Optical and CFD investigation of flow and mixture formation in a DI-H2ICE

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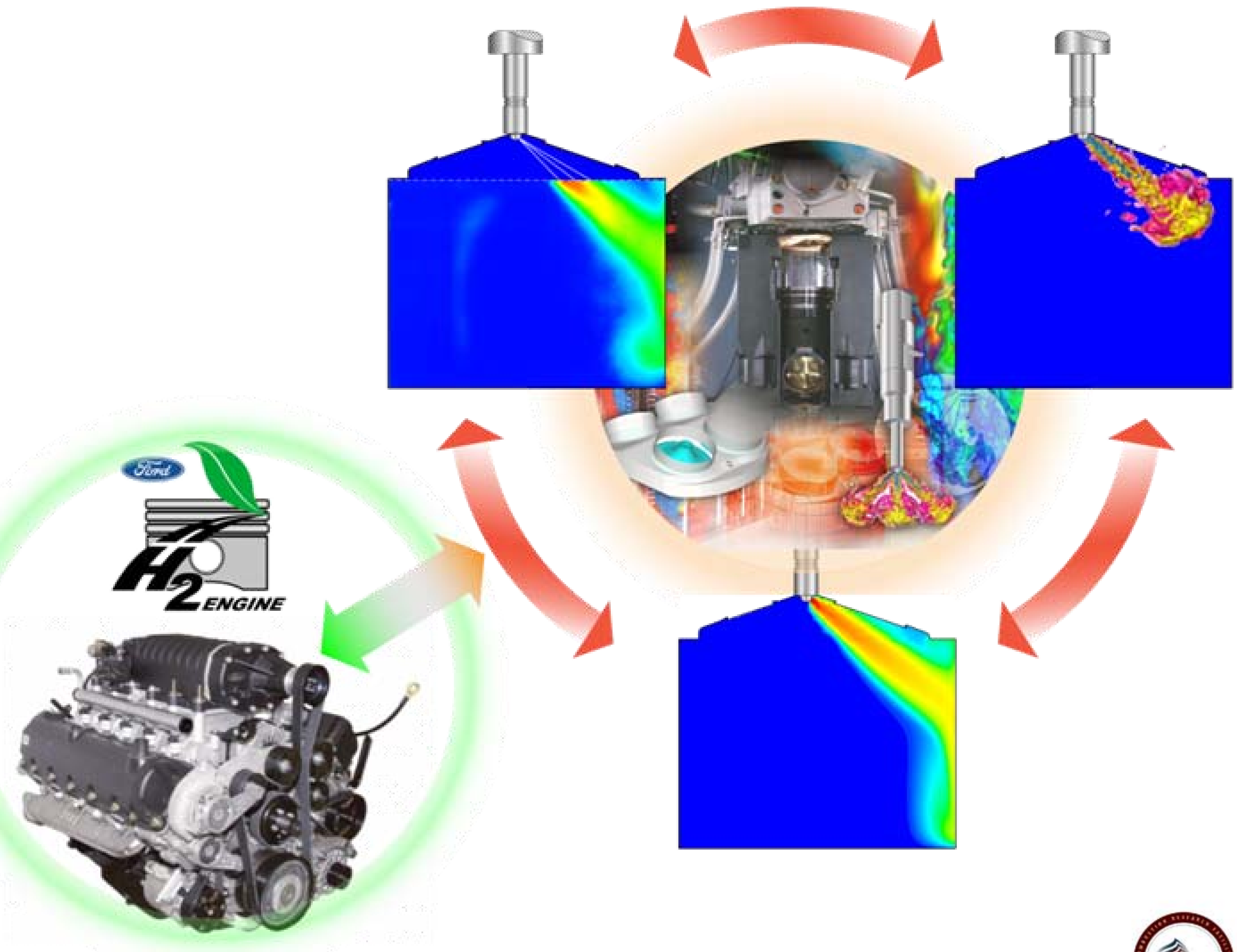
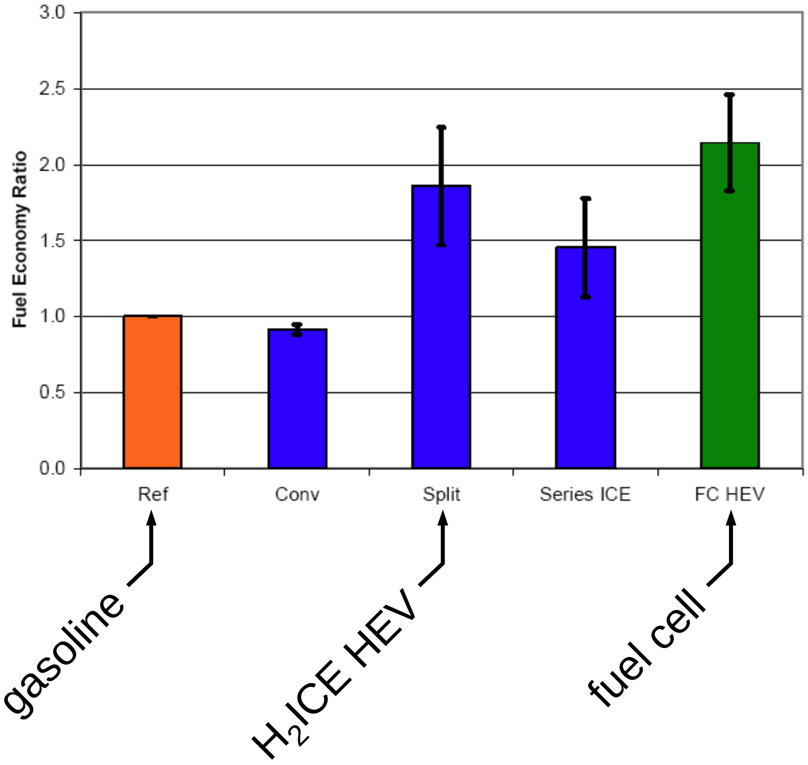


Sponsor:
DOE / OVT
Program Manager:
Gurpreet Singh

Vehicles with advanced hydrogen-fueled engines are competitive with systems based on fuel cells.

- Hydrogen engines build on existing, mass-produced, cost-effective technology.
- Advanced high-efficiency hydrogen engines are based on direct injection (DI).
- Higher power density, better efficiency, lower NOx are possible with DI.
- Relies on control over fuel-air mixing despite complex flow and short time scales

Vehicle-system modeling by ANL*



Insight into in-cylinder processes needed → Optical engine, Simulation

Data from optical engine provide physical understanding and simulation validation.

