SAND2013-4376C

Frontiers in Combustion Research, Sandia and Collaborators

Art Pontau

Deputy Director, Transportation Energy Center

Sandia National Laboratories

Livermore, CA

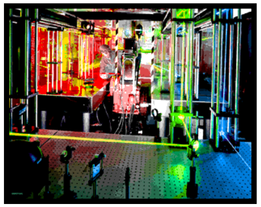
June 4, 2013

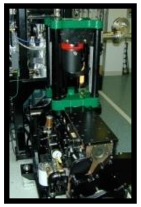
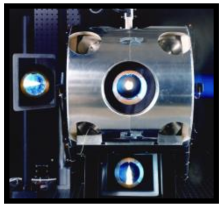
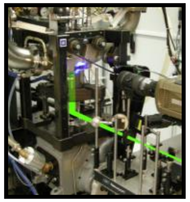
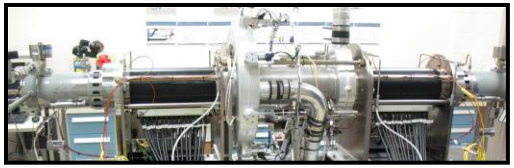
U.S. Department of Energy (DOE)
Energy Efficiency and Renewable Energy Program (EERE):
Engine Combustion Research Connects to Needs of Industry

- Mission: Provide the combustion and emission science base needed by industry to develop high-efficiency, clean engines for future fuels.
- Integral part of DOE/industry advanced engine and fuels programs.
- Sponsor is DOE Office of Vehicle Technologies
- Strong collaborations with industry, universities, and other national labs.
- 25 staff, technologists and post docs; plus visitors

Working with industry to develop the science-base for next-generation engines for future fuels.

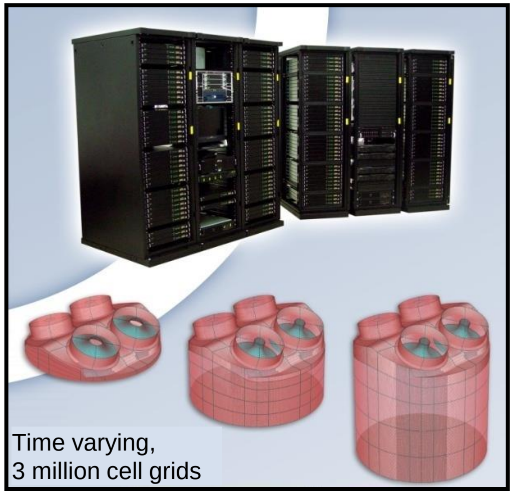
- Advanced combustion strategies for enabling high-efficiency engines
  - SI, Diesel, and Low-Temperature Combustion (HCCI, PCCI, …)

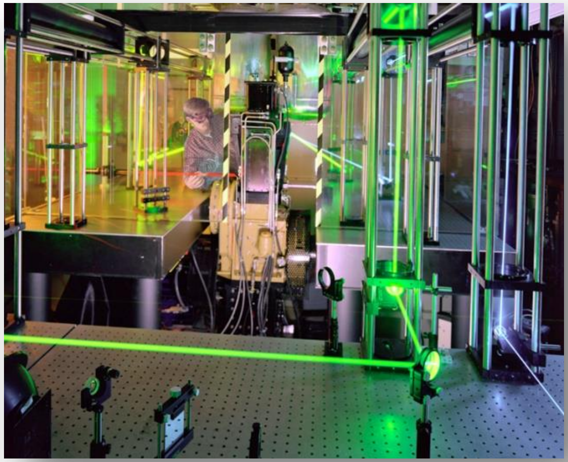
- Future fuels
  - adv. Petroleum
  - bio-fuel
  - gas-to-liquid
  - oil sand and shale
  - natural gas & H_2

- Next generation computational tools
  - massively parallel machines

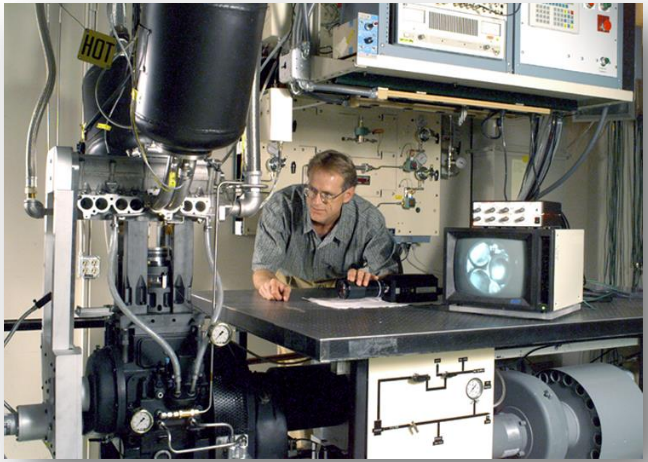


Engines Research Focuses on Improving Efficiency, Reducing Emissions

Heavy-Duty Diesel Engines

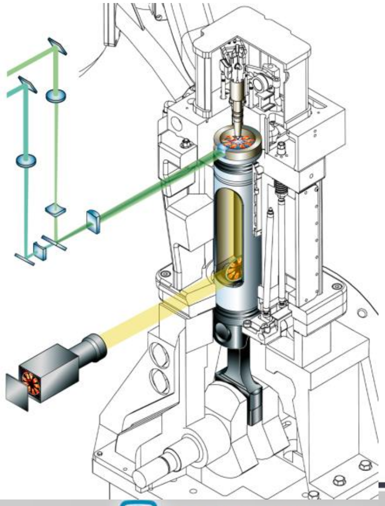


Alternative Fuels



Gasoline Engines

- Partnerships with industry characterize the program
- Laser-based optical diagnostics.
- Optically accessible, realistic engine conditions
- Simulation/modeling



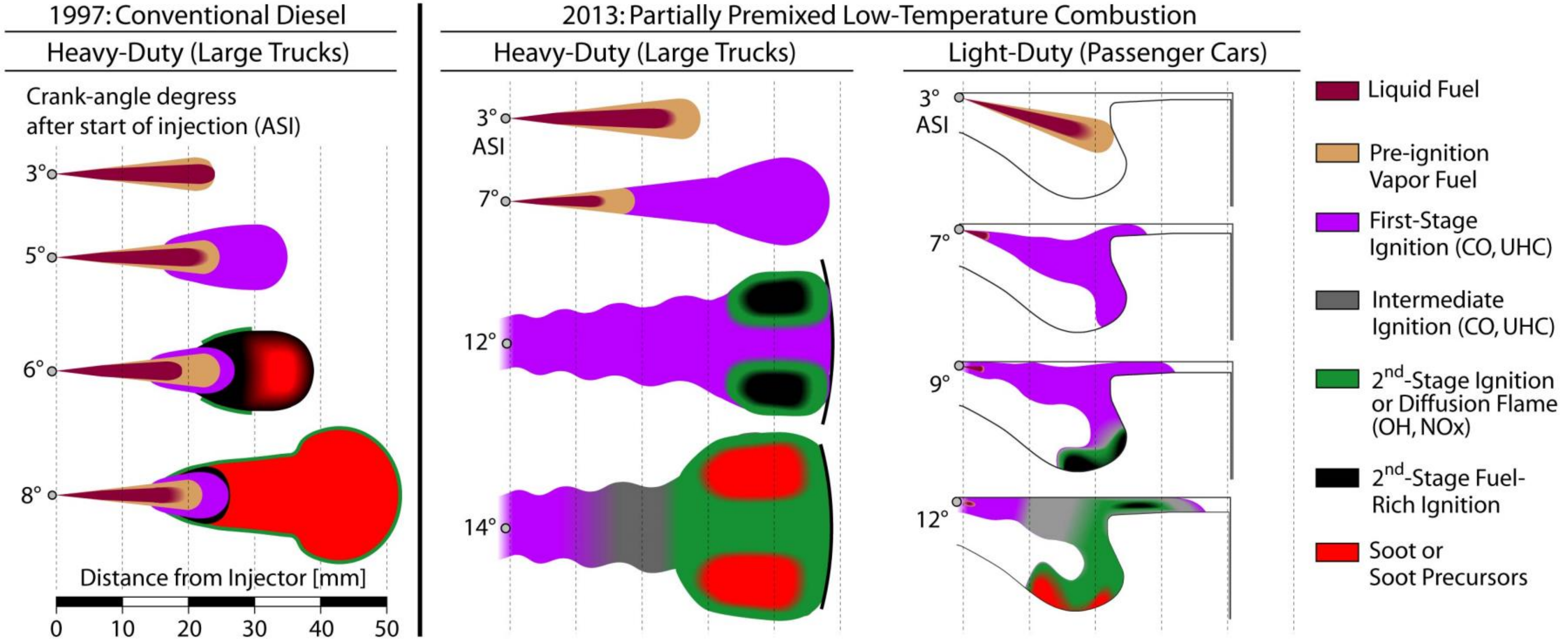
Newly developed conceptual model for diesel LTC combustion describes in-cylinder processes *(SNL-Musculus)*

