IMPROVING SPRAY MODELS FOR ADVANCED COMBUSTION STRATEGIES

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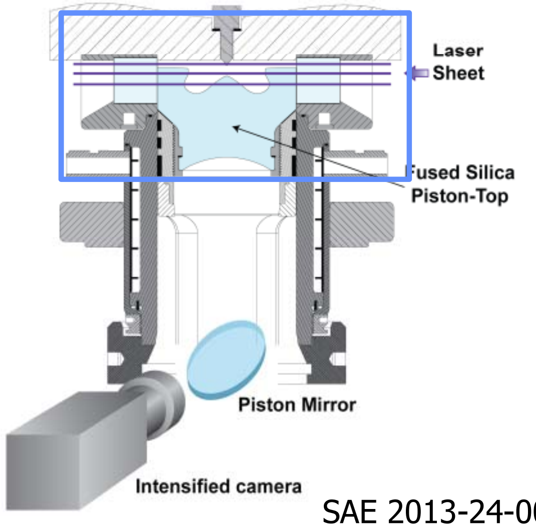
Sandia National Laboratories

Transition to large-scale computations

- Understand the ‘locality effects’ of flow, compositional and thermal non-uniformities on combustion
- Prepare the path towards comprehensive flow and transport modelling (LES, DNS) and future engine studies with full engine geometry

- First KIVA4 implementation (Torres, 2006) as the base code ✓
  - Need for a framework that is tailored to internal combustion engine simulations
  - Buggy but enabled support for unstructured geometries
- Large-scale combustion chemistry ✓
  - Sparse Analytical Jacobian chemistry solver (‘SpeedCHEM’)
  - High-Dimensional cell Clustering
- Extended and improved spray modelling ✓
- Parallelization of the flow field and spray solution ⌛

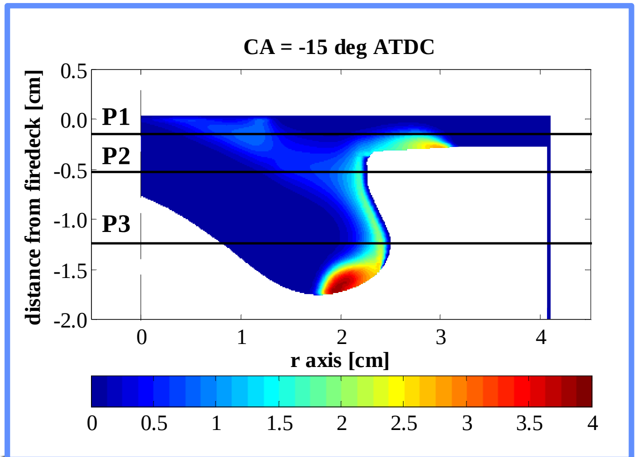
PPC mixture preparation experiments

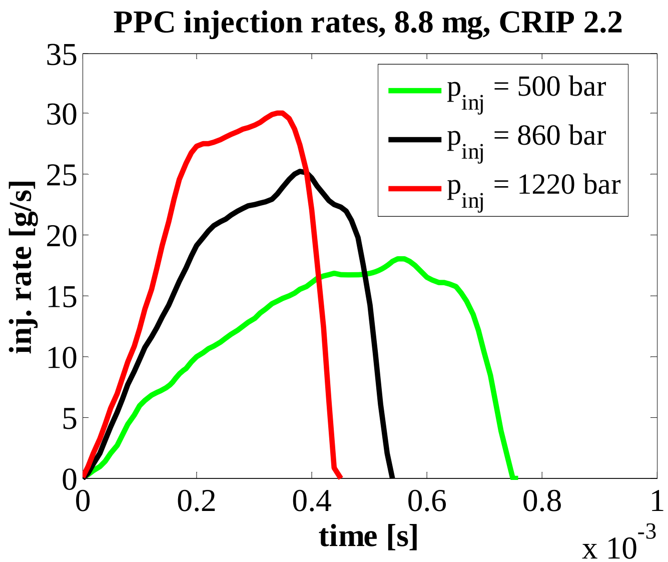


SAE 2013-24-0061

Experiments carried out at Sandia National Laboratories by P.C. Miles, D. Sahoo, S. Busch

- Optically-accessible Sandia-GM 1.9L engine
- Bosch CRI2.2 7-hole injector
- Variable swirl ratio intake: Rs = 1.5 to 4.5
- Fuel for mixture preparation studies: PRF25
- PLIF equivalence ratio measurements





