the same national laboratory’s optical engine program might generate even more interesting results.
- Response: Collaborations in the area of ducted fuel injection as well as detailed characterization of the CRC surrogate fuels have been established.

Collaborations and Coordination with Other Institutions

ECN6, 10-11 September 2018 @ Technical University of Valencia, Spain, prior to THIESEL

- More than 100 attendees representing academic, national lab, and industry technical leaders from around the world
- Topic Coordinators, Speakers, and Contributors from >30 different institutions:
  - United States (11):
    - General Motors, Argonne National Laboratory, Oak Ridge National Laboratory, Sandia, UMass Amherst, University of Wisconsin, University of Michigan, Oregon State University, Artium Technologies, Penn State University, Georgia Tech
  - International (21):
    - Chalmers University (Sweden)
    - University of Brighton (U.K.)
    - Technical University of Eindhoven (Netherlands)
    - Technical University of Denmark (Denmark)
    - RWTH Aachen University, University of Duisburg-Essen Technical University of Darmstadt, Siemens CD Adapco (Germany)
    - IFPEN, CORIA, University D'Orleans (France)
    - CMT-Technical University of Valencia University of Oviedo, CIEMAT (Spain)
    - University of Perugia, CNR-Istituto Motori Technical University of Milano (Italy)
    - University of New South Wales University of Melbourne (Australia)
    - KAUST (Saudi Arabia), Aramco (Saudi Arabia)

Cumulative (2010-2019)

Experimental Contributions
>75 measurements/diagnostics from >20 institutions

Modeling Contributions
>40 institutes have submitted ECN cases

64 Publications in ScienceDirect referencing "ECN" in 2018 and 2019

38 SAE Publications referencing "ECN" in 2018 and 2019

Remaining Challenges/Barriers

Advanced high efficiency engine strategies will continue to rely on direct injection making the study of injector internal dynamics and flows as well as rate-of-injection and spray mixing and combustion characteristics critical to engine research

- The influence of internal and near-nozzle flows on spray plume dispersion, plume-to-plume interactions, and spray collapse must be clarified to support better design of mixture preparation for all combustion strategies relying on direct-injection
- A database characterizing liquid penetration and spray-wall interactions under controlled conditions is needed to support accurate simulation of wall-wetting and fuel-film formation – and subsequent design to minimize cold-start/re-start emissions
- Designers need to understand how next generation of high-pressure, short-injection-duration fuel systems can enhance control of mixture preparation that is needed for stratified operation
- Wall wetting or liquid in bulk charge creates fuel-rich, PM-forming combustion and is not completely explained by fuel physical properties (distillation curve) or soot metrics (PMI index)
- Wall film thickness is difficult to quantify, well-controlled soot measurements from wall films are challenging but necessary, soot chemistry may vary depending on engine operating conditions
- Establishing and expanding quantitative databases with injector, spray, combustion and pollutant formation datasets that inform model development is essential.
- Robust quantitative mixing measurements remain challenging, but are essential for progress in CFD

Proposed Future Research (FY19-FY21)

- Gasoline direct-injection activities
  - Quantify soot in spark/laser ignited gasoline sprays in vessel, compare to engine data (FY19)
  - Explore effectiveness of multiple injections to limit liquid penetration for reduced soot from wall wetting but also to understand bulk gas and droplet mixing (FY19)
  - 1D DNS in CONVERGE of wall film with flame interaction (FY19)
  - Further development of line-of-sight absorption diagnostic for mixture fraction imaging (FY20)
  - Diagnostic development for characterizing wall-impinging sprays (FY20-21)
  - Extend soot extinction imaging of soot in films for quantitative measurements (FY21)
  - ECN: Establish and compile a database characterizing liquid penetration and spray-wall interactions under controlled conditions to support CFD efforts and designs to minimize cold-start/re-start emissions (FY19-FY21)
- Diesel research activities
  - Investigate sources of plume dispersion and initial near nozzle ROI transients via imaging of transient internal flows (including cavitation) using transparent nozzles (FY19)
  - Assess impacts of trans-critical spray phenomenon on the atomization, vaporization, and mixing processes under reacting and non-reacting conditions (FY19)
  - Investigate cool-flame (and cool-flame wave associated with TCI) and high-temperature ignition and flame stabilization—phenomena that remain challenging for CFD (FY20)
  - Diagnostic development for quantitative soot imaging orthogonal to wall, wall heat transfer, and wall temperature control (FY19-20)
  - Collaborative efforts toward the development of accurate PAH chemistry and soot inception models for use in CFD codes (FY19-21)