Motivation:

– 1997: Conventional diesel conceptual model (left) is foundation of understanding for industry
– 2013: Need new conceptual model to aid development low-temperature combustion (LTC)

Impact of new LTC conceptual model:

– Describes LTC operating condition effects on spray, mixing, combustion, efficiency, emissions
– Supported by years of optical data and simulations in heavy-duty (left) and light-duty (right)



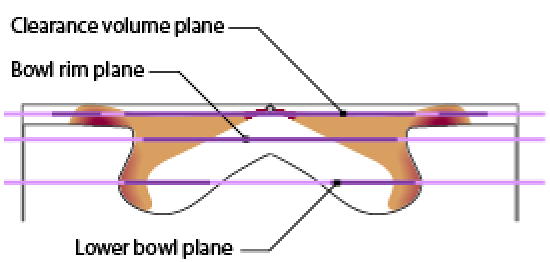
Diesel LTC fuel-air distribution measurements clarify the mixing processes critical to operation (SNL-Miles)

Motivation:

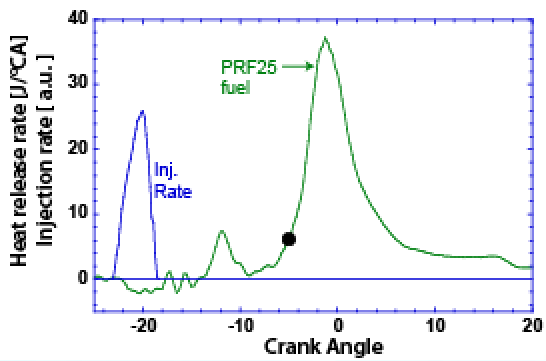
- Dominant sources of UHC and CO at light-load from LTC combustion include crevices and over-lean mixture formation
- First-of-kind, quantitative fuel-air distribution measurements in light-duty engines required to understand and verify UHC and CO sources, and provide model validation data for challenging swirl and wall interaction conditions

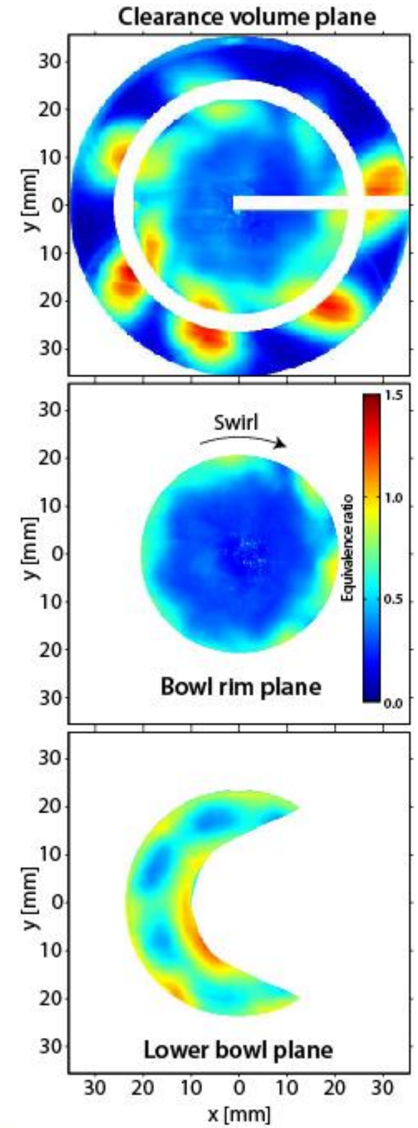
Results on sources of UHV and CO:

- Substantial over-lean mixture exists in the upper-central regions of the bowl and clearance volume -
- Despite MBT timing, fuel penetrates to near the cylinder walls and will be forced into the ring-land crevice during high temperature heat release
- Fuel-rich mixtures persist within the squish volume with<ϕ> < 2



Darkened areas of the laser sheet indicate visible regions





Planar-imaging thermometry shows the source of thermal stratification critical to HCCI operation (SNL-Dec)

Motivation:

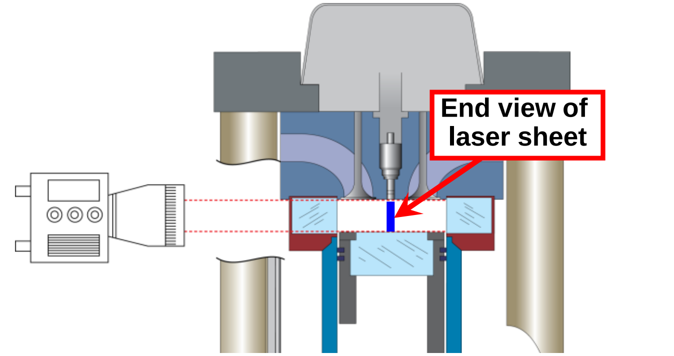
- Natural thermal stratification (TS) in an HCCI engine enables much higher loads
- Increasing TS has a high potential to extend the high-load limit and/or increase efficiency.
- An understanding of TS is required to realize potential

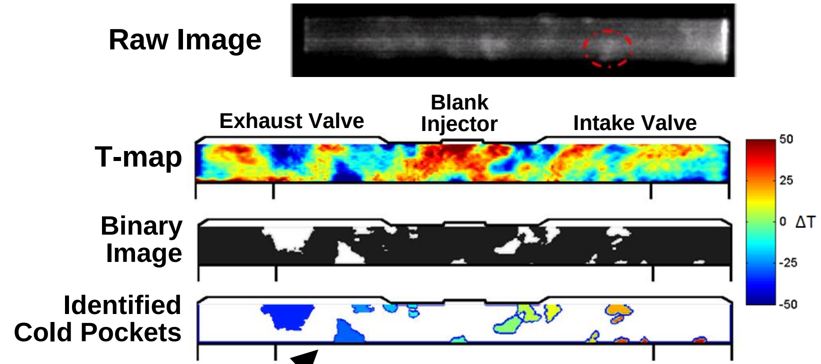
Method:

- Establish side-view technique to obtain thermal images of bulk gas & boundary layer simultaneously.

Accomplishments:

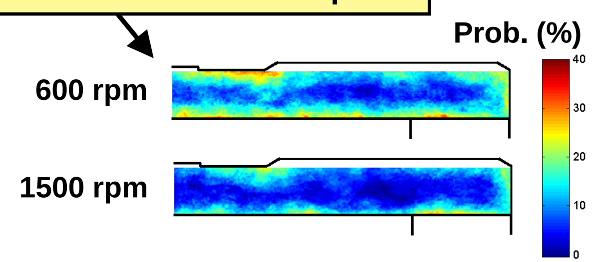
- TS occurs as cold regions dispersed intermittently throughout the otherwise-hot bulk-gas.
  - Develops progressively during latter part of compression stroke.
- TS is turbulent in nature ⇒ no evidence of flows transporting cold wall-gas into central region.
- TS results from turbulent structures of cold gas extending from the walls into the bulk gas.
- Amount of TS varies with operating conditions.