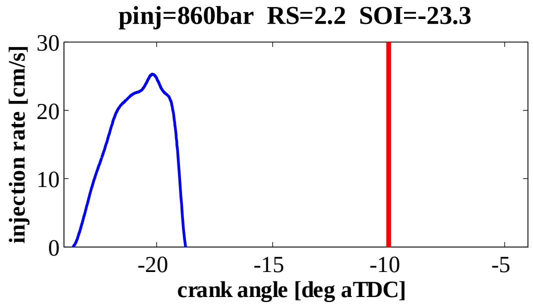
PPC mixture preparation validation

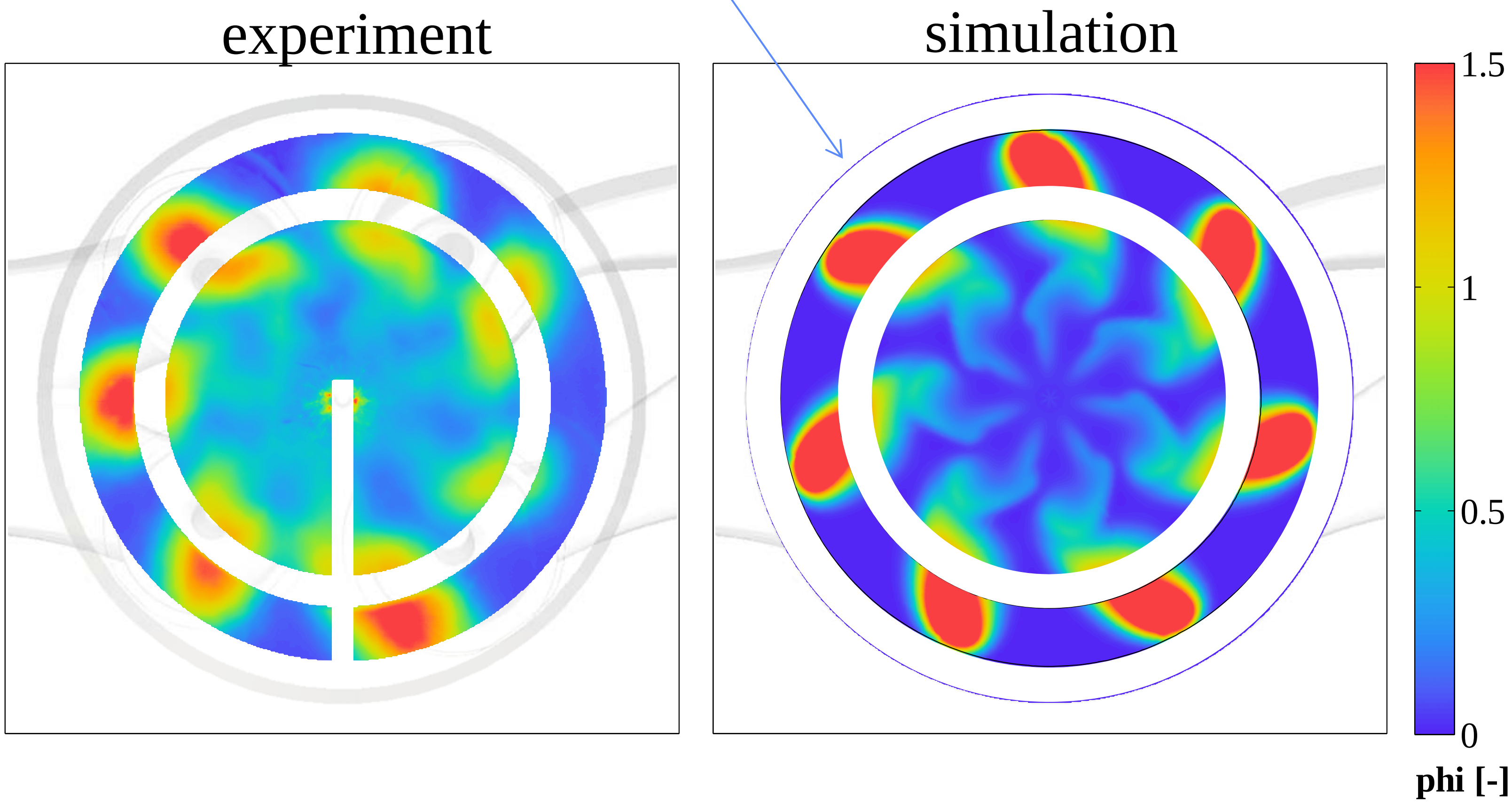
sector mesh

P1 (squish)