Numerical Simulation	Optical Measurements	Metal Engine
ANL, LLNL, Sandia	Sandia	Argonne Ford (not DOE funded)

- Automotive-sized optical engine
- Spatially resolved measurements of in-cylinder processes
  - Fuel distribution
  - Flow field
  - Combustion

$\left.\begin{array}{l}\text{Fuel distribution}\\ \text{Flow field}\end{array}\right\}$ Mixture formation

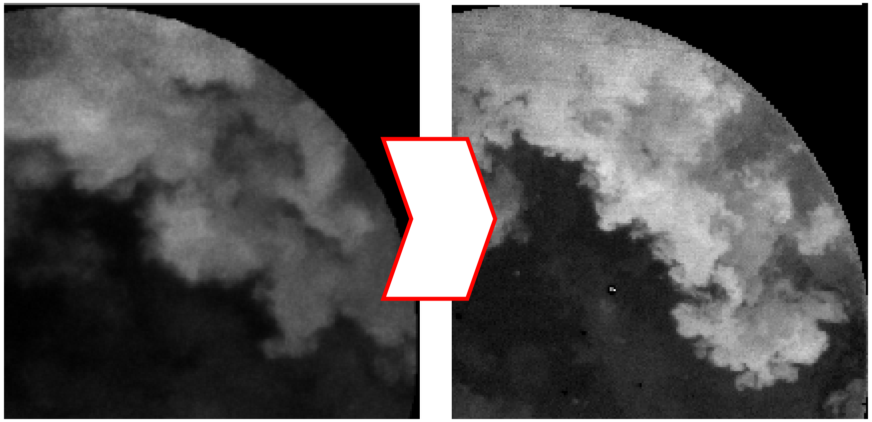
Goals:

Fundamental understanding of in-cylinder processes in H2ICEs

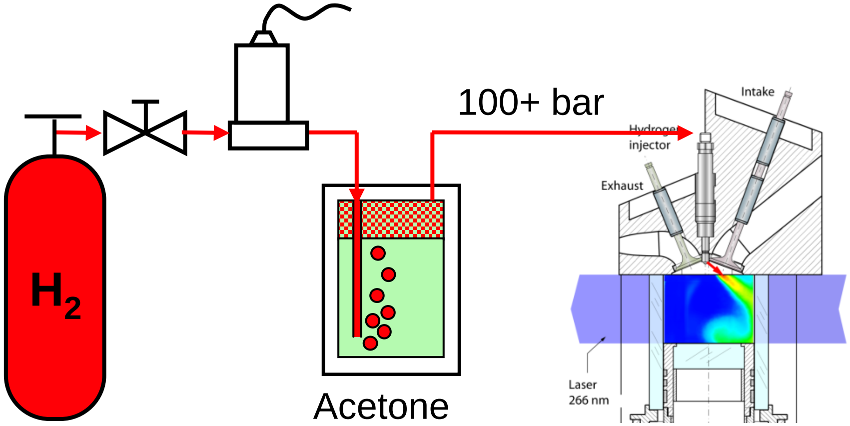
Predictive design capabilities through validated simulations

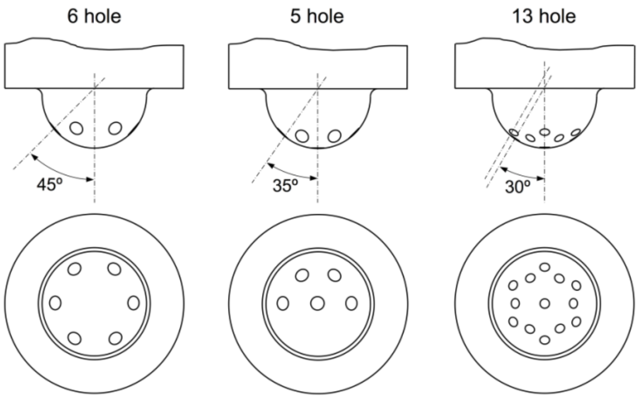
Expand science base for both gas and liquid-fueled engine development

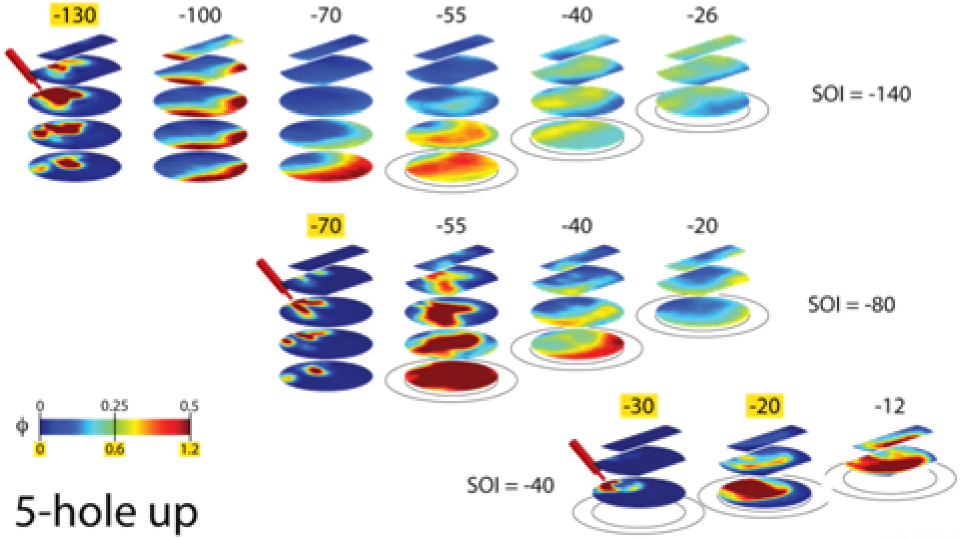
Last year, accurate fuel imaging was developed and used to study multi-hole injectors.



Improved diagnostics and tracer seeding enable accurate fuel imaging at any injection pressure.







This year: Interaction of intake flow and injection, Validation of industry-type simulation tools.

