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Sandia National Laboratories

Detailed evaporation modelling for gasoline direct injection: iso-octane vs. E30

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Program Managers: Gurpreet Singh, Michael Weismiller

Co-Optimization of Fuels & Engines

U.S. DEPARTMENT OF ENERGY | NNSA

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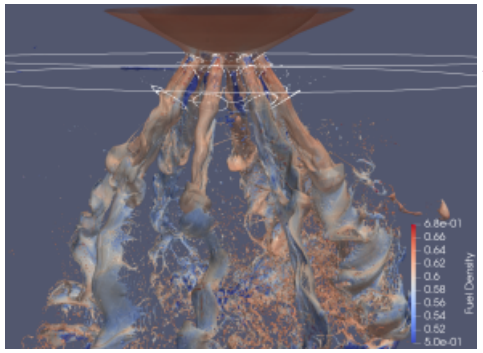
Co-Optima approach

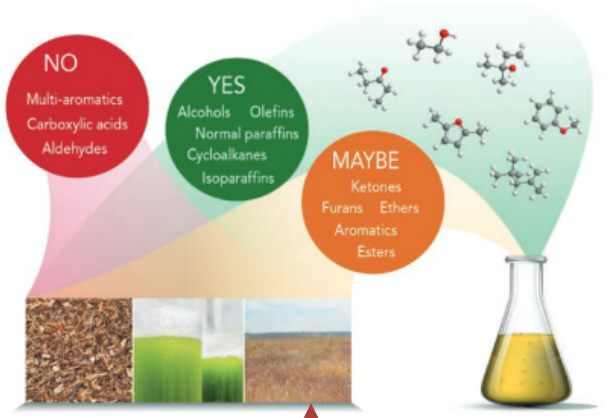


Direct Fuel Injection simulation

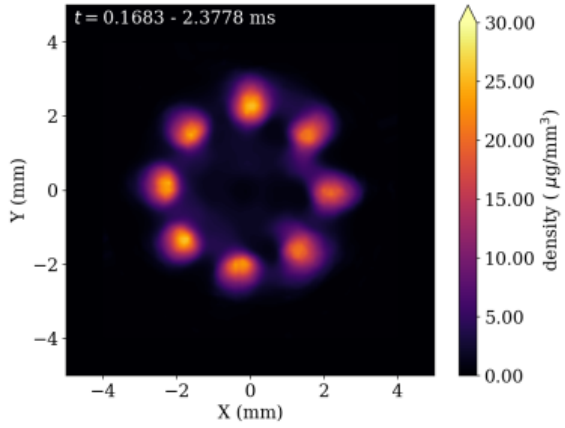
Spray

Fuel

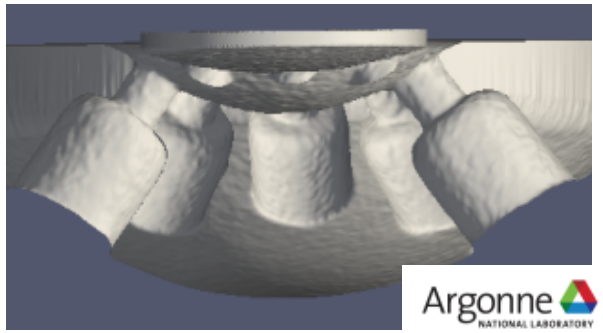
Hardware

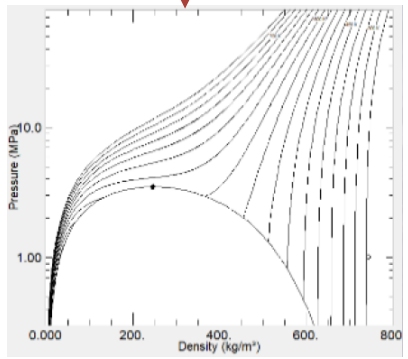


Surrogate composition and thermo-physical