CA = -10.0

Squish mixing = slightly underestimated





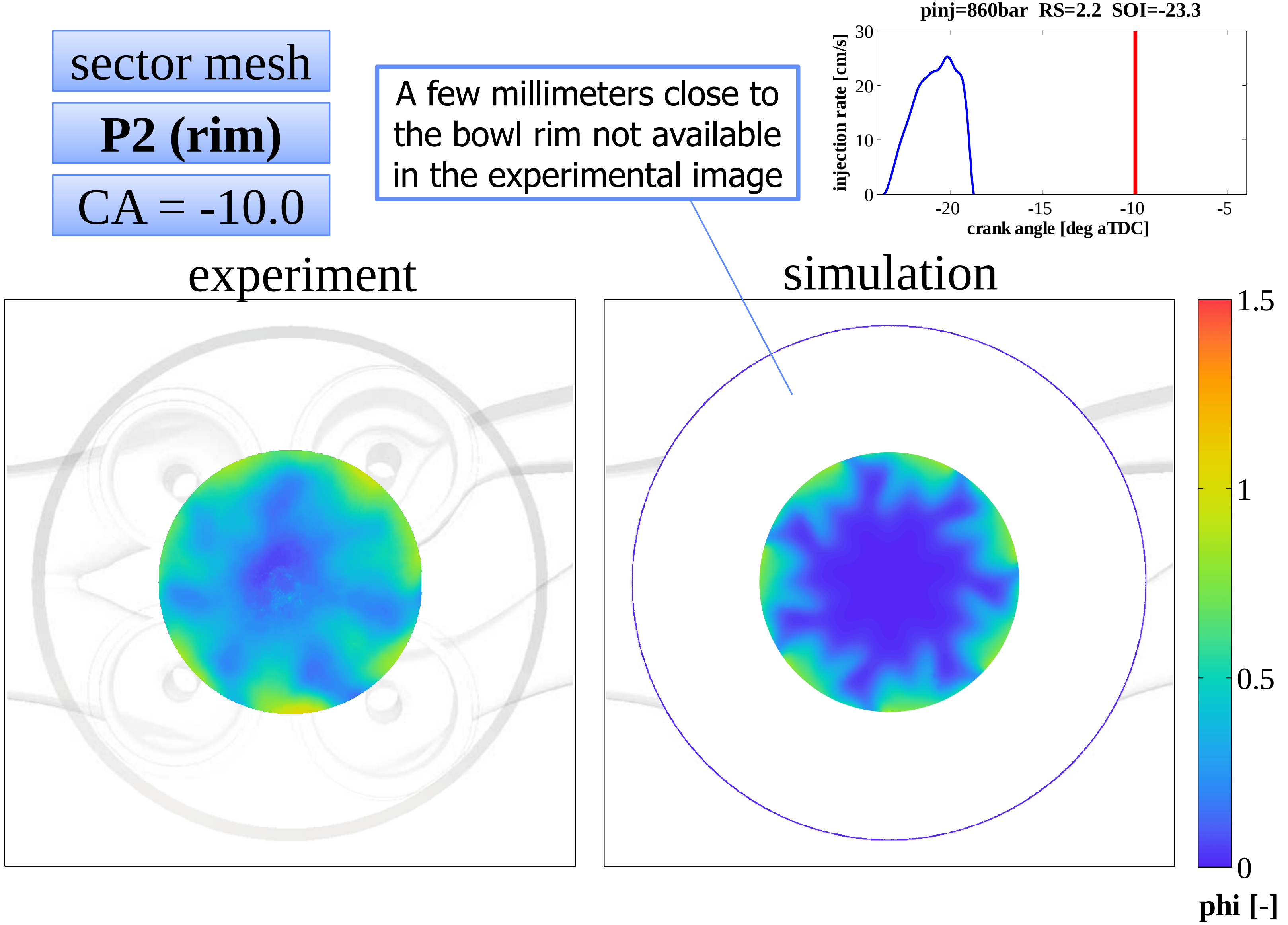
PPC mixture preparation validation

sector mesh

P2 (rim)

CA = -10.0

A few millimeters close to the bowl rim not available in the experimental image



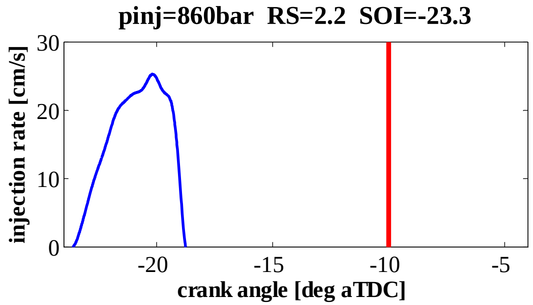
PPC mixture preparation validation

sector mesh

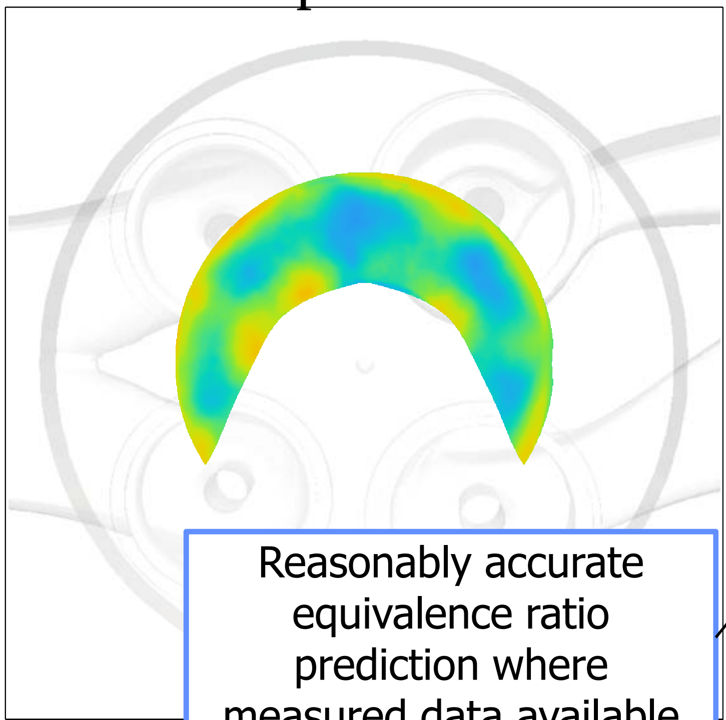
P3 (bowl)

CA = -10.0

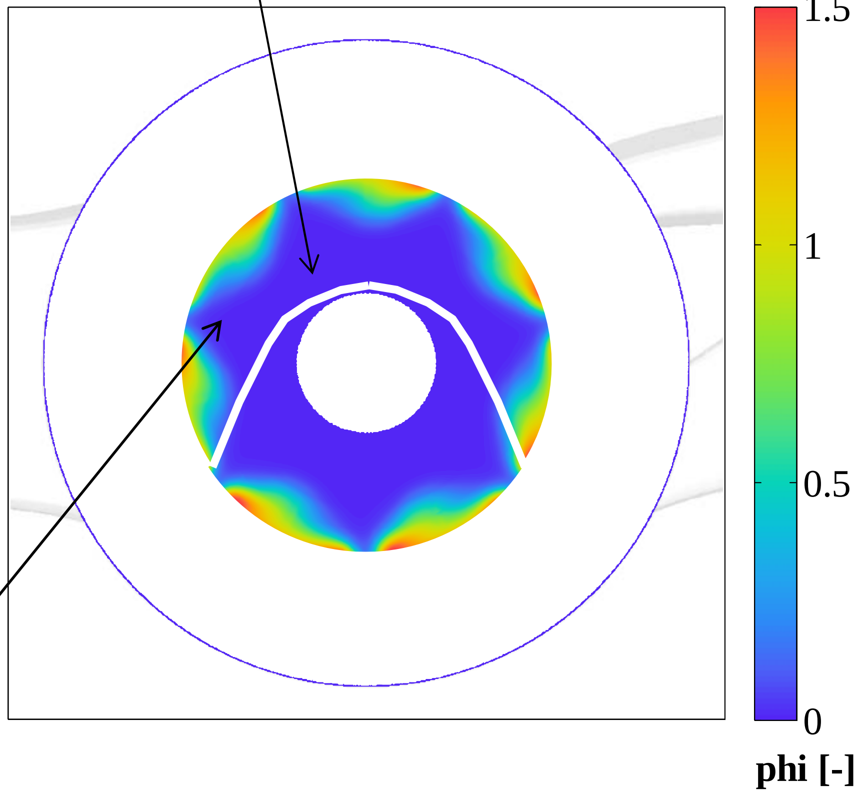
Slight underprediction of jet penetration reaching back up to the centerline



experiment



simulation



Reasonably accurate equivalence ratio prediction where measured data available

Spray modelling improvement effort

✓ Current spray model validation
(unstructured code, sector mesh same to SAE2013-01-1105)

✓ Flow prediction validation
(unstructured full engine model, generalized RNG k-ε closure)
(CaF 2013, submitted; THIESEL 2014, submitted)