Detailed study of mixture preparation in **simple, yet instructive configuration**

Sandia

Assemble data package for simulation initiation: solid model, BCs

Optical data to examine areas of concern for simulations:

- Base flow field
- Flow / wall interaction
- Flow / injection interaction

Argonne

Grid generation

Initial calculation

Convergence study

Refined simulations

LLNL/Wisconsin

Grid generation

Initial calculation

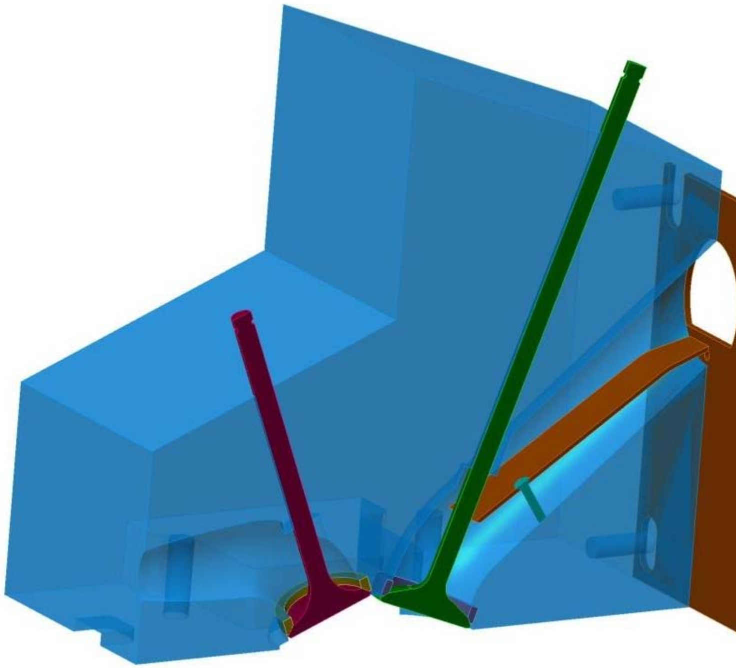
Convergence study

Refined simulations

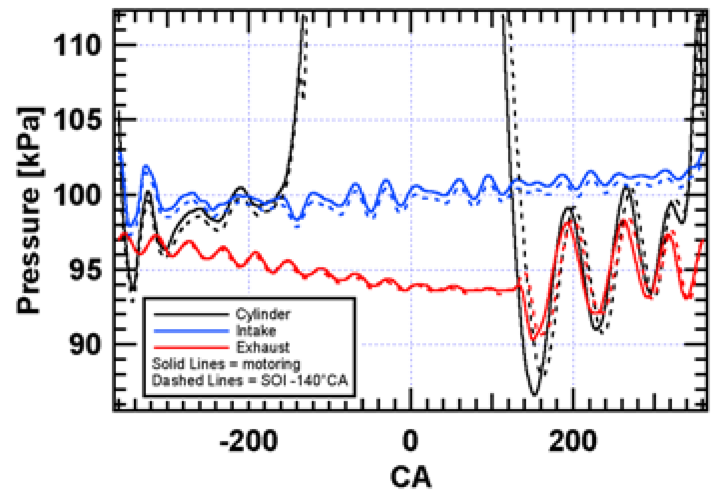
Cross-comparison of experiment and simulations, coordination of improvements.

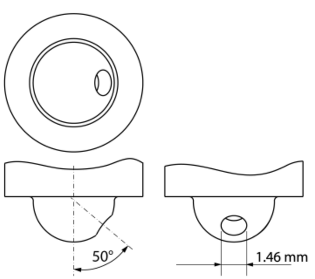
Integrate data in ECN (web data base)

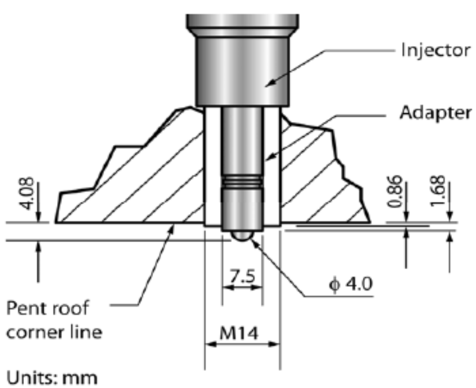
An engine data package, including a detailed solid model of the head, was assembled.



Engine head solid model
+
Other geometry
Flow rates
Valve and injector timings
Pressure traces
Temperatures