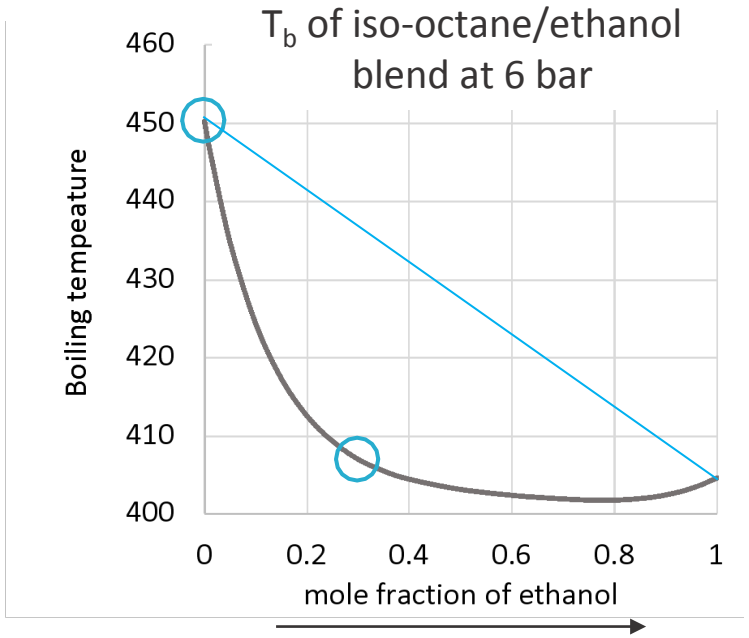


X-Ray imaging





Co-Optima challenges



1. Gasoline/ethanol blends do not behave like an ideal mixture (alcohol is a polar substance and iso-octane is non-polar):
   - Non-linear effects (azeotrope)

2. Do individual species need to be individually tracked?
   - Infinitely fast (infinite-conductivity model) vs. finite thermal and mass diffusion

$$\mathrm{Pe}_l = \frac{K_s}{D_l} = \frac{surface\ regression\ rate}{liquid\ interdiffusion\ rate}$$

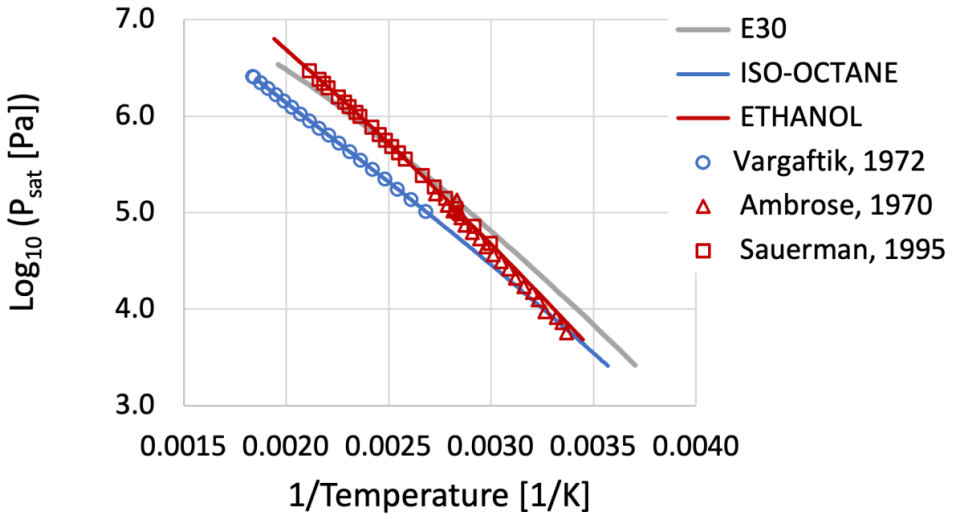
(for spherical symmetry: $\mathrm{Pe}_l = \frac{\dot{m}_v}{4\pi R D_l \rho_l}$)

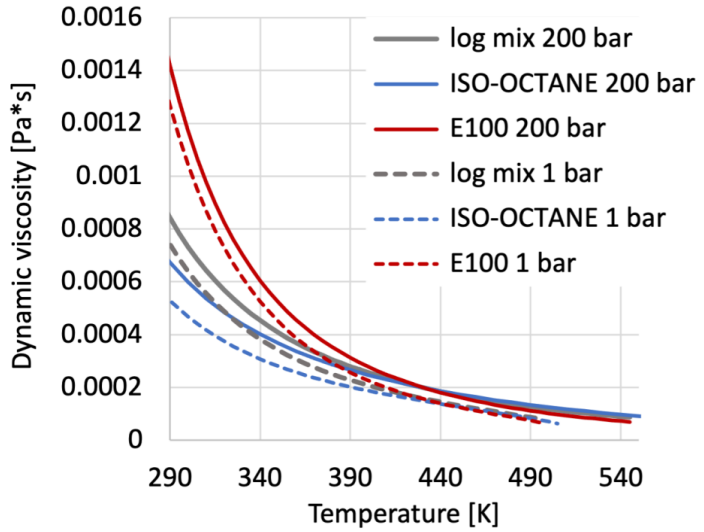
   - There are two limit cases:

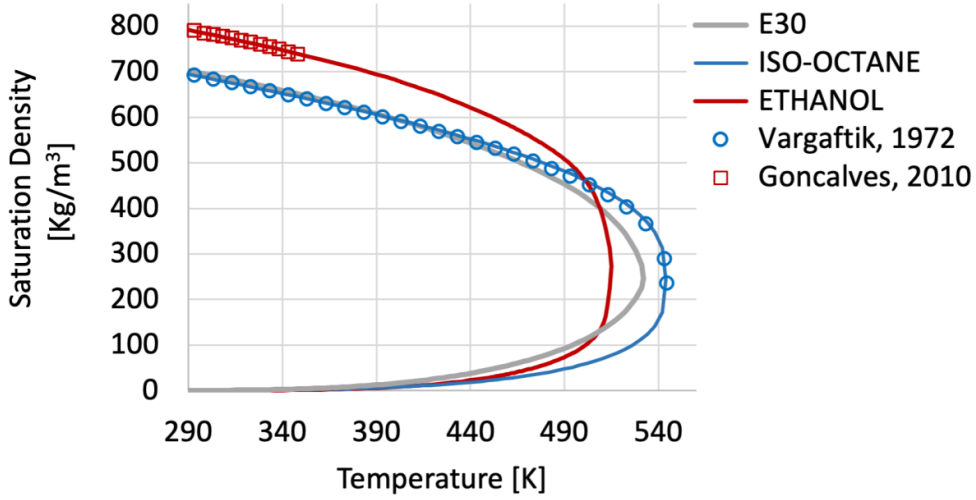
Pe << 1: distillation

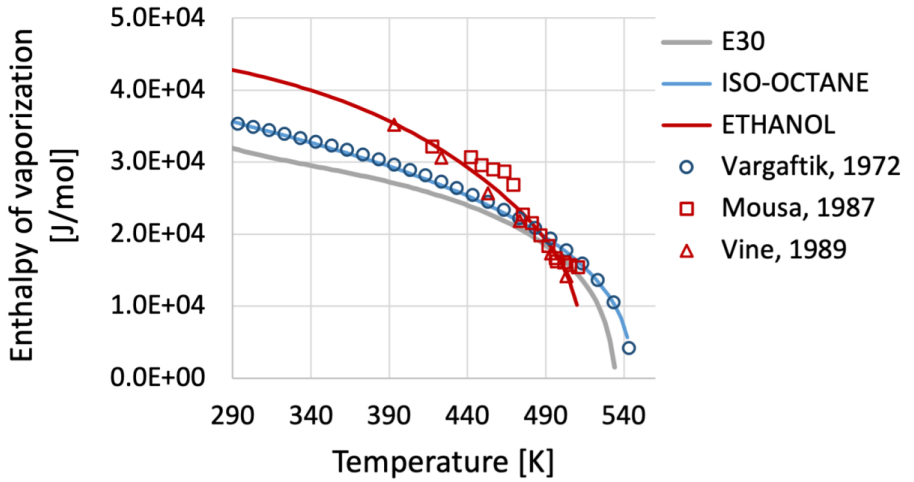
Pe >> 1: co-evaporation

Mixing rules based on the Helmholtz energy of the components with departure function for E30









Computational approach: the interface-capturing code CLSVOF

In collaboration with FSU and the LBNL AMReX co-design center

- Sharp-interface discretization of multi-phase Navier-Stokes equations:
  - ✓ Moment of Fluid interface representation [1]
  - ✓Adaptive Mesh Refinement (AMReX)
  - ✓ Large Eddy Simulation (WALE)
  - ✓ Fully compressible formulation [2]
  - ✓ Non-conformal moving wall boundaries [3,4]
  - ✓ Cavitation [5]
  - ✓ Evaporation and boiling [6,7]

[1] M. Jemison, et al., J. Sci. Comput. 54(2-3) (2013) 454-491.