→ Spray model improvement and calibration
(Sandia ECN spray experiments)

↓

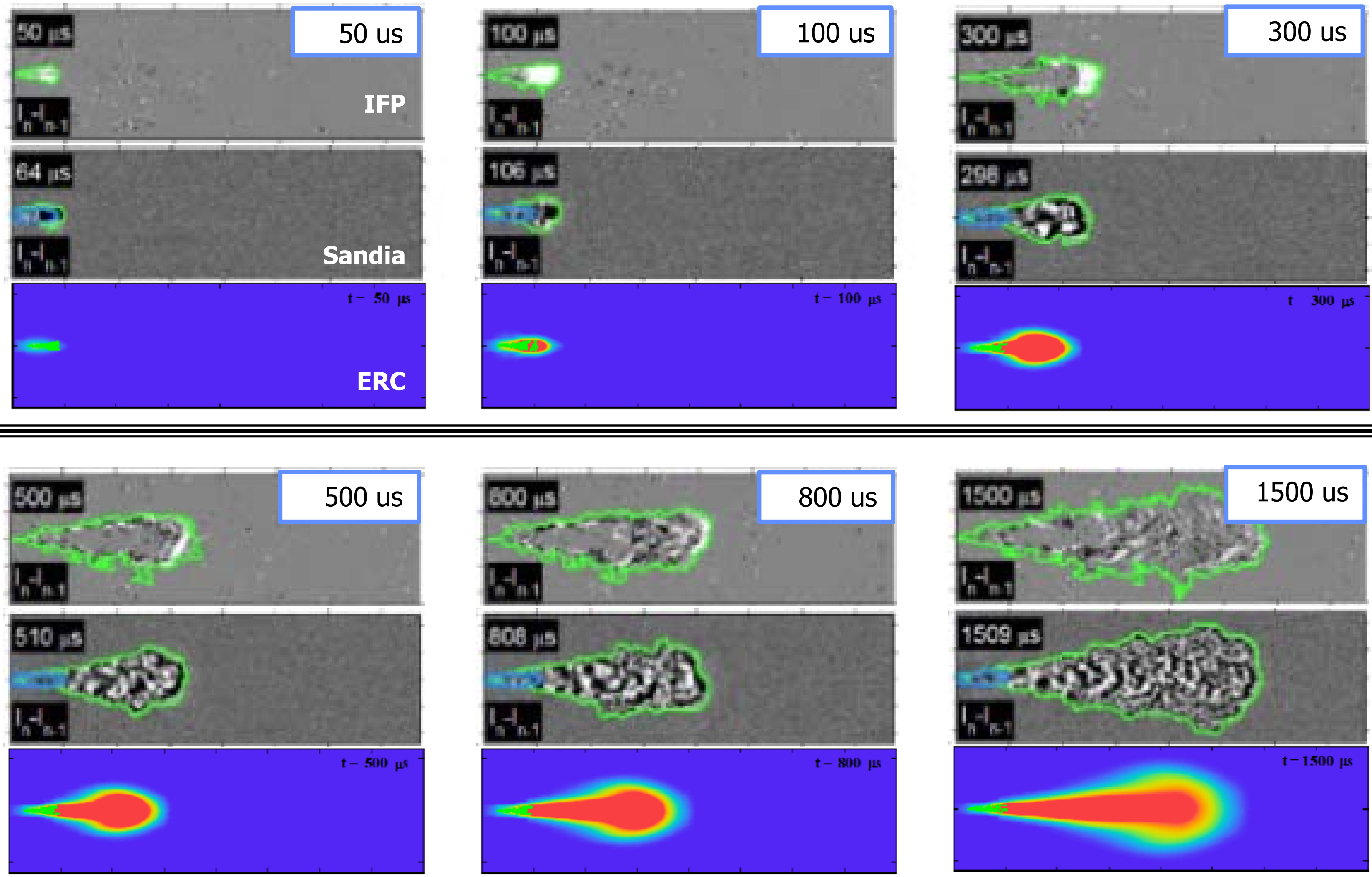
Spray A

Injection-induced turbulence effects on near-nozzle flow	Model study to capture near-SOI transient

Sandia Spray A modeling

900K, 60 bar, t_{ini} = 1.5 ms

- [contour] fuel vapor mass fraction, in the range [0, 0.05]
- [green dots] liquid phase distribution projection



Spray constants GA study

- Multiple interacting spray models → hard to isolate the effects of each model
- Hard to validate each of these isolated phenomena against experiments
- May be aided by future DNS simulations

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A GA optimization to answer these questions:

→ What **parameter regions** should we move in?

→ When we used to calibrate the spray constants, how much were we **tweaking the gas-phase** prediction too?

→ Is there an **optimal calibration set**, and, does this include "historically used" values or does it suggest new ones, which better fit the newest and highly confident Sandia experiments?

Spray constants GA study

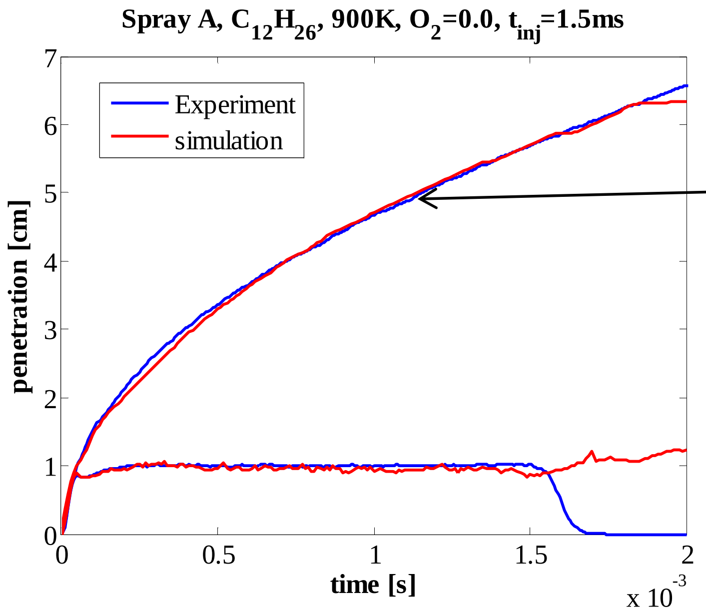
6 model variables

Variable	name	std value	range	to
RT time constant	C_{RT}	1.0	0.05	50.0
RT wavelength cnst.	$C_{\Lambda RT}$	0.1	0.01	10.0
KH decay timescale cnst.	B_1	40.0	10.0	100.0
Gas-jet Stokes number	St	3.0	0.1	5.0
Gas-jet entrainment cnst.	K_{entr}	0.7 (ideal=0.45)	0.3	3.0
Max gas-jet velocity frac.	γ	0.6	0.2	0.9