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

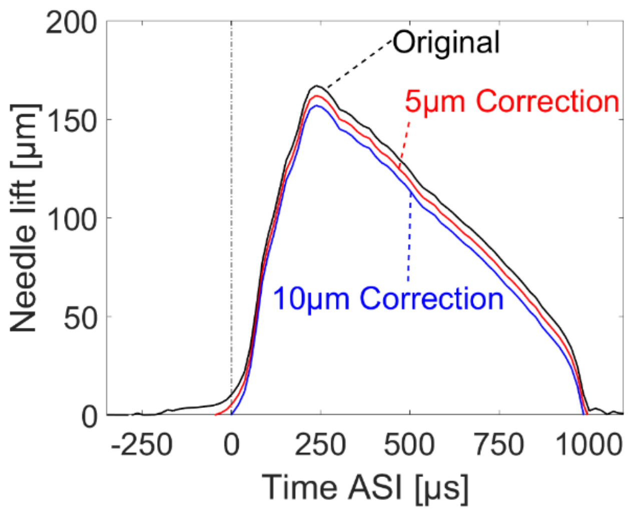
Presentation Summary

- Project is relevant to the development of high-efficiency, low-emission engines, which all use direct-injection sprays
  - Observations in controlled environment lead to improved understanding/models for engine development
  - We address specific challenges facing current injection systems as well as future concepts
- FY19 approach yields increased understanding of key phenomena
  - Quantitative, high-speed measurements of soot field in laser-ignited GDI sprays provide critical target data for model improvement
  - High-throughput facility offers unique opportunity for tomography of GDI sprays leading to better characterization of injector/injection, fuel, and ambient effects
  - Characterization of trans-critical behavior and associated impact on spray mixing is critical to inform models
- Collaboration through the ECN used as a tool to accelerate research and provide a pathway for improved CFD tools used by industry
- Future plans will continue research in gasoline and diesel sprays using unique tools and facilities