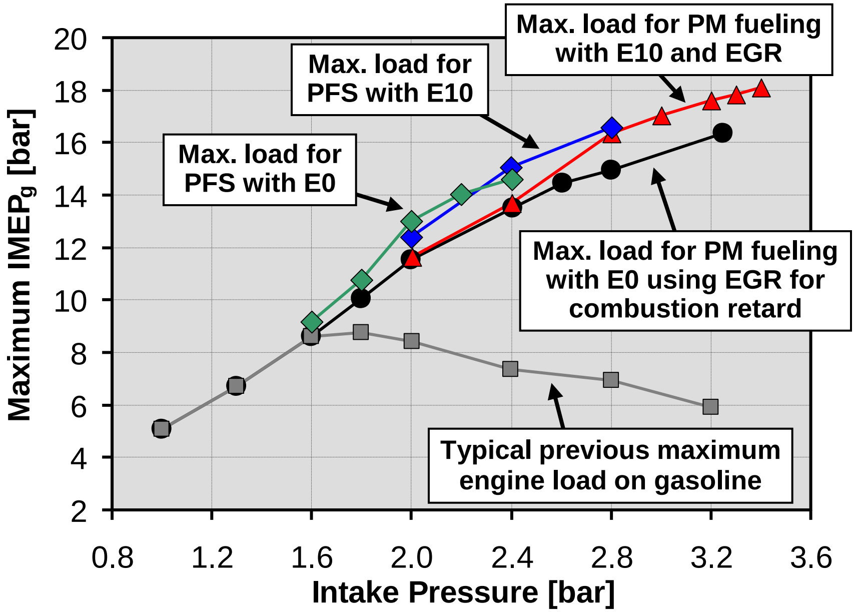
Almost all cold "pockets" are turbulent structures attached to firedeck or piston top.

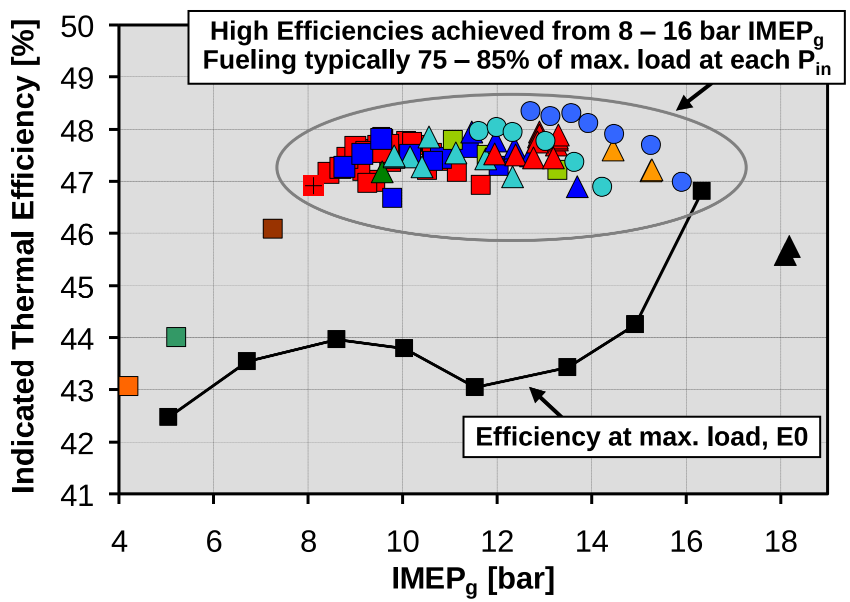
Probability of cold structures increases with decreased speed.



Boosting and fuel stratification using E10 substantially increase HCCI load range and efficiency (SNL-Dec)

- **Previously:** Improved understanding of boosted HCCI enabled higher loads on conventional 87-octane gasoline (E0).
  - **Load limit = 16 bar IMEP$_g$**, premixed (PM)
- **E10**: Blend 10% ethanol with gasoline.
  - Reduces EGR requirement with boost.
  - More air in cylinder allows higher fueling.
  - <u>**Load limit = 18 bar IMEP$_g$**</u>, premixed
- **Partial Fuel Stratification (PFS)**
  - Gasoline (E10) becomes ϕ-sensitive with boost allowing PFS to reduce heat release rate.
  - Provides higher loads without knock at lower boost pressure.
- **Thermal efficiency of 47 – 48% over 8 to 16 bar IMEP$_g$ range.**

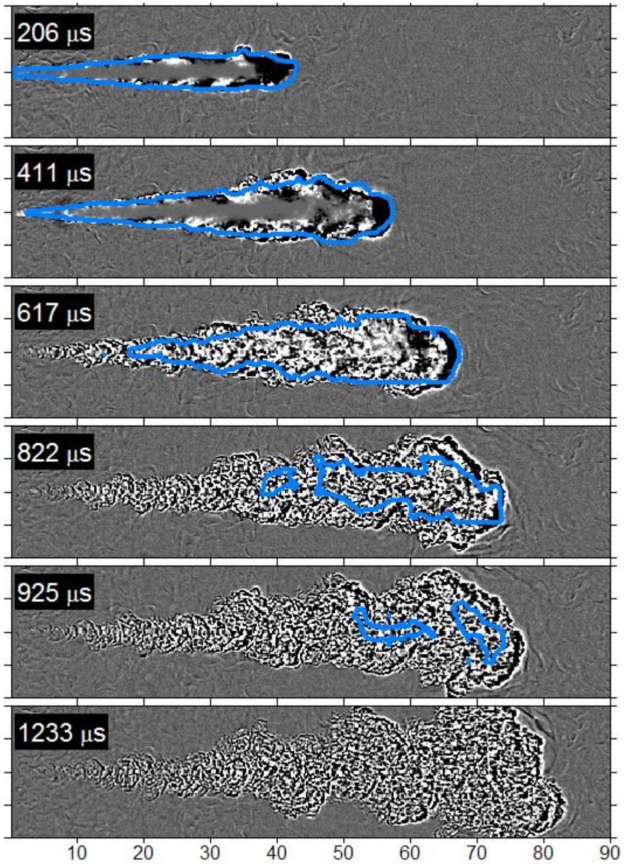




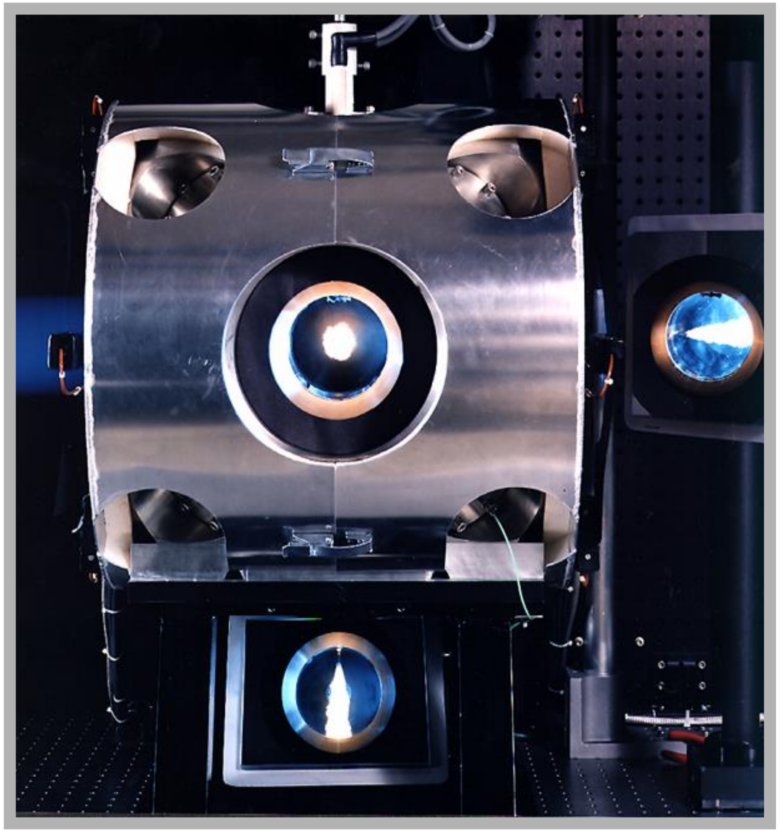
The role of spray combustion research for high-efficiency engines.

- Future high-efficiency engines use direct injection.
  - Diesel, gasoline direct injection, partially-premixed compression ignition
- Complex interactions between sprays, mixing, and chemistry.
  - Two-phase system, including multiple injections
  - Spray-induced mixture preparation
  - Complicated internal flows within injectors
- Optimum engine designs discovered only when spray modeling becomes predictive.
  - Predictive modeling shortens development time and lowers development cost.
  - Makes efficient engines more affordable.
- Relevant to EERE Advanced Combustion Engine research and development goals.