5 Spray A objectives

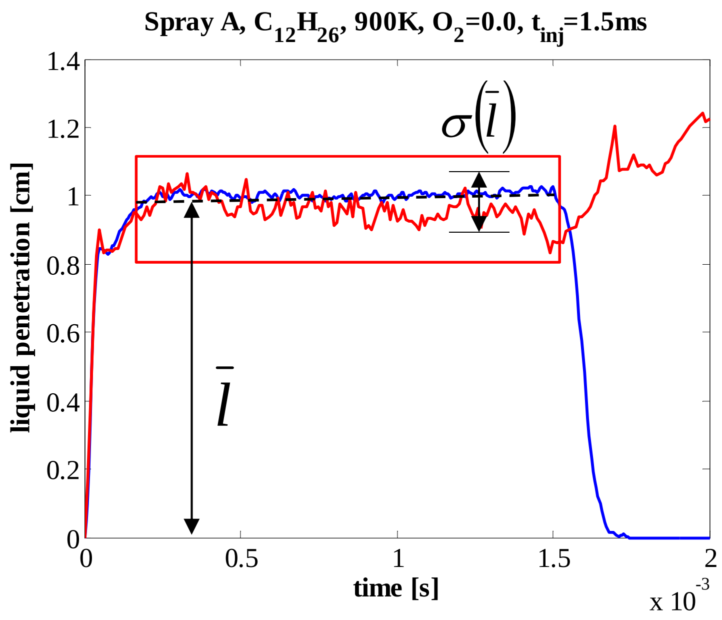
Phenomenon	merit
1) Vapor penetration	integral mean squared error (MSE)
2) Vapor dispersion	mean integral MSE (future addition)
3) Liquid ramp	integral MSE
4) Steady liquid region	mean peneration error
5)	penetration stdev error

Spray A objectives



1) MSE on predicted vapor penetration

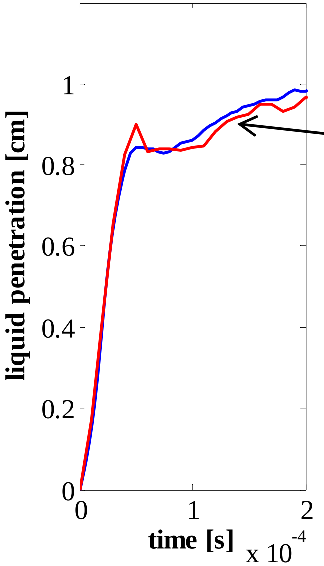
$$f_1 = \frac{1}{t}\int_0^t \left(\frac{\left(v_{sim}(\tau) - v_{exp}(\tau)\right)}{v_{exp}(\tau)} \right)^2 d\tau$$



4,5: error on mean and stdev of steady liquid length

$$f_4 = \frac{\left|\bar{l}_{sim} - \bar{l}_{exp}\right|}{\bar{l}_{exp}}; \quad f_5 = \frac{\left|\sigma(l_{sim}) - \sigma(l_{exp})\right|}{\sigma(l_{exp})};$$

Spray A objectives

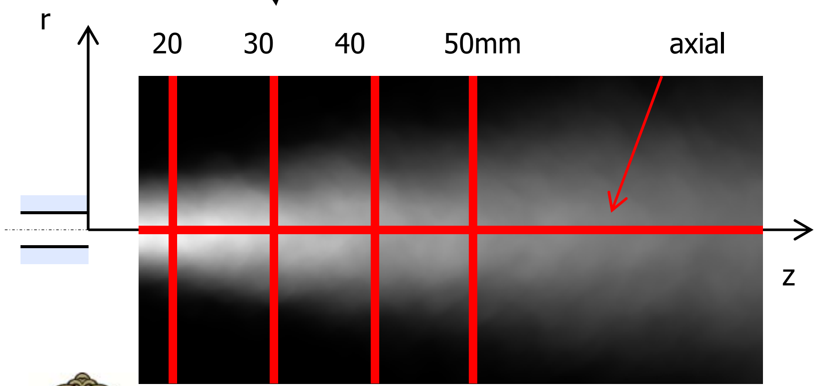


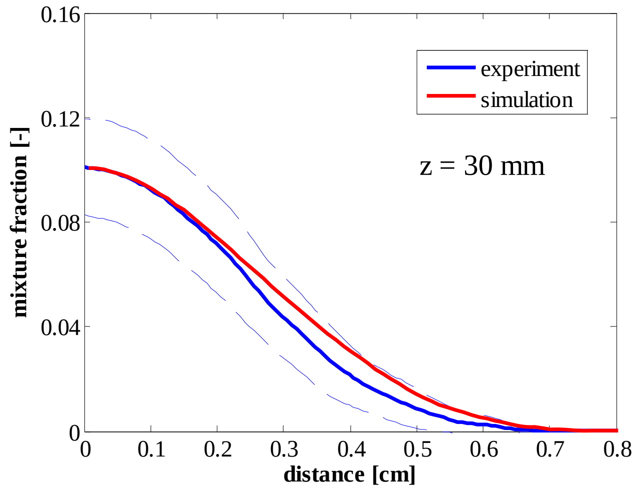
3) liquid penetration on the ramp up

$$f_3 = \frac{1}{t_{ramp}} \int_0^{t_{ramp}} \left(\frac{\left(l_{sim}(\tau) - l_{exp}(\tau) \right)}{l_{exp}(\tau)} \right)^2 d\tau$$