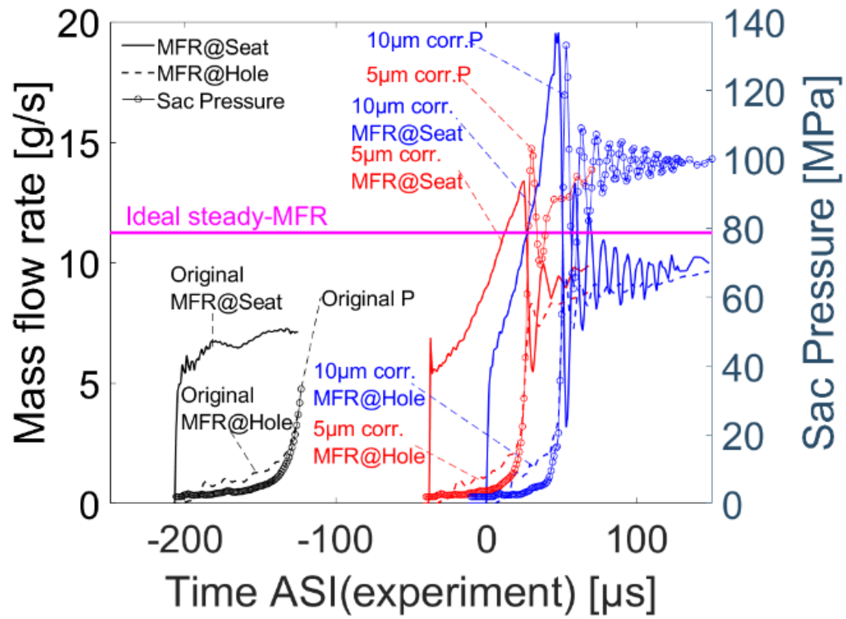
Technical Backup Slides

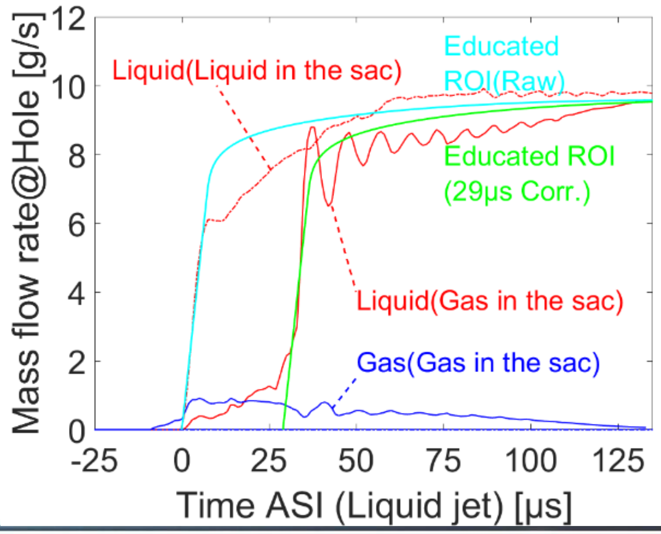
Injector deformation influences ROI at startup; models must implement correct ROI to capture early penetration behavior

- Finite element analysis performed for nozzle elasticity
- CFD simulation with needle profile correction