Schlieren: vapor boundary
BLUE: liquid boundary



Experimental approach utilizes well-controlled conditions in constant-volume chamber.



- Well-defined ambient conditions:
  - 300 to 1300 K
  - up to 350 bar
  - 0-21% O_2 (EGR)
- 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.

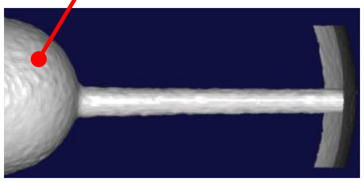
Objectives/Milestones

- Aid the development of computational models for engine design and optimization (ongoing).
  - Lead an experimental and modeling collaboration through the Engine Combustion Network with >100 participants (http://www.sandia.gov/ECN)
  - Target conditions specific to low-temperature diesel and DI gasoline.
    - ECN activities focus on quantification, standardization, leveraging, detailed analysis.
    - Provides a pathway from experimental results to more predictive CFD modeling.
    - Activities, progress, and future directions listed under ECN2 Workshop proceedings.
    - Represents major advances in terms of diagnostics, modeling tools, and so forth.
- (1) Expand datasets to a larger range of conditions for more extensive model evaluation, including
- (2) Apply quantitative soot diagnostics in optically thick diesel sprays, providing opportunity for needed improvement in PM predictions.
- (3) Evaluate liquid/vapor penetration and plume-plume interactions in DI gasoline sprays, forming unique model-target dataset.

ECN collaborative research at specific target conditions

Injector

90° C, 1500 bar

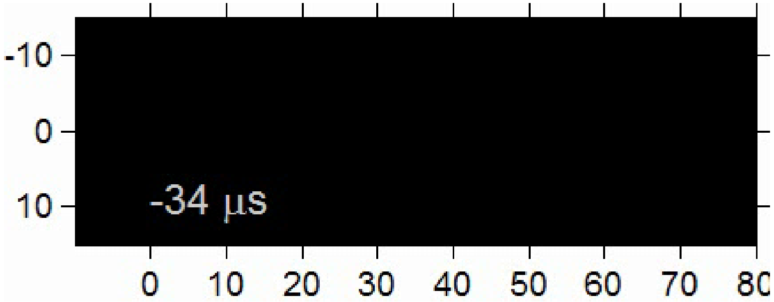


Internal nozzle geometry

Ambient

900 K, 60 bar

Spray A

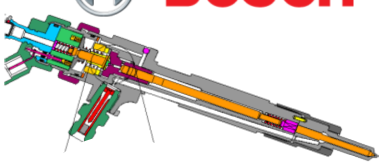


Other defined targets:

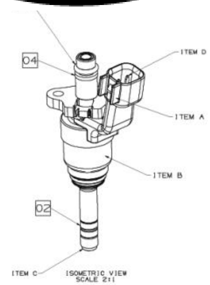
- Spray H (baseline n-heptane)
- Spray B (3-hole version of Spray A).
- Gasoline DI and engine flows.

- Opportunity for the greatest exchange and deepest collaboration.
  - Understanding facilities/boundary conditions.
  - Understanding diagnostics and quantification.
  - Standardize methodologies for post-processing.
- Leverages the development of quantitative, complete datasets.
  - Unique diagnostics to build upon past understanding.
  - Moves from “qualitative” to “quantitative”.
  - Sharing results/meshes/code/methods saves time and effort.
- Methodology now applied to parametric variants about Spray A.

BOSCH



DELPHI



Measurements to date at Spray A conditions

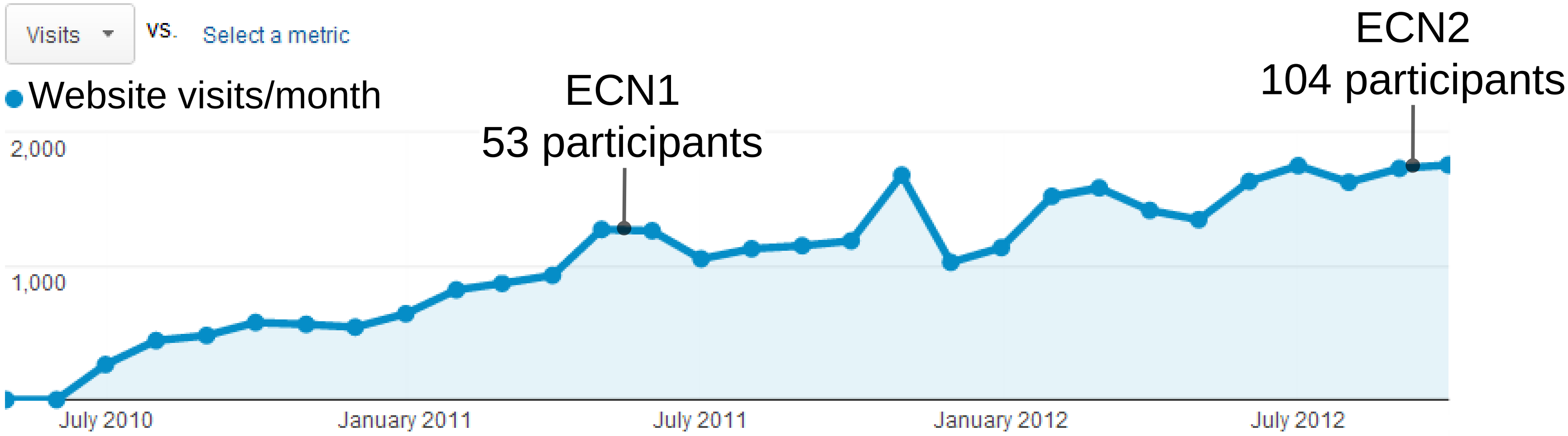
26 types of experiments

10 different international institutions

Quantity	Experiment	Contributors (Inst. and/or person)
Gas T distribution	fine-wire TC, variable diameter TC	CAT, CMT, Sandia, IFPEN, TU/e, KAIST, Chalmers
Nozzle internal temperature	thermocouple	Sandia, CAT, IFPEN, CMT, TU/e, Aachen, Chalmers
Nozzle surface temperature	laser-induced phosphorescence	IFPEN (Louis-Marie Malbec, Gilles Bruneaux)
Nozzle geometry	x-ray tomography	CAT (Tim Bazyn), Infineum (Peter Hutchins)
Needle movement/noz. geom.	phase-contrast imaging	Argonne (Alan Kastengren, Chris Powell)
Nozzle geometry	silicone molds	CMT (Raul Payri, Julien Manin)
Nozzle exit shape	optical microscopy, SEM	Sandia (Julien Manin, Lyle Pickett), TU/e
Mass rate of injection	bosch tube method	CMT, KAIST
Rate of momentum	force piezo	CMT, Sandia, CAT
Total mass injected	gravimetric scale	CMT, Sandia, IFPEN
Nozzle Cd, Ca	momentum + mass	CMT, Sandia
Liquid penetration	Mie scatter	IFPEN, Sandia, CMT, CAT, TU/e
Liquid penetration	Diffused back illumination (DBI)	Sandia, CMT, IFPEN, TU/e
Liquid optical thickness	laser extinction	Sandia (Julien Manin, Lyle Pickett)
Liquid structure	long-distance microscopy	Sandia, CMT (Julien Manin, Lyle Pickett)
Liquid vol. fraction (300 K)	x-ray radiography extinction	Argonne (Alan Kastengren, Chris Powell)
Vapor boundary/penetration	schlieren / shadowgraphy	Sandia, IFPEN, CAT, CMT, TU/e
Fuel mixture/mass fraction	Rayleigh scattering	Sandia
Velocity (gas-phase)	PIV	IFPEN (L.-M. Malbec, G. Bruneaux, M. Meijer)
Ignition delay	high-speed chemiluminescence	Sandia, CAT, CMT, IFPEN, TU/e
Lift-off length	OH or broadband chemilum.	Sandia, IFPEN, CAT, CMT, TU/e
Transient lift-off/ignition	intensified OH chemiluminescence	Sandia, IFPEN, CAT, CMT, TU/e
Pressure rise/AHRR	high-speed pressure	Sandia, IFPEN, TU/e
Soot luminosity/Radiation	high-speed luminosity imaging	Sandia, IFPEN, CAT, CMT, TU/e, DTU
Soot volume fraction	laser-induced incandescence, laser extinction, DBI	IFPEN/Duisberg-Essen, Sandia (Scott Skeen)