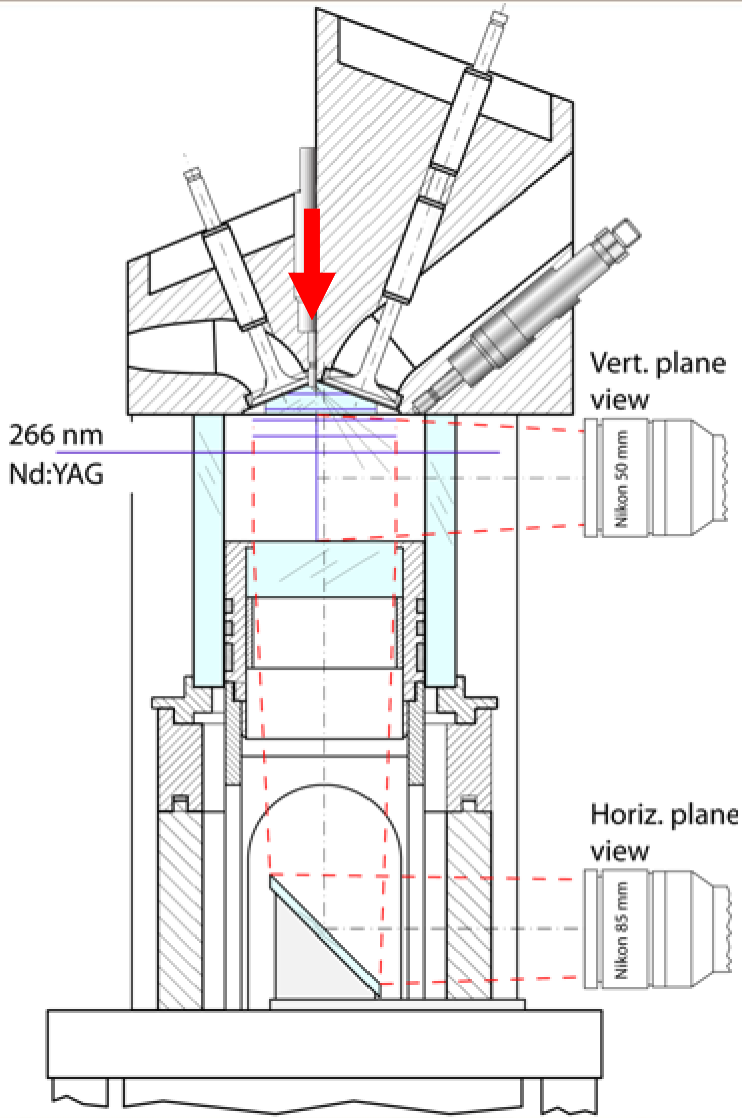




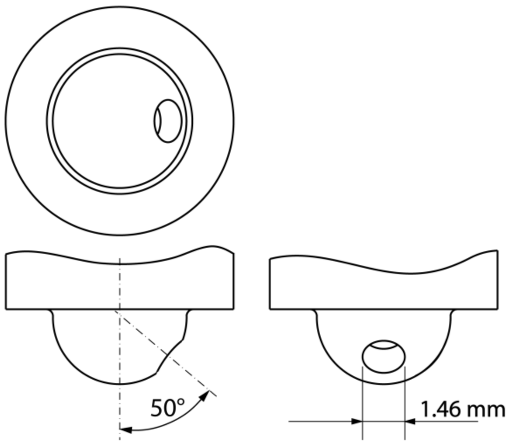


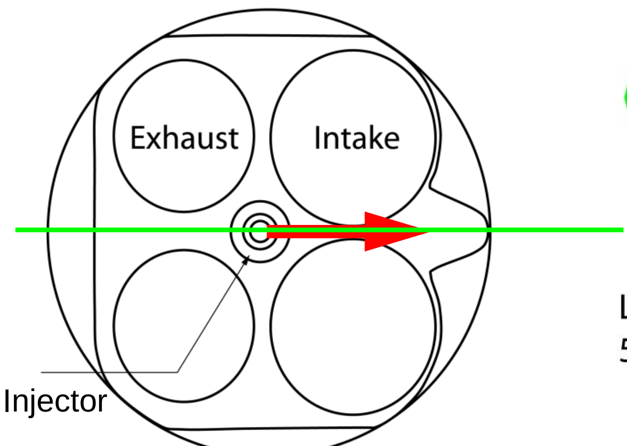
The engine is a passenger-car sized single-cylinder engine with optical access.

Engine specifications and testing conditions	
Bore	92 mm
Stroke	85 mm
Displacement	565 cm^3
Compression ratio	11
Speed	1500 rpm
Equiv. fired IMEP	2.5 bar
p_{intake}	1.0 bar
$p_{injection}$	100 bar
Global Equiv. Ratio/molar fraction	0.25/0.095
Injection duration	17.5 °CA
Start of injection	**-140 °CA**

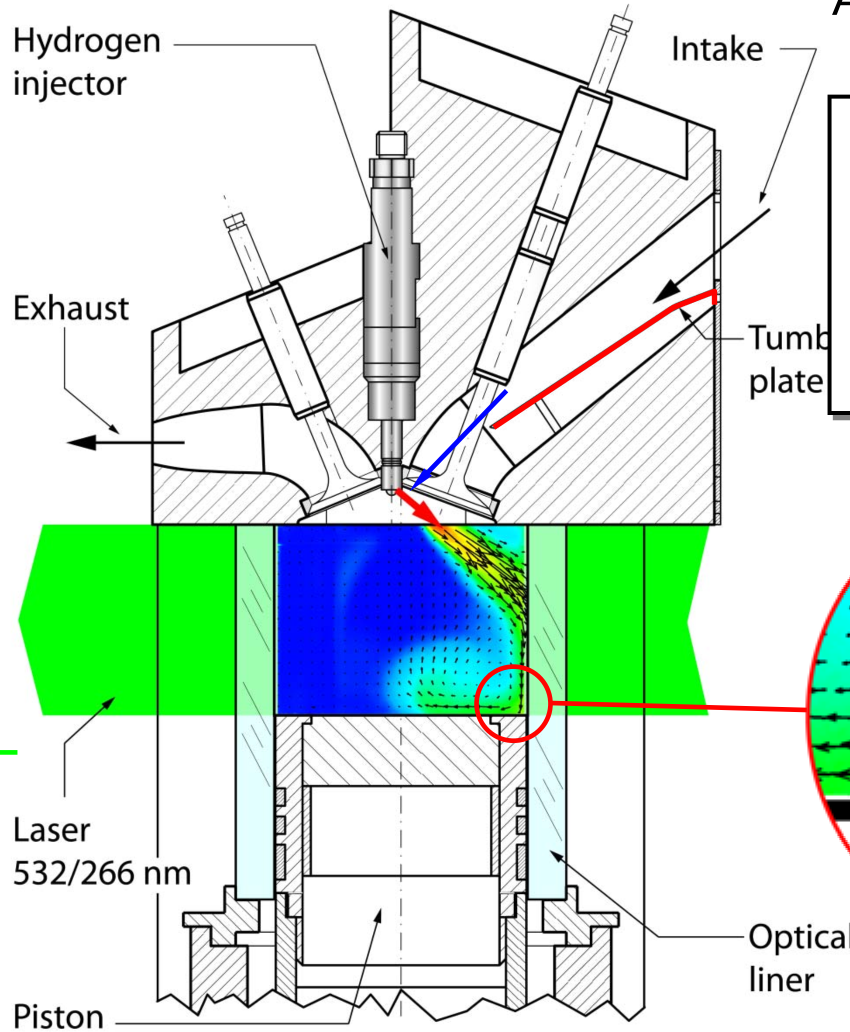


A single-hole injector avoids jet-jet interaction. Measurements ideally suited for simulation validation.