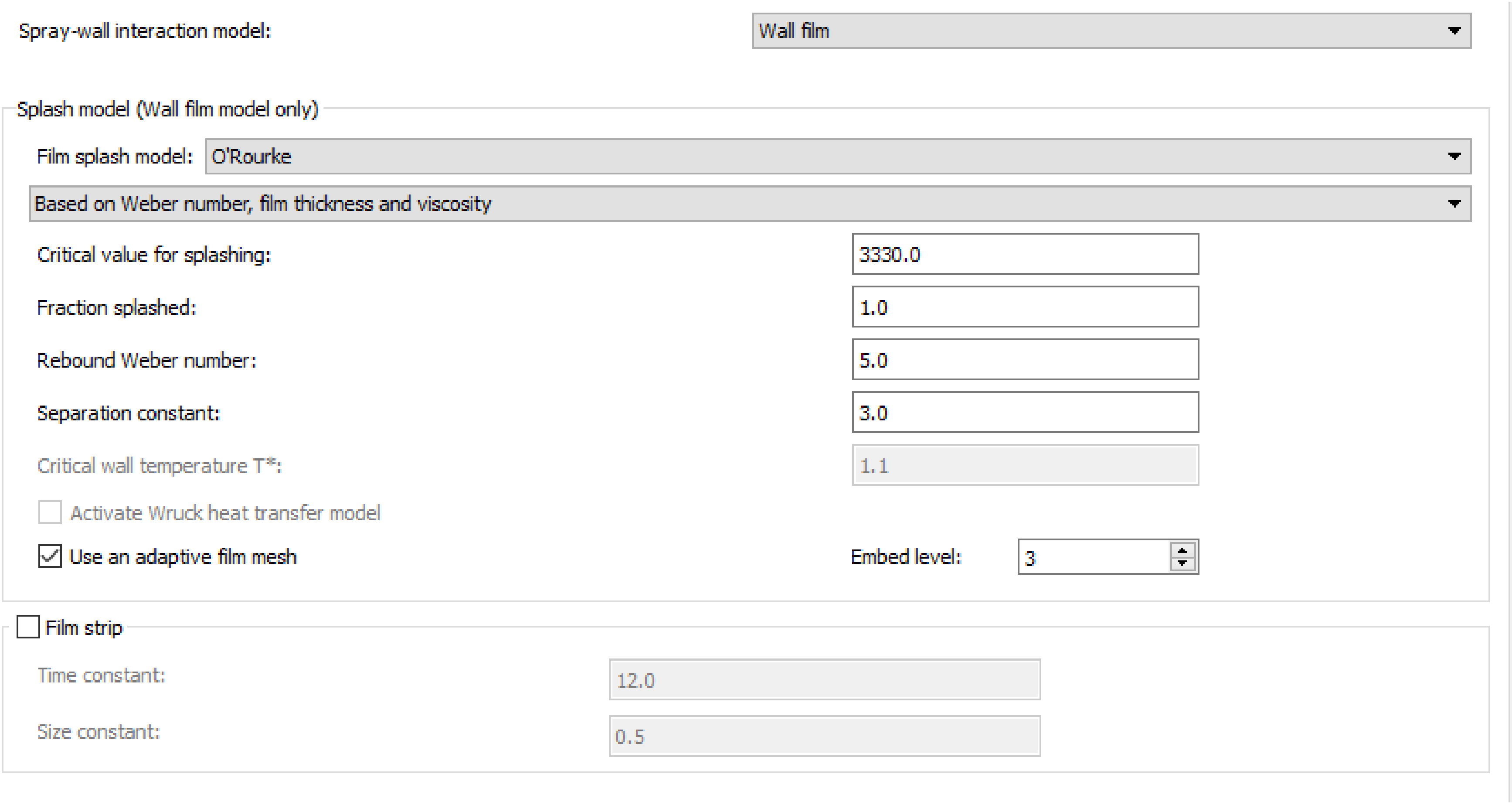


Yasutomi et al., SAE PFL, Sandia, 2019





Backup Slide: Converge Wall Model



Close collaboration and pathway to better CFD tools

Experiment

Sandia, Argonne, IFPEN, CMT, CAT, GM, Delphi, Bosch, TU/e, Ist. Motori, Mich. Tech., Meiji, Infineum, Chalmers, KAIST, Aachen, Melbourne, Brighton, Michigan, Artium

CFD codes used

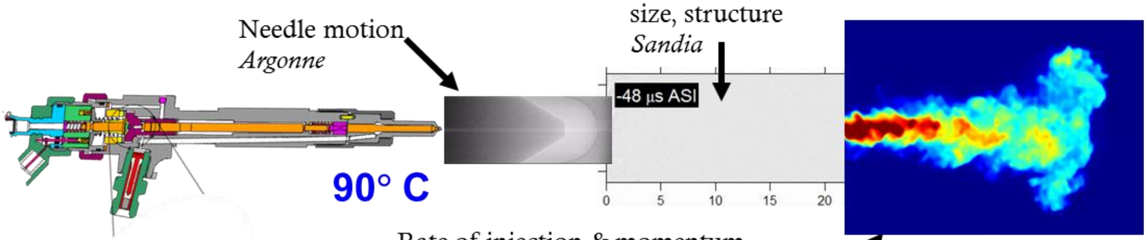
CONVERGE
Star CD
Open FOAM
KIVA
ANSYS Fluent & CFX
FORTE
RAPTOR
other research codes…

CFD approaches

RANS
LES
High-fidelity LES
Eulerian-Eulerian
Eulerian-Lagrangian
Dense fluid
many spray and combustion variants…

Modeling submissions

Sandia, Argonne, IFPEN, CORIA, KAUST, Aramco, CMT, PoliMi, Perugia, UMass, UNSW, Istituto-Motori, Oviedo, CIEMAT, Penn St., TU/e, UW-Madison, Purdue, ETH-Zurich, Aalto, Aachen, DTU, Cambridge, Georgia Tech, Chalmers, Darmstadt, Siemens, GM…



ECN organization

- Monthly web meetings
- Workshop organizers gather experimental and modeling data, perform analysis, understand differences, provide expert review
- Very tight coordination because of target conditions

Most industry use ECN data to test their CFD practices