Past
FY13

Workshops organized with voluntary participation (for ECN2: 8 experimental, 16 modeling teams)

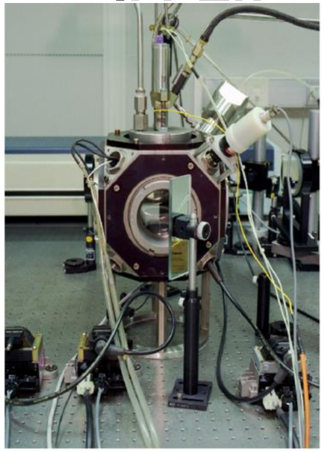


Organizers facilitate side-by-side comparison and analysis to provide an expert review of the current state of the art for diagnostics and engine modeling:

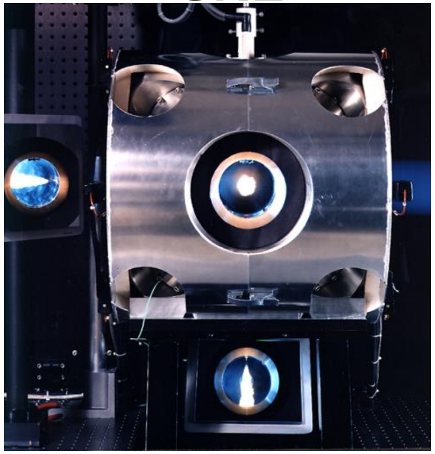
- ECN2 overall organization:
  - Gilles Bruneaux (IFPEN), Lyle Pickett (Sandia)
- Internal Nozzle Flow
  - Chris Powell (Argonne), David Schmidt (UMassAmherst), Marco Arienti (Sandia)
- Spray Development and Vaporization
  - Julien Manin (Sandia) , Sibendu Som (Argonne), Chawki Habchi (IFPEN)
- Mixing and Velocity
  - Louis-Marie Malbec (IFPEN), Gianluca D'Errico (Pol. Milano)
- Ignition and Lift-off Length
  - Michele Bardi (CMT), Evatt Hawkes (UNSW), Christian Angelberger (IFPEN)
- Soot
  - Emre Cenker (Duisburg/IFPEN), Dan Haworth (Penn St.)
- Gasoline Sprays
  - Scott Parrish (GM)
- Engine Flows
  - Sebastian Kaiser (Duisburg-Essen)

Ignition and lift-off length measurements are consistent for different types of HP-HT facilities.