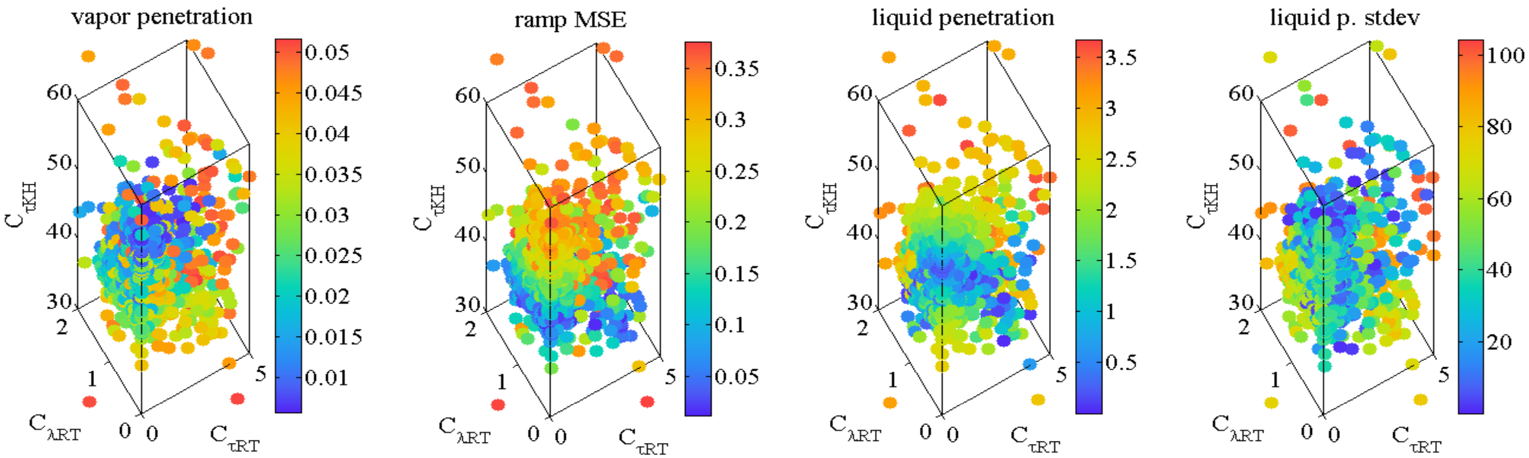
2) Mean integral vapor dispersion MSE (under development)

$$f_2 = \frac{1}{5} \left(MSE\big|_{z=20} + MSE\big|_{z=30} + MSE\big|_{z=40} + MSE\big|_{z=50} + MSE\big|_{axis} \right)$$





Results: breakup model constants



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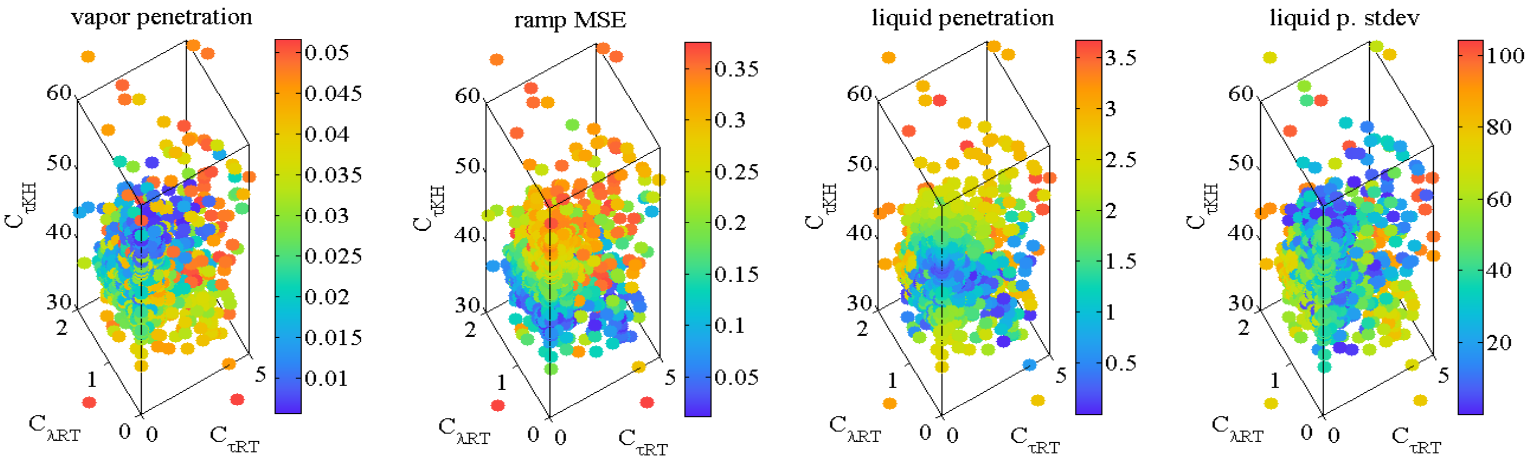
Coordinates → the variables

Colors → merit: the bluer, the better

Results: breakup model constants



KH decay time scale constant (B_1)