[2] M. Jemison, M. Sussman, M. Arienti, J. Comput. Phys., 279, (2014) 182-217.

[3] M. Arienti and M. Sussman, Int. J. of Multiphase Flow 59: 1-14 (2014).

[4] M. Arienti and M. Sussman, Int. J. of Multiphase Flow 88, 205-221 (2017).

[5] M. Arienti, E. Wenzel, B.A. Sforzo, C.F. Powell, Proceedings of the Combustion Institute (2020).

[6] E. Wenzel and M. Arienti, ILASS-Americas (2021).

[7] E. Wenzel and M. Arienti, “A conservative framework for the modeling and simulation of evaporation in compressible flow systems” – submitted to JCP.

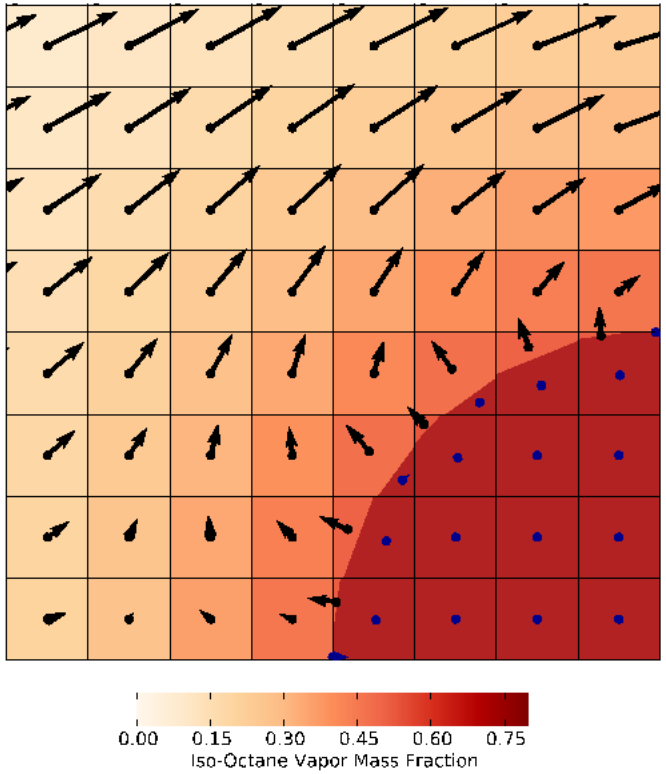
Droplet in crossflow example: relevance of Stefan flow

- E30 has lower vapor pressure, generally leading to larger evaporation rate
- High rates of evaporation provide insulating layer of cool gas and thicken boundary layers
- In turn, the phase change rate depends on the boundary layer thickness

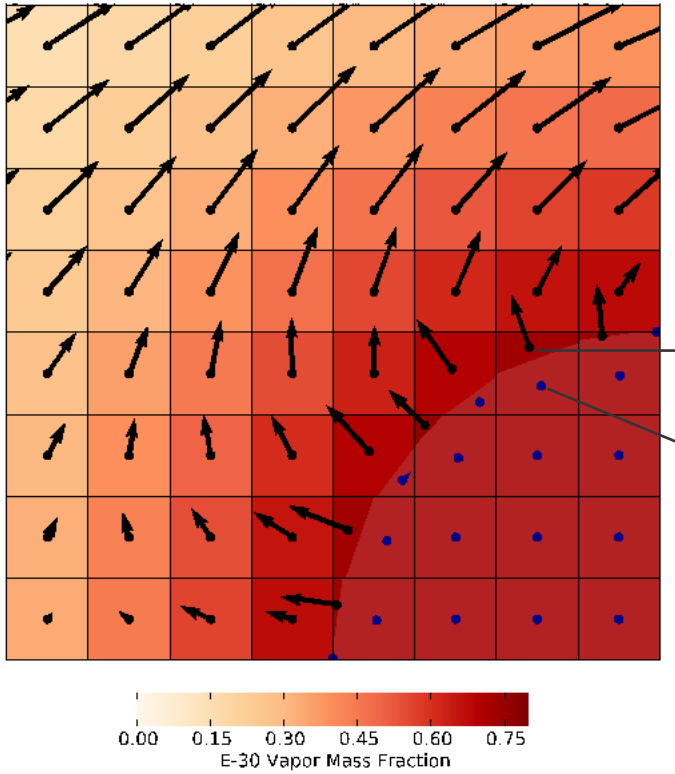
U_{cross} = 10 cm/s

P_g = 3 bar
T_g = 573 K
T_l = 362 K

Iso-octane



E30



Gas phase centroid

Liquid phase centroid

Computational challenge

- Problem: phase change introduces velocity discontinuity at the interface
  - Directly applying the divergence operator would impose an unphysically large momentum increment
- Solution:
  - Introduce cell-centered, phase-specific velocity