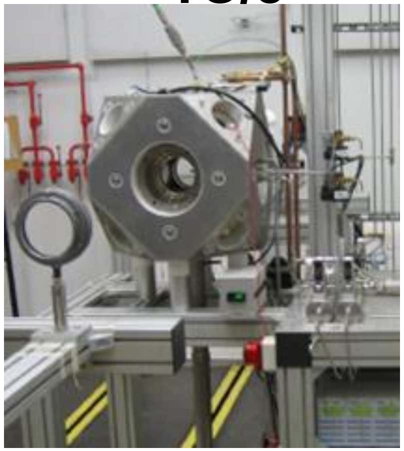
IFPEn



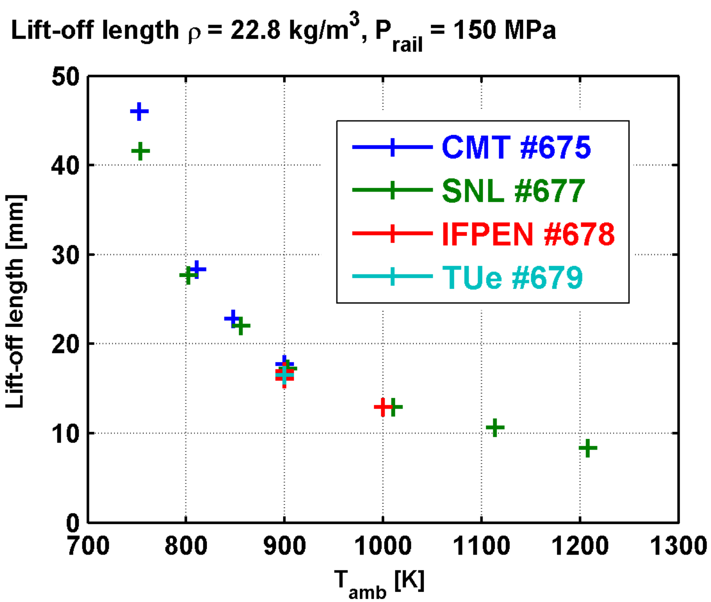
SNL

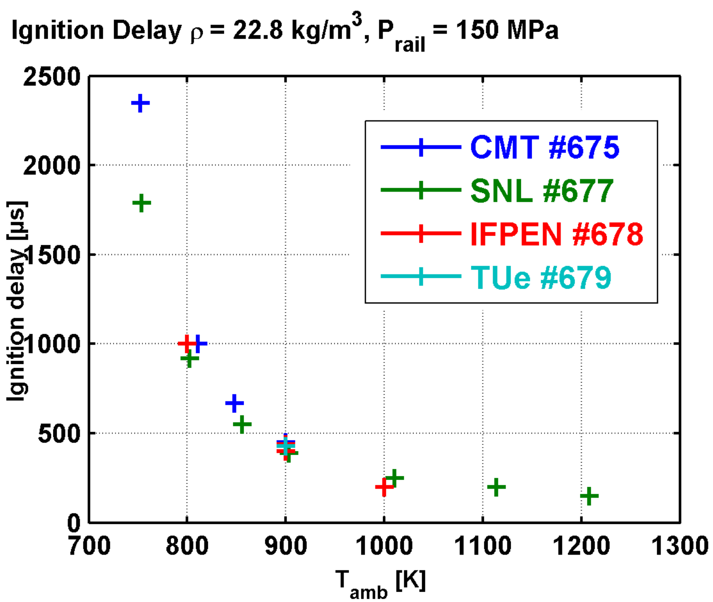


TU/e



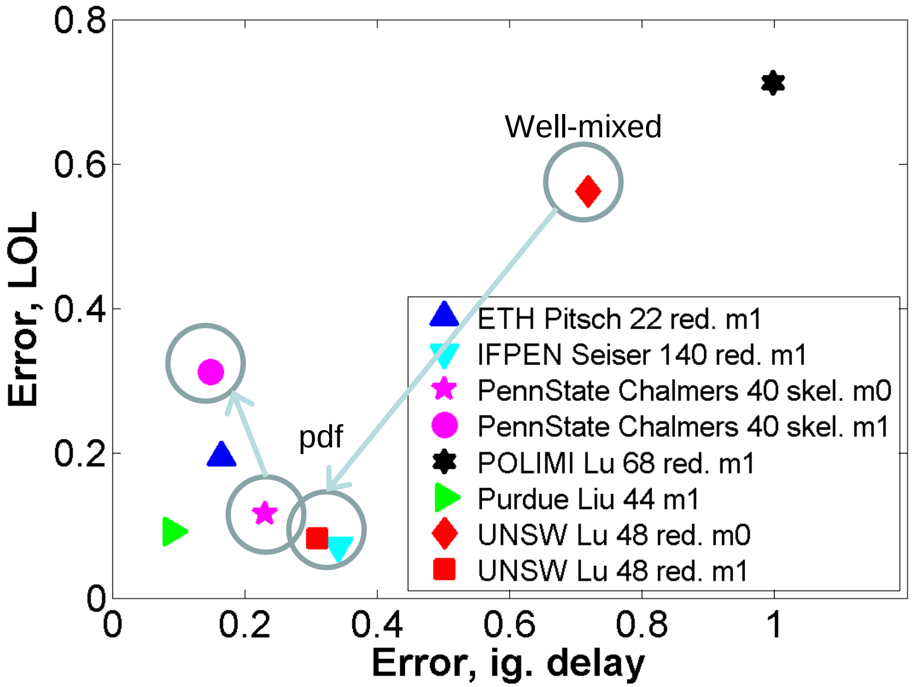
CMT



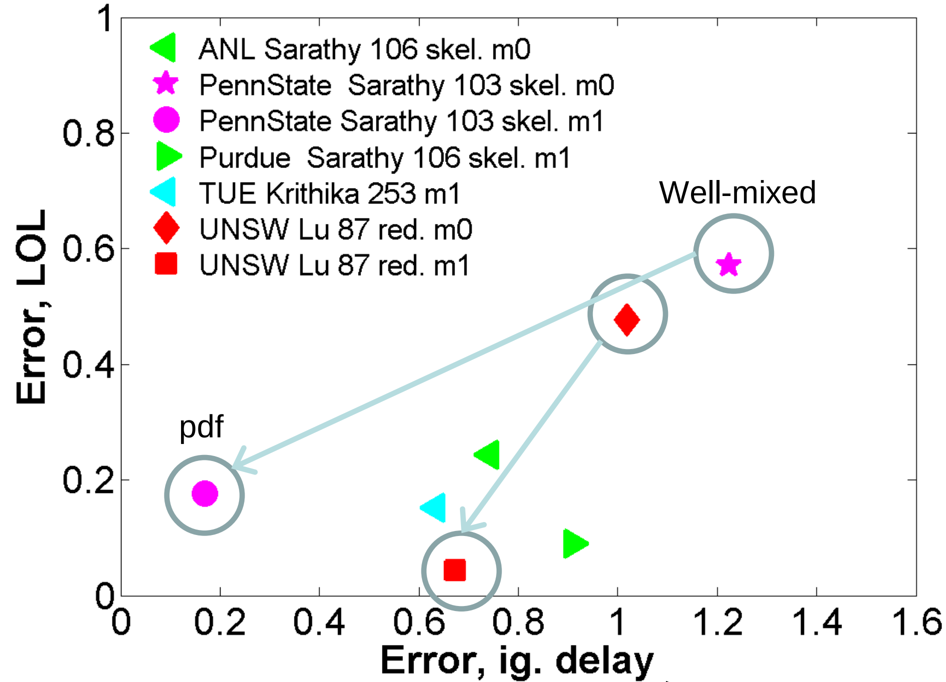


ECN2 parametric variations show modeling improvement, but no superior combustion model.

C_7H_{16}, 21% O_2, 14.8 kg/m^3, 150 Mpa



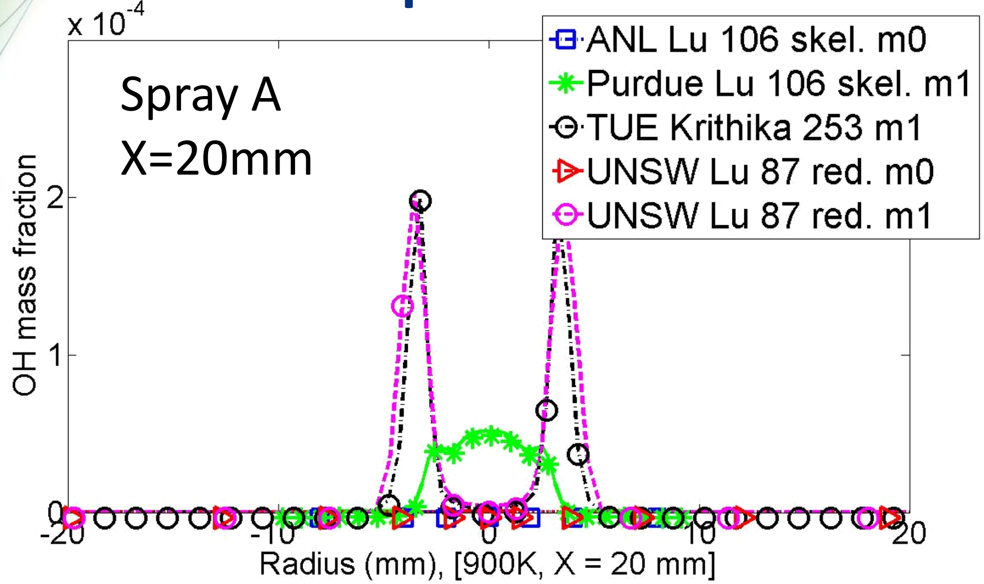
$C_{12}H_{26}$, 15% O_2, 22.8 kg/m^3, 150 Mpa

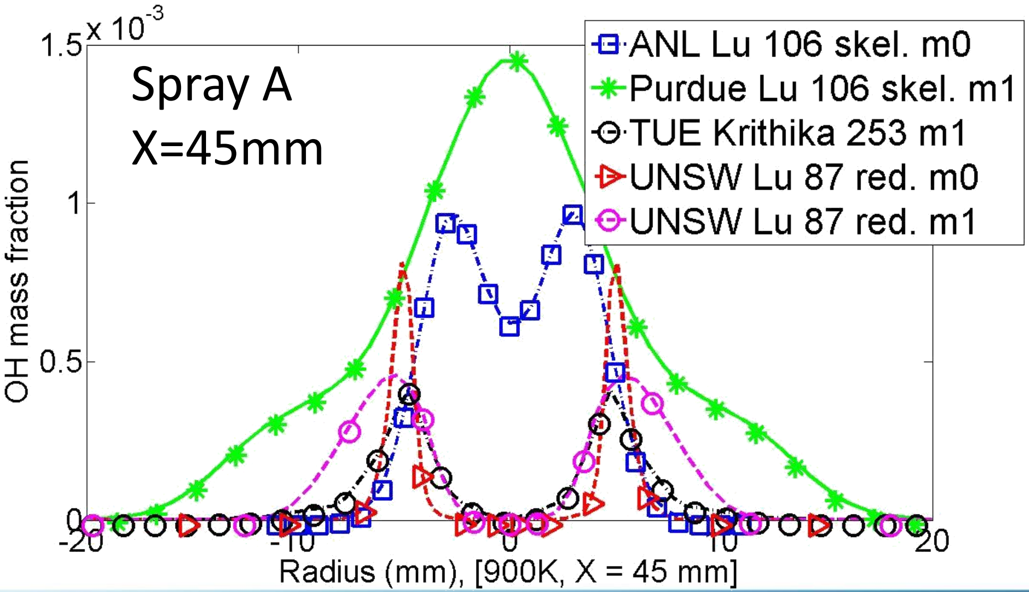


No ignition at 900 K at ECN1 !

- Difficult to achieve predictive ignition delay and lift-off length.
  - Lift-off length predictions better than ignition delay.
  - Predictions better for n-heptane than n-dodecane.
- Serious questions remain about the chemical mechanisms and combustion models.
  - More advanced combustion models (pdf) show improvements for one set of data, but not others.
  - Errors of 20-40% could easily translate to sooting vs non-sooting sprays.

Side by side analysis reveals differences in models, and points to the need for further experiments.