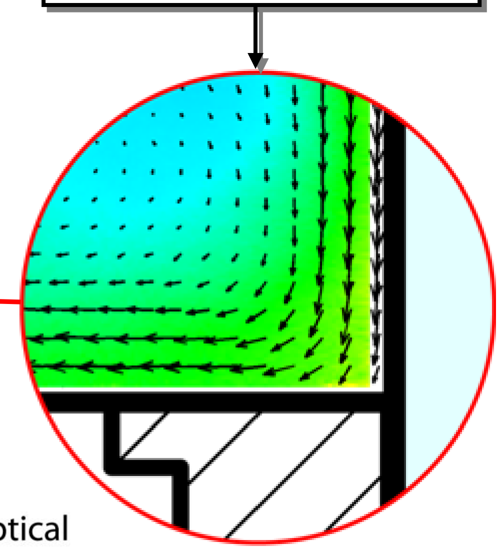


Acetone PLIF + PIV

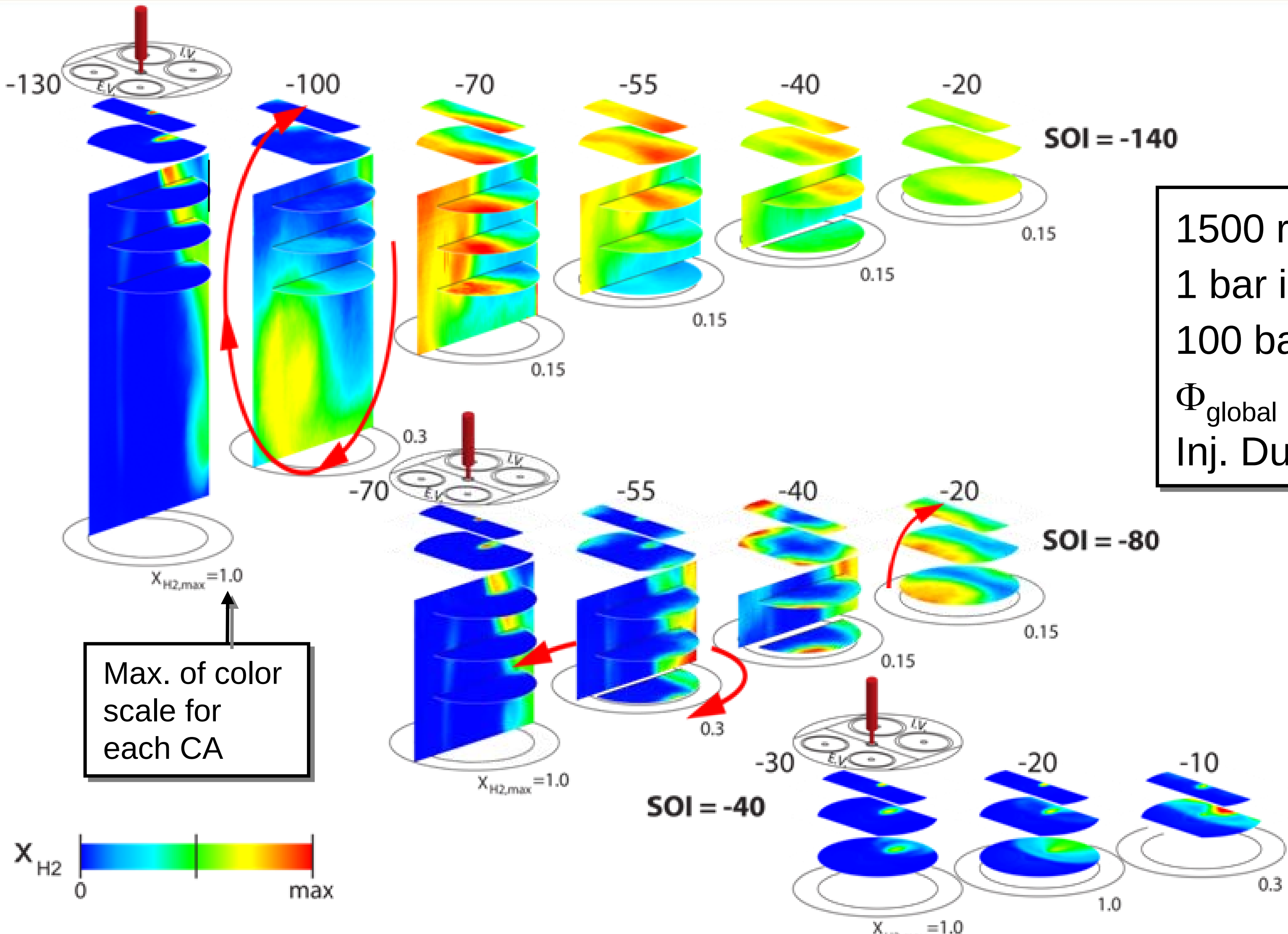


Unique measurements

- full bore & stroke
- almost to walls
- quantitative



Cross-plane imaging of the fuel concentration gives an overview of large-scale convection.



1500 rpm
1 bar intake pressure
100 bar injection p.
Φ_{global} = 0.25
Inj. Duration 17.5ºCA

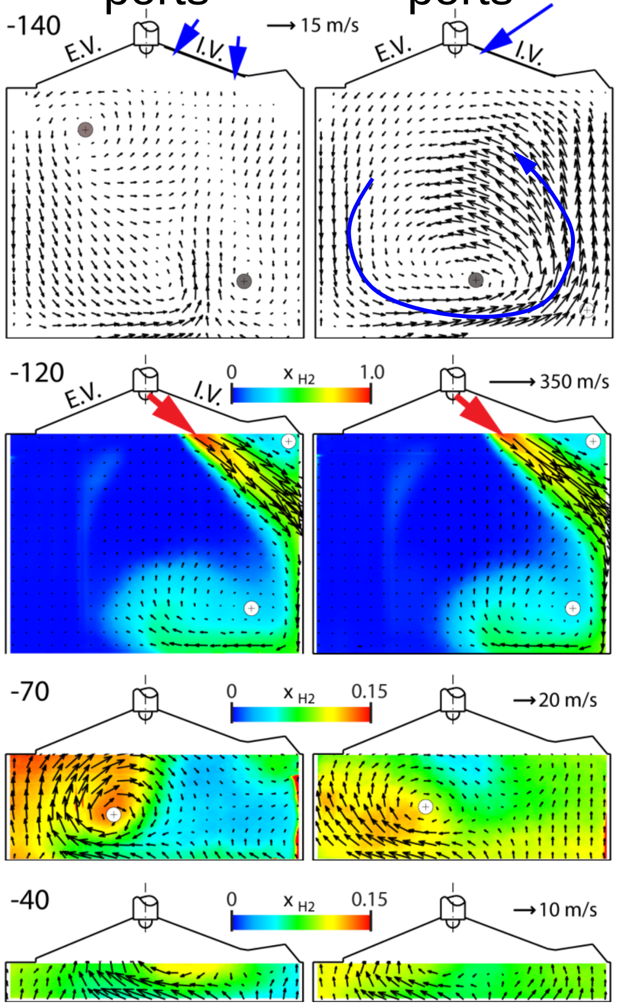
Enhanced tumble significantly changes bulk convection and mixing.

Low-tumble ports | High-tumble ports

Just before injection

At the end of injection

During com-pression



SOI = 140ºCA, p_{inj} = 100 bar

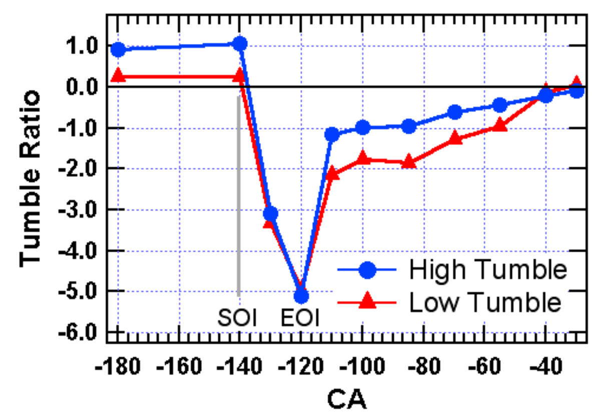
Mean velocity and hydrogen mole-fraction

Intake modification increases tumble by 4x.