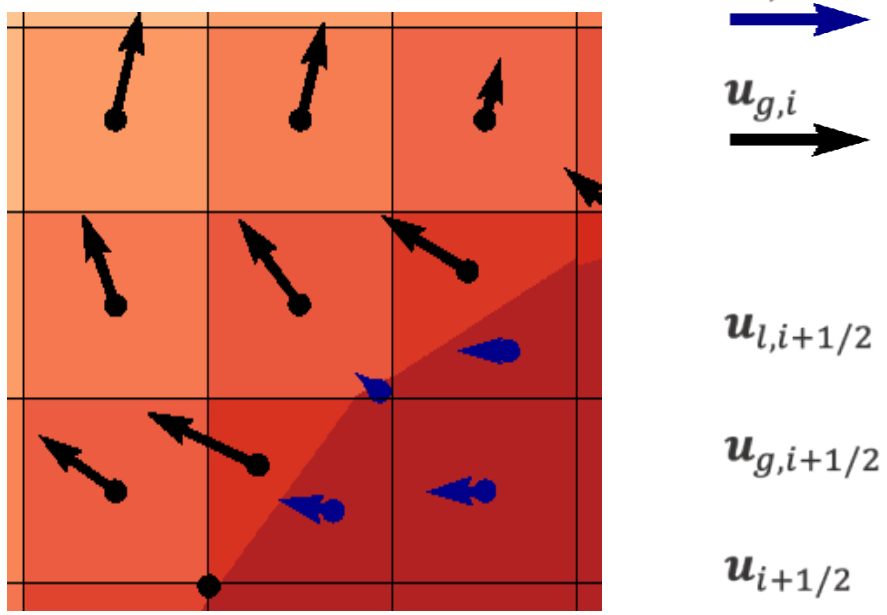
$$u_{g,i}^{n+1} - u_{l,i}^{n+1} = \dot{m}_i^d \left(\frac{1}{\rho_{g,i}^a} - \frac{1}{\rho_{l,i}^a} \right) n_x^d$$

$$\phi_{g,i}^{n+1} \rho_{g,i}^{n+1} u_{g,i}^{n+1} + \phi_{l,i}^{n+1} \rho_{l,i}^{n+1} u_{l,i}^{n+1} = \rho_i^{n+1} u_i^{n+1}$$

  - Introduce face-centered, phase specific velocity

$$u_{g,i+1/2}^{n+1} = \frac{\sum_j u_{g,j}^{n+1} W_{ij}}{\sum_j W_{ij}} \qquad u_{l,i+1/2}^{n+1} = \frac{\sum_j u_{l,j}^{n+1} W_{ij}}{\sum_j W_{ij}}$$