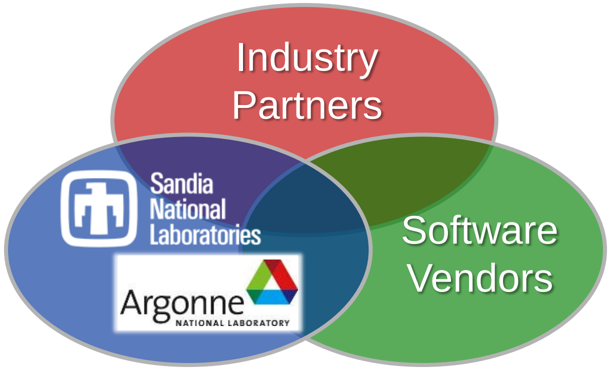


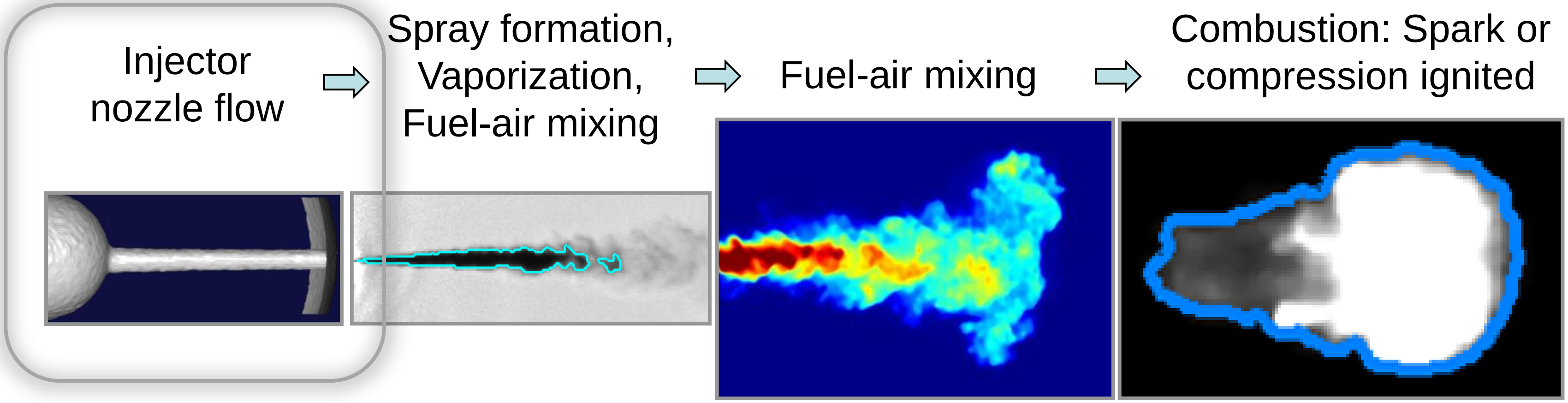
- Lift-off length:
  - Expt: 17.5 mm
  - ANL: 22.8 mm
  - Purdue: 20.3 mm
  - Tue: 18.1 mm
  - UNSW m0: 27.0 mm
  - UNSW m1: 16.8 mm

- Similar lift-off length but very different OH profiles.
- ECN experimental participants plan to perform planar OH measurements.

A proposed
Spray Combustion Consortium (SCC)

“Delivering Experimentally-Validated, Predictive Nozzle Flow Models and Understanding”





Overview of the proposed consortium

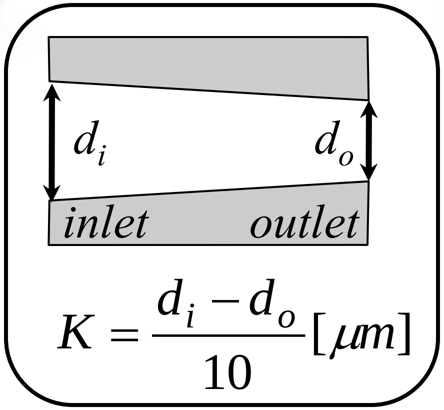
- An industry funded consortium enabling highly leveraged outcomes.
- Primary outcomes:
  - Validated nozzle flow models that couple to spray/combustion models
  - New understanding of nozzle flows
- Partners: Industry, software vendors, and key national labs in the field.
  - Team provides direct path from understanding to validated models.
- Major benefits to partners:
  - Multi-year lead-time in a critical technology area for future engines & injectors.
  - Firsthand understanding of the design implications
  - Comprehensive understanding of new modeling tools that are developed and a multi-year lead time with respect to their development and use.
  - A highly leveraged investment, through partner funding and use of DOE resources.
  - Access to state-of-the-art expertise, research tools, software, and a high-performance computing cluster.
  - A showcase for software vendors.
- Funding /duration: $3.6M over 3 years ~ 8 partners at $150K/year/partner.

Why now is right time to pursue internal nozzle flow research.

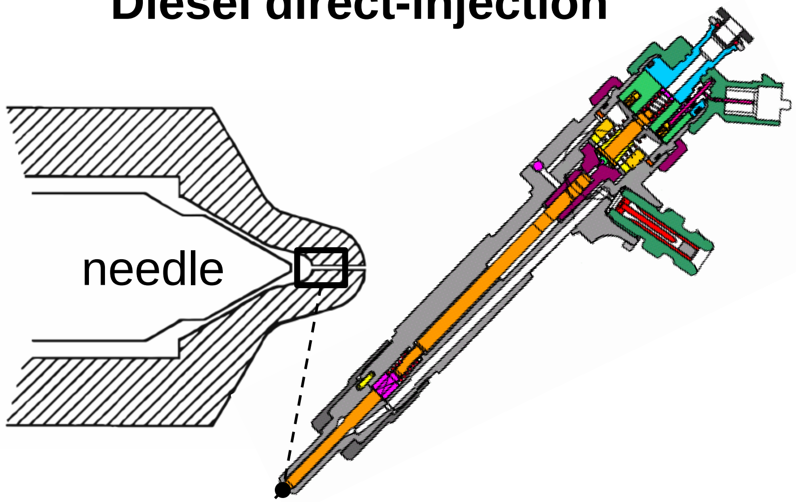
- Nozzle exit flow conditions critical to predictive spray modeling.
- Offers new combustion control possibilities through injector design.
- New enabling research capabilities are emerging:
  - Real-size, real-condition transparent nozzle research (1500 bar).
  - High-speed long-distance microscopy imaging using unique, pulsed lighting (<50 ns, >200 kHz).
  - Quantitative diagnostics for vapor fraction using x-ray beams with high spatial resolution (5 μm) - Argonne.
  - Internal nozzle geometry and needle movement characterization with unprecedented accuracy.
  - High-fidelity LES employing accurate numerical methods and unique capabilities for treating:
    - compressible flows
    - real-fluid properties
    - large-density gradients (cavitation, flash vaporization)
    - dense-fluid phenomenon, including supercritical conditions at orifice exit

Focus on critical nozzle flow processes.