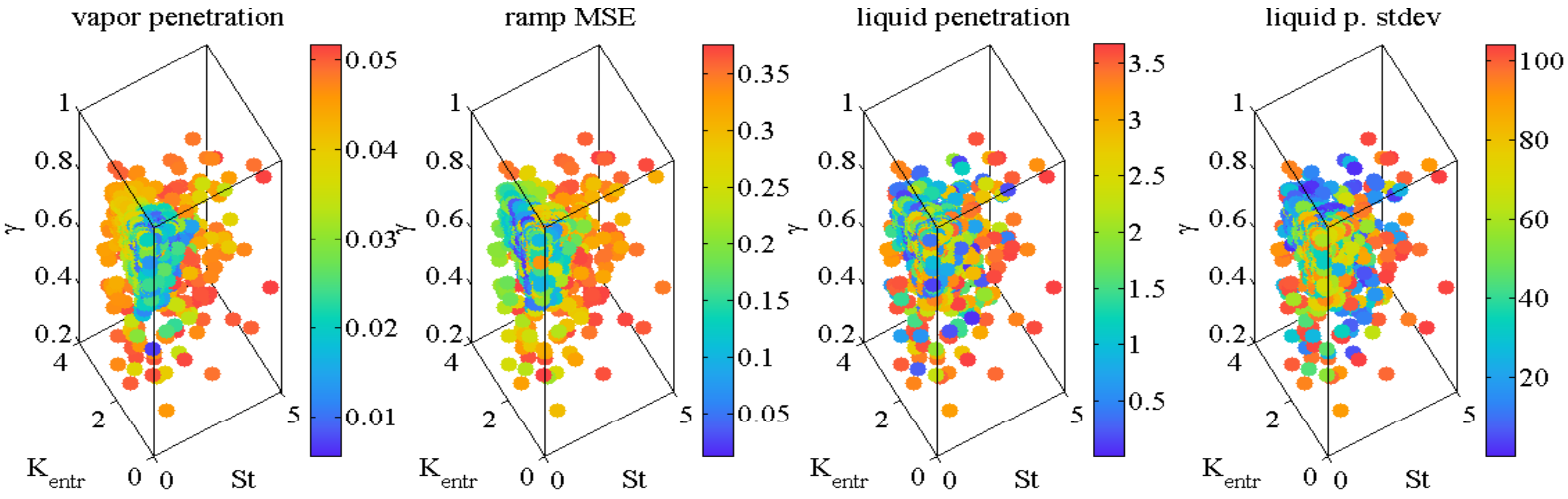
- affects the liquid ramp phase (→ RT breakup not occurring yet), not the steady-state
- Vapor penetration: **B_1 > 50** → we do not want breakup to compensate for turbulence!

-Liquid ramp: **$B_1 \in [35 – 44]$** → converging to the widely validated B_1 = 40

RT model constants (wavelength $C_{\lambda RT}$, timescale $C_{\tau RT}$)

- Crucial to liquid length prediction, which is "a tiny bit" after RT breakup happens
- the RT timescale seems to have optimal values **~ $C_{\tau RT}$ = 3.7**; or **$2 < C_{\tau RT} < 4$**

Results: gas-jet model constants



Very definite behavior for vapor penetration and liquid ramp

γ ϵ [0.7 – 0.9] → Better to apply most of the effective gas-jet velocity

Kentr ϵ [0.6 – 0.9] for vapor penetration,

[0.8 – 1.5] for liquid ramp → slightly higher than currently used

Stokes ϵ [0.8 – 1.0] ← Significantly smaller than the value St = 3.0 suggested in (Abani and Reitz, 2008) for steady gas-jet modelling →

Study of
Stokes number effects

GA optimization summary

■ Confirms complex interactions among the models

■ Suggests that the Stokes number calibration used for steady gas-jet modelling is overestimated → needs a deeper study

■ Confirms standard "historically used" and well validated values (e.g., $B_1 = 40$)

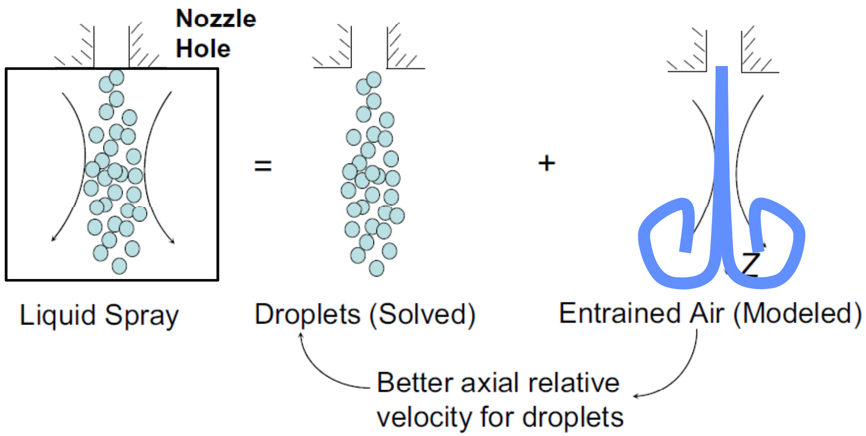
↓

■ Currently setting up a more comprehensive optimization study:

- Large number of individuals and generations
- GRNG turbulence → validated for vapor penetration
- Inclusion of jet dispersion merit as an objective

■ Final validated calibration set will be used for grid resolution study

Gas-jet model Stokes number study



Eddy generation frequency in the modeled gas-jet equal to particle responsiveness in the spray jet drops

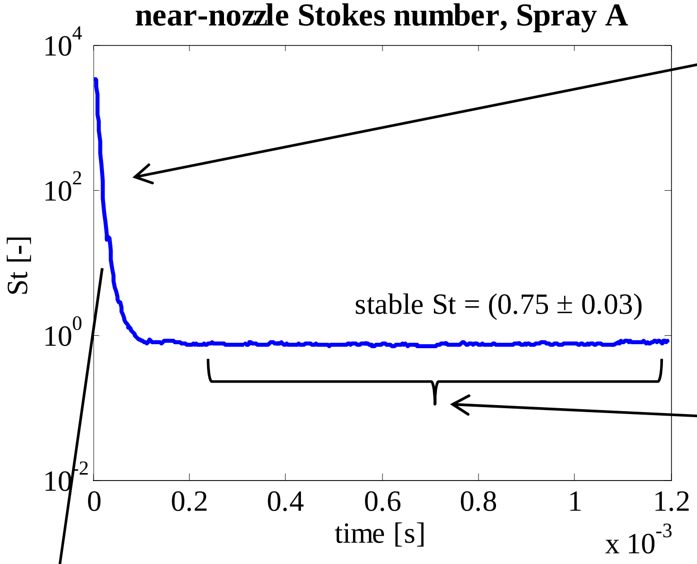
$$\frac{f_V x}{U_{flow}} = Strouhal \approx Stokes = \frac{\tau_I}{\tau_p}$$