Injection and tumble are in counter-flow.

High tumble retards fuel convection and increases mixing.

Injection disrupts flow, but momentum difference high vs. low tumble is preserved.



The wall jet retains the patterns of free jets. This could be important for sub-model extension.

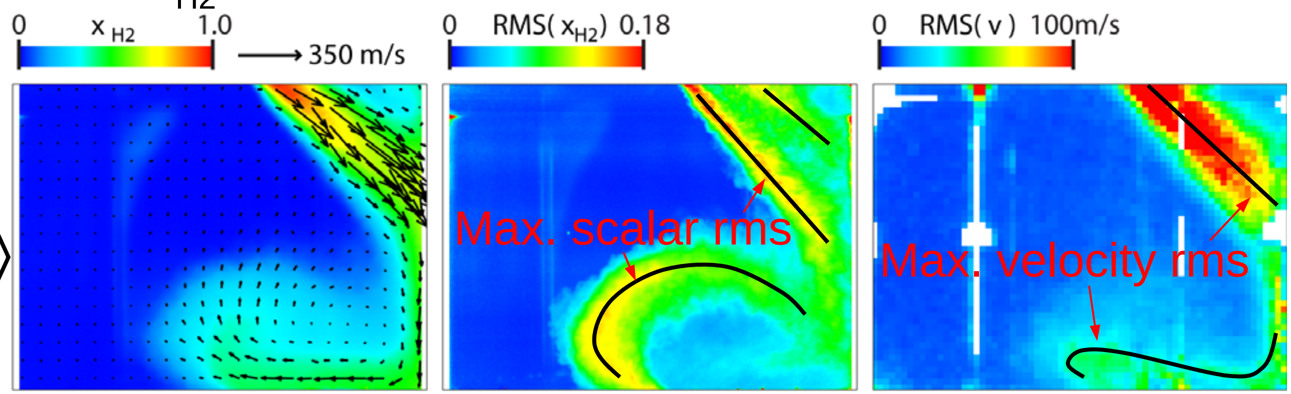
Structural similarities between free jet and transient wall jet

-120°CA At the end of injection

mean v
mean x_{H2}

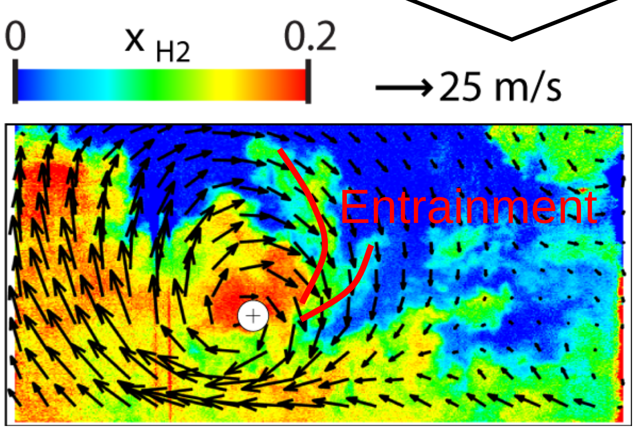
RMS (x_{H2})

RMS (v)



single-shot x_{H2}
mean v

-85ºCA



Peak in scalar fluctuations in wall jet is "outside" of peak velocity fluctuation
→ Similar to free jet

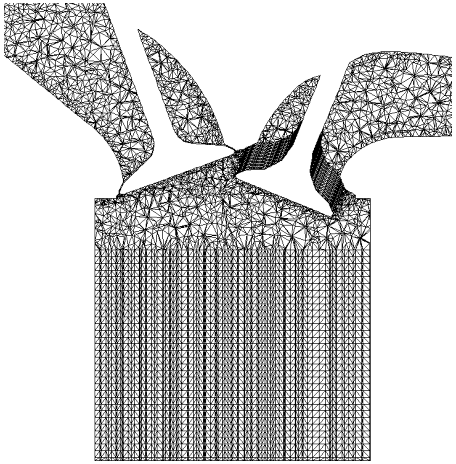
Intermittent fuel-rich structures are at ~45º with respect to mean velocity
→ Similar to free jet

Jet model extension?

Comparing different CFD approaches promises unique insight into their strengths and weaknesses.

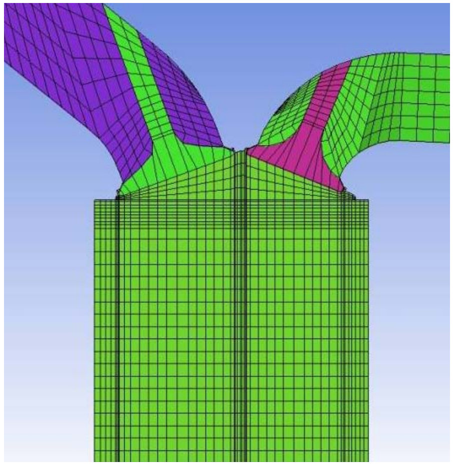
Initiated 18 months ago

FLUENT simulation at Argonne NL.
- Commercial code
- No jet sub-model
- 1.2M gridpoints, parallel on 8 cores
- Partially unstructured mesh
- GAMBIT mesh generator



Just started

KIVA 3V simulation at LLNL.
- Source code accessible
- Sub-model for H_2 jet
- 80k gridpoints, single core
- Block-structured mesh
- ICEM-CFD mesh generator



First target:

Mixture formation with single-hole nozzle,

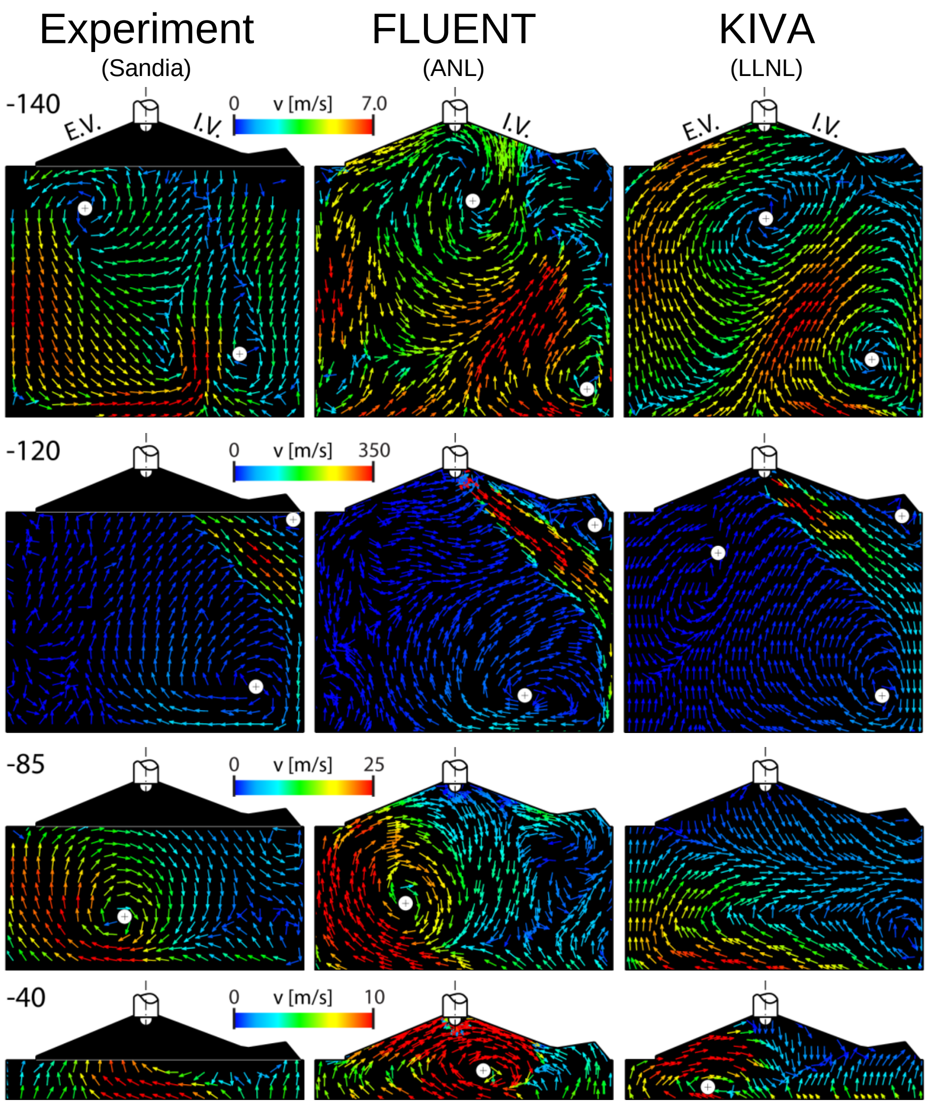
SOI = -140 ºCA

The simulations are able to predict the mean flow field reasonably well.

Just before injection

At the end of injection

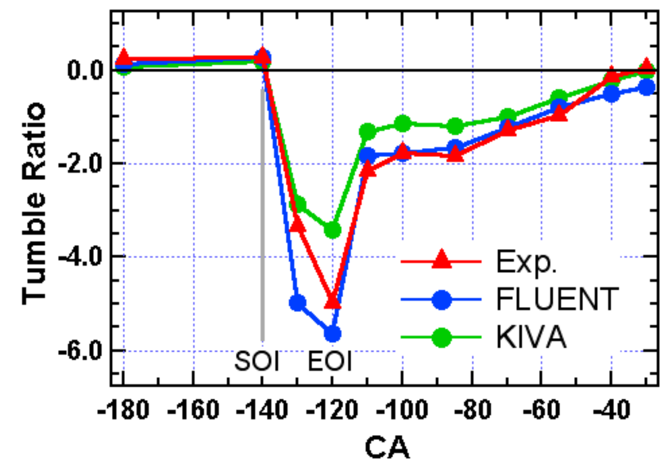
During com-pression



SOI = 140ºCA, low tumble

Mean velocity

Both simulations predict pre-injection flow accurately.



FLUENT captures convection accurately.

KIVA captures main features OK.

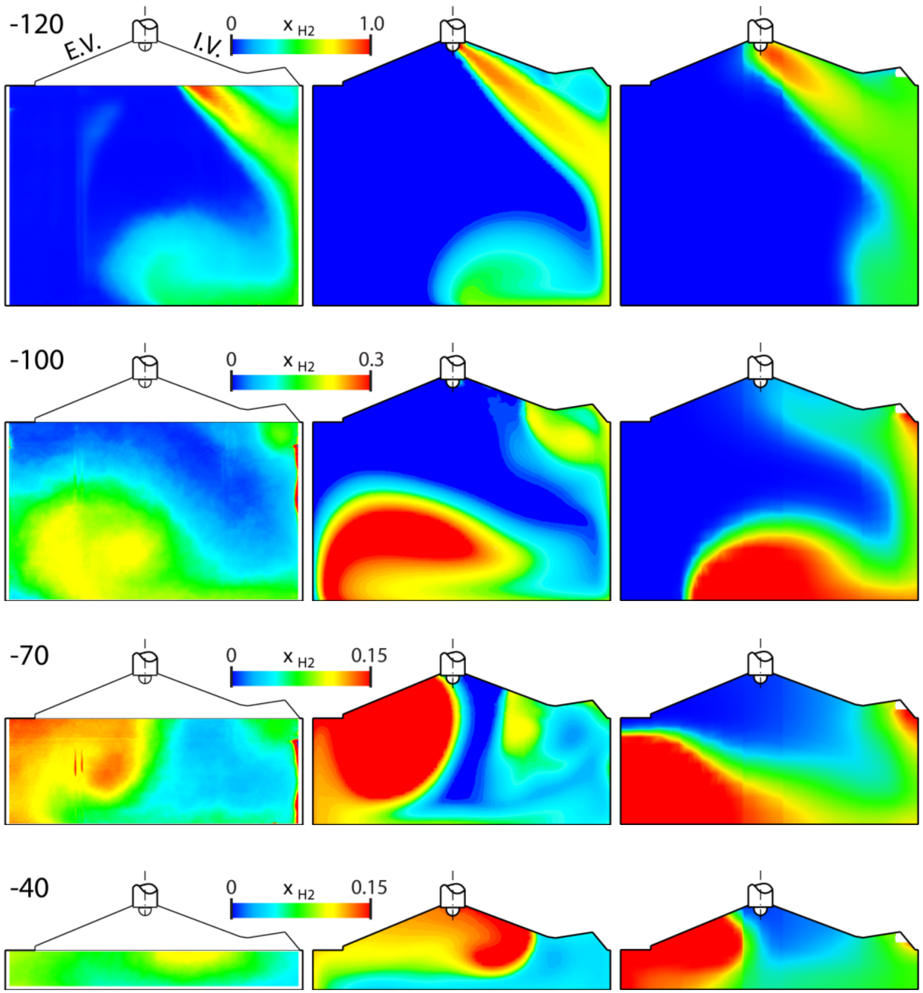
Fuel convection is predicted well by FLUENT. Mixing is under-predicted by both simulations.