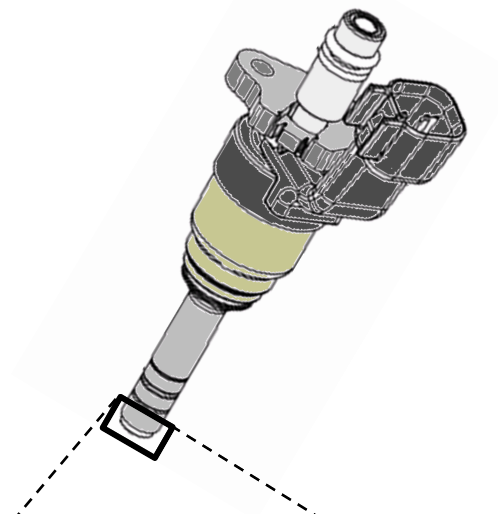
Orifice shape



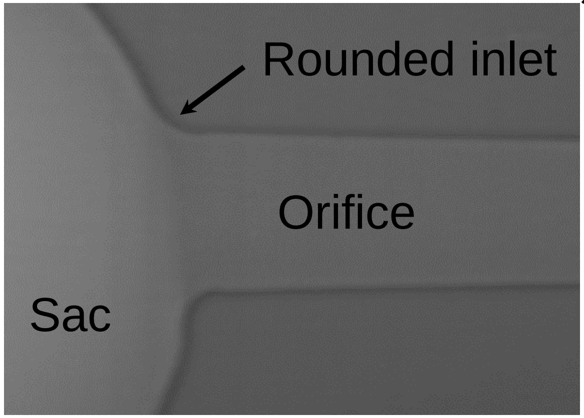
Diesel direct-injection



Gasoline direct-injection

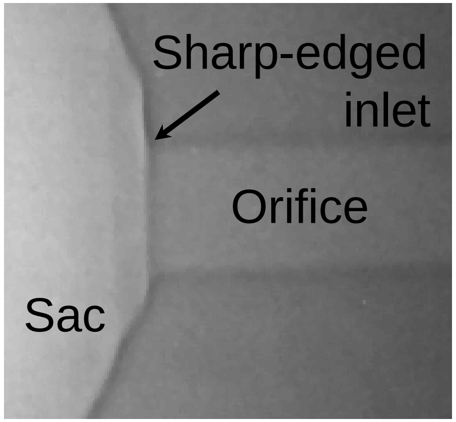


KS: K = 1.5, smooth



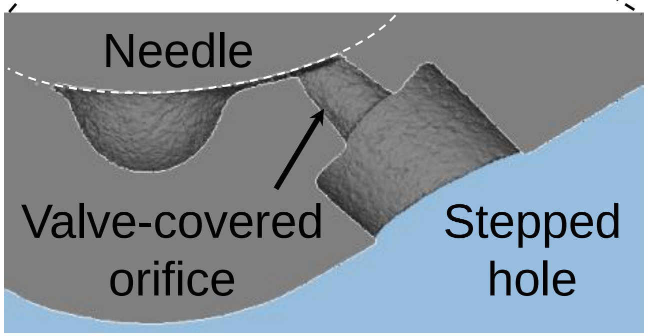
Minimal cavitation expected

K0: K = 0, sharp



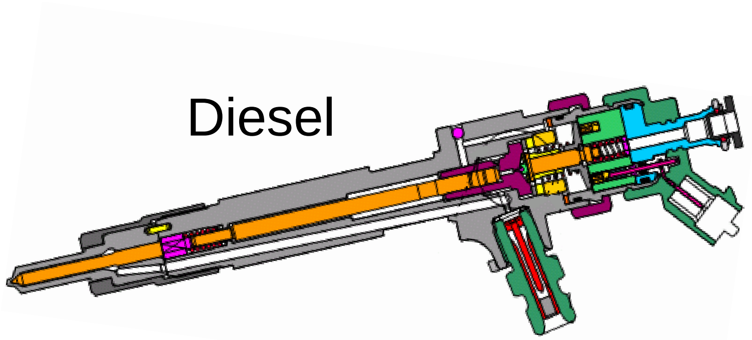
Cavitation expected

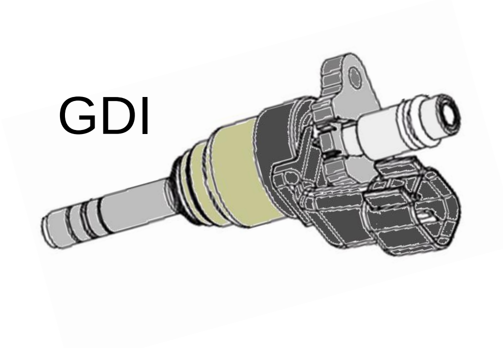
GDI: VCO stepped hole
K < 0



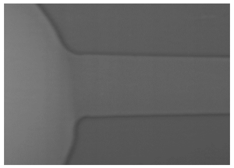
Valve interaction
Flash boiling

Experimental Scope

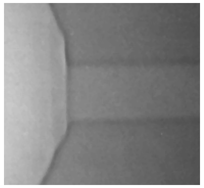




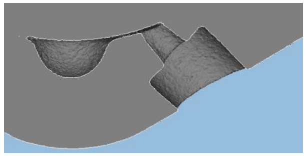
KS
(minimal cavitation)



K0
(cavitation expected)



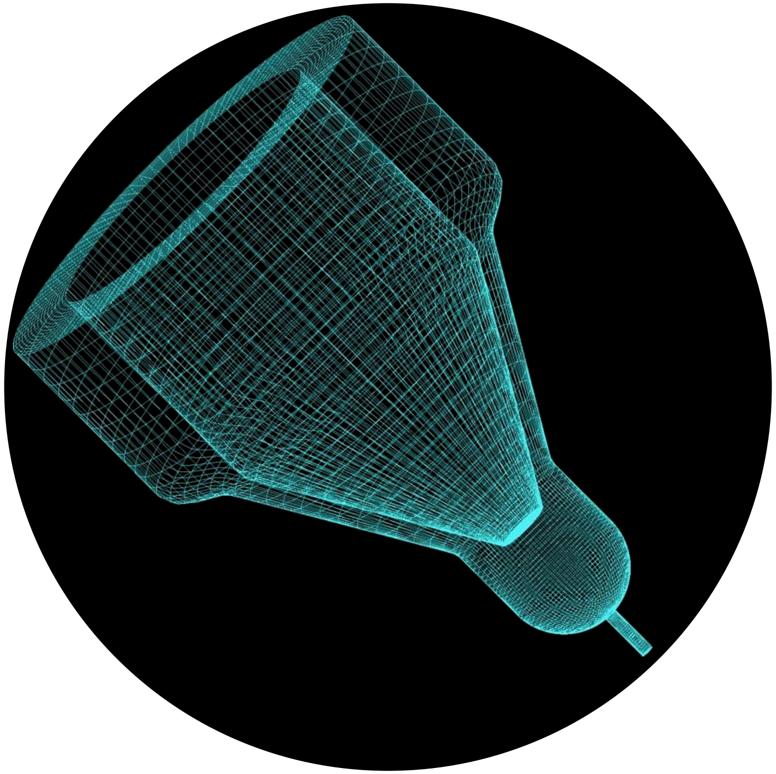
GDI
(valve interaction, flash boiling)



- Three real-scale transparent injector nozzle types with metal counterparts.
  - Metal counterparts will be Engine Combustion Network (ECN) targets, providing leveraging of all ECN work focused on downstream spray research.
- Fabricate nozzles and prepare optical (Sandia) and x-ray (Argonne) experiments.
- Develop first-of-kind database for model development/validation:
  - Characterize nozzle geometries, needle movement, flow performance, …
  - Quantification of vapor and fuel distribution inside and at the exit of nozzles

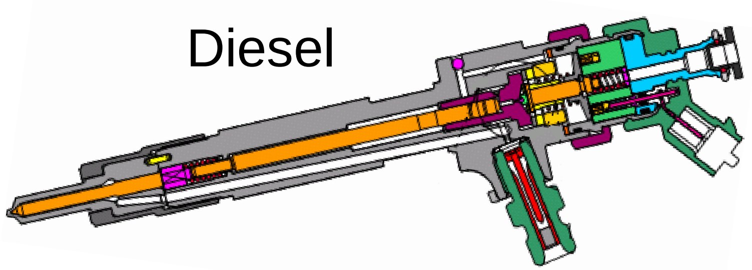
Sandia's high-fidelity LES modeling provides powerful complement to the experiments.

- Theoretical framework … (Comprehensive physics)
  - Fully-coupled, compressible conservation equations
  - Real-fluid equation of state (high-pressure phenomena)
  - Detailed thermodynamics, transport and chemistry
  - Multiphase flow, spray
  - Dynamic SGS modeling (no tuned constants)
- Numerical framework … (High-quality numeric's)
  - Dual-time stepping with generalized preconditioning (all-Mach-number formulation)
  - Staggered finite-volume differencing (non-dissipative, discretely conservative)
  - Massively-parallel
- Extensively validated, ported to all major platforms

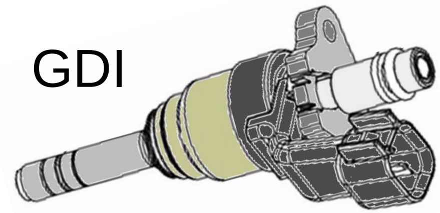


Modeling Scope

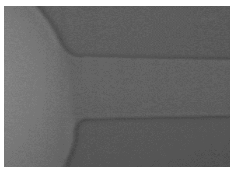
Diesel



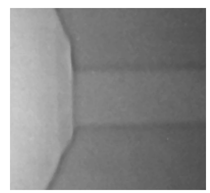
GDI



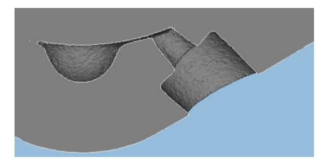
KS
(minimal cavitation)



K0
(cavitation expected)



GDI
(valve interaction, flash boiling)



- Commission computer cluster (>1000 cores) and initiate high-fidelity LES
  - Near first principles simulation (compressible flow, real fluid properties, cavitation, wall effects, flash boiling, moving geometries, geometric details).
  - Model smooth (KS) to complex (K0, GDI) nozzles
  - Extends experimental database and understanding
- Detailed LES and engineering model comparisons establish best practices
- **Software vendors develop improved engineering models for commercial codes**
  - **Release periodic updates to partners**