→ Assumed to be a model **calibration parameter → St = 3**

- A noticeably smaller range [0.8 – 1.0] suggested by the GA optimization
- The constant value can be replaced by a local estimation, exploiting injection-induced turbulence effects at the nozzle

Gas-jet model Stokes number study

- Stokes calculation from RNG k-ε predicted integral length scale **at the nozzle**

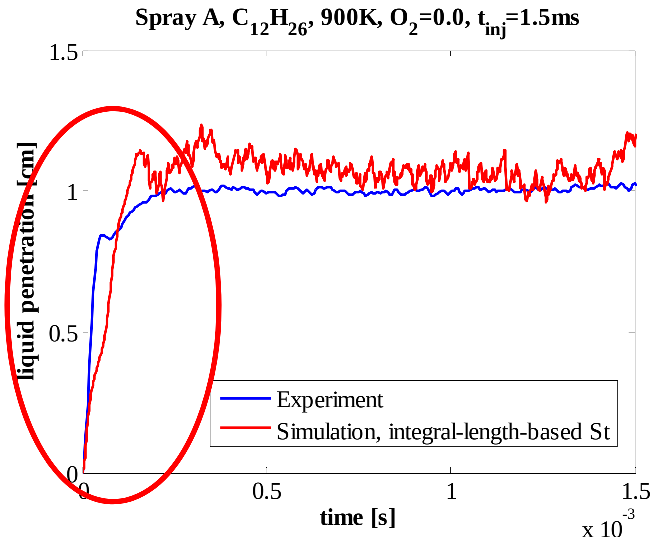


Initial slope → jet-induced turbulence not yet developed in the nozzle cell

Reasonable – the CFD model is underresolved at the nozzle!

A very stable region during steady-state injection

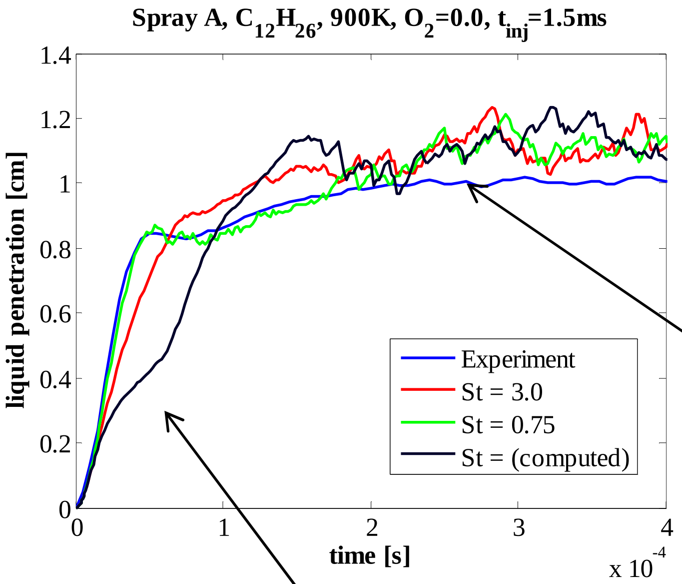
high St → significantly delayed liquid length development near SOI

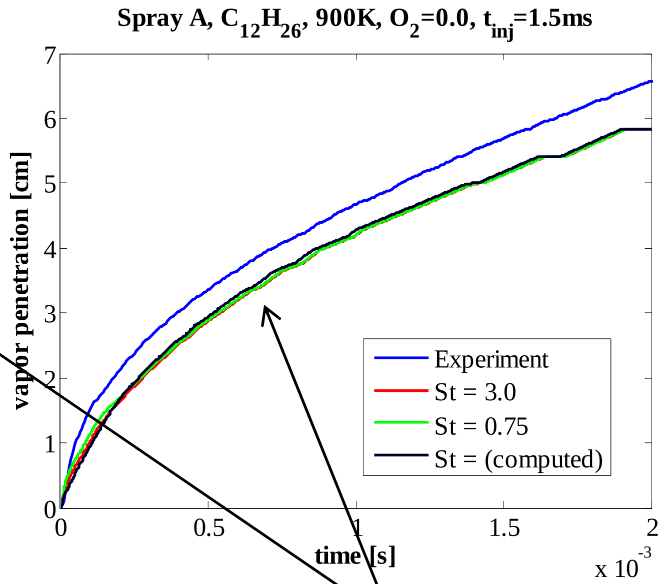


Stokes number crucial to modelling jet-induced turbulence effects on drop penetration

Gas-jet model Stokes number study

- Constant Stokes, **St = 3.0** (gas-jet model), **St = 0.75** (as in the steady part)
- Variable Stokes, **St = (computed at nozzle local cell)**





Significantly affects the initial liquid core development transient

Limited effects over steady-state liquid and vapor penetration

Excellent match of the initial development "bump" with **St = 0.75**

Further research directions

Spray

- Extend GA optimization and carry the improved calibration over to engine simulations

Fluid solution

- Parallelization for large-scale computations
- The KIVA lesson: a simple (Jacobi!) preconditioner can be very robust, and work very well (30+ years) if tailored to the problem (= coarse but topology-changing mesh)
- The most used ILUTP+BiCGStab solver "just works well" → possible to improve preconditioning the physical relationship of the pressure-velocity coupling is exploited

Chemistry

- Chemistry solver now scales linearly with problem size (sparse analytical Jacobian)
- → Need to move to scaling much less-than-linearly with the problem size

  → adjoint-sensitivity-aided partitioned (ASAP) clustering

Turbulence & Transport

- We are correctly modeling neither turbulent nor molecular transport
- Simple, linear isotropic turbulence models fail even over a simple gas jet case → but widely used for engines!
- Accurate transport modelling → diffusion, viscosity, etc

Thanks! Questions?

Acknowledgements

D.O.E. Office of Vehicle Technologies, P.M. Gupreet Singh
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