Experiment (Sandia) | FLUENT (ANL) | KIVA (LLNL)

Mean hydrogen mole fraction

At the end of injection

During com-pression



LLNL’s jet model in KIVA predicts turbulent diffusion in free jet well, but not jet penetration.

FLUENT accurately captures fuel convection, but under-predicts dispersion.

→ Could result in problems for combustion part of simulation

Currently, KIVA sim. is inaccurate in convection and dispersion.

→ May need mesh refinement (only 80k cells now)

Future work will continue to target fundamental issues of H_2ICE combustion in collaborative work.

Support validation of mixture-preparation phase in simulations

- Complete velocity measurements (pent-roof region, horizontal plane)
- Assess refined simulations

Understand stratified hydrogen combustion and pollutant formation

- High-speed imaging of flame front propagation
- Develop diagnostics to examine pollutant formation (NOx, Temperature)

Investigate advanced operating strategies

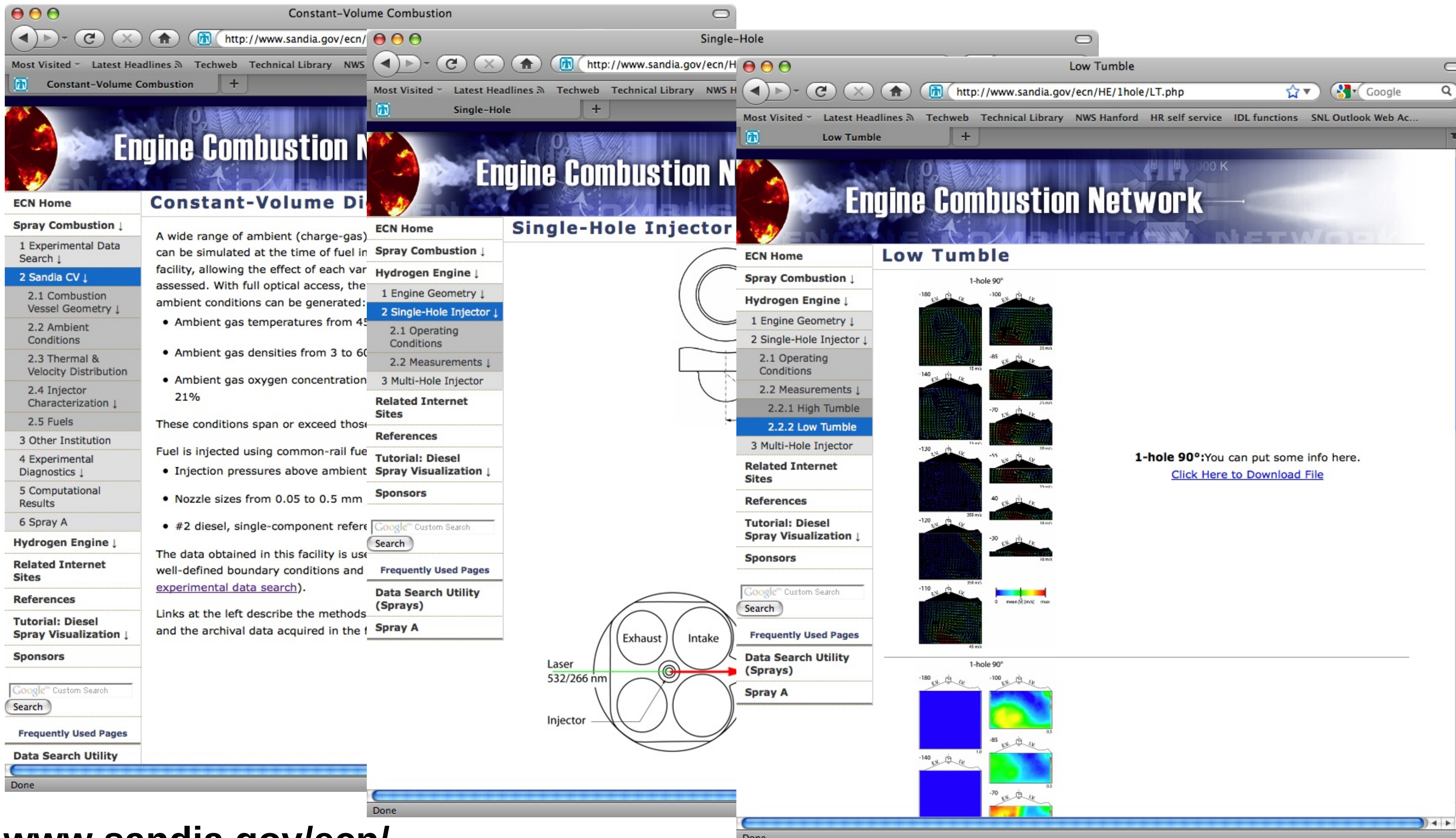
- EGR, Multiple injections, …
- Gaseous fuels other than H_2 ?

Continue and improve collaborations

- Coordinate work with Ford, ANL, LLNL, and other partners
- Integrate imaging data into Engine Combustion Network

Validate, learn from, and advance simulations

Boundary conditions and experimental data will be available via the Engine Combustion Network.



www.sandia.gov/ecn/

In summary, a focus on simulation validation is driving towards predictive tools for H2ICE optimization .

(1) Collaborations with Argonne and Lawrence-Livermore Labs were initiated to advance industry-type 3D CFD as a predictive tool for H2ICE optimization.

- Assembled data package, including detailed engine geometry.
- Argonne NL: FLUENT, Lawrence-Livermore NL: KIVA-3V.

(2) Quantitative imaging of fuel mole-fraction and flow field with a single-hole injector showed interaction of injection and intake-induced flow.

- Enhanced intake-induced tumble significantly alters convection and mixing.
- Both pre-injection flow and small differences in geometry influence mixture formation when changing nozzle pointing *(not discussed in this presentation).*

(3) Unique data set allowed for detailed assessment of the simulations' accuracy in predicting DI mixture formation.

- FLUENT is accurate in fuel convection, underpredicts dispersion.
- KIVA needs more resolution; convection and dispersion less accurate.
- Experimental data are/will be available on web via Engine Combustion Network.