Velocity field diagram



Computational challenge

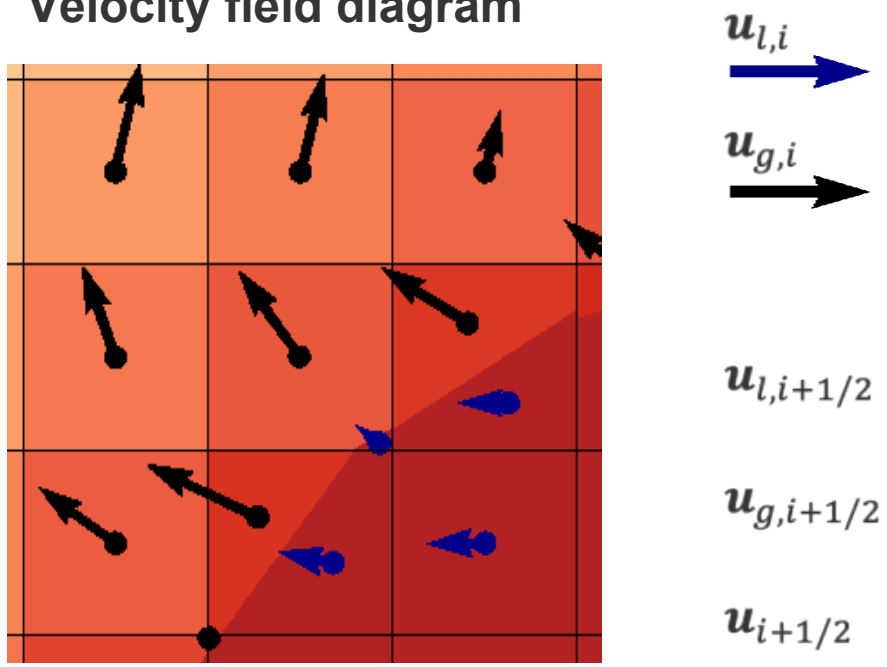
- Problem: phase change introduces velocity discontinuity at the interface
  - Directly applying the divergence operator would impose an unphysically large momentum increment
- Solution:
  - Solve augmented single-fluid pressure equation
  - Conservatively extract phase-specific velocities from single-fluid velocities

$$\phi_{g,i}^{n+1}\rho_{g,i}^{n+1}u_{g,i}^{n+1} + \phi_{l,i}^{n+1}\rho_{l,i}^{n+1}u_{l,i}^{n+1} = \rho_i^{n+1}u_i^{n+1}$$

$$u_{g,i}^{n+1} - u_{l,i}^{n+1} = \dot{m}_i^d \left(\frac{1}{\rho_{g,i}^a} - \frac{1}{\rho_{l,i}^a} \right) n_x^d$$

  - Transport all conserved quantities with phase-specific velocities; transport MOF quantities with liquid-phase velocity; apply consistency constraints

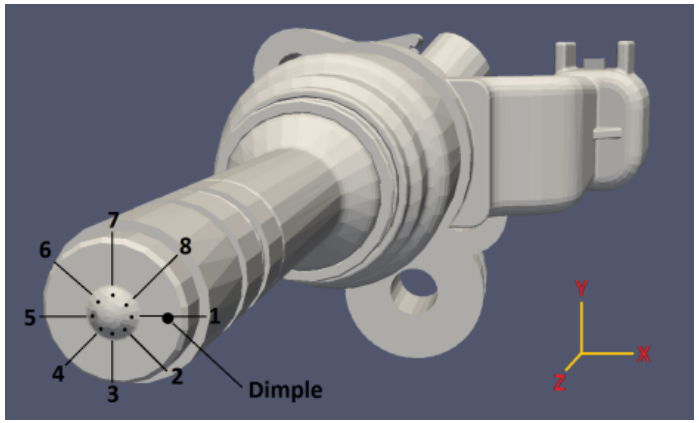
Velocity field diagram



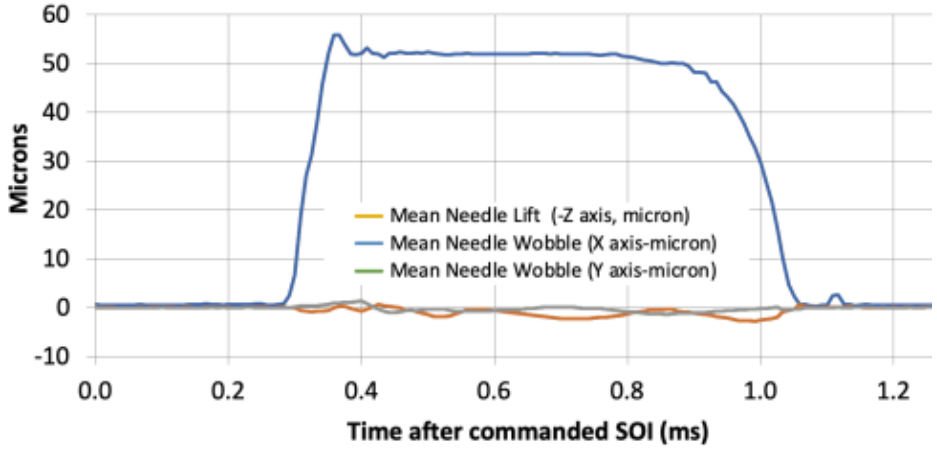
Fully open vs. closing pintle and near-injector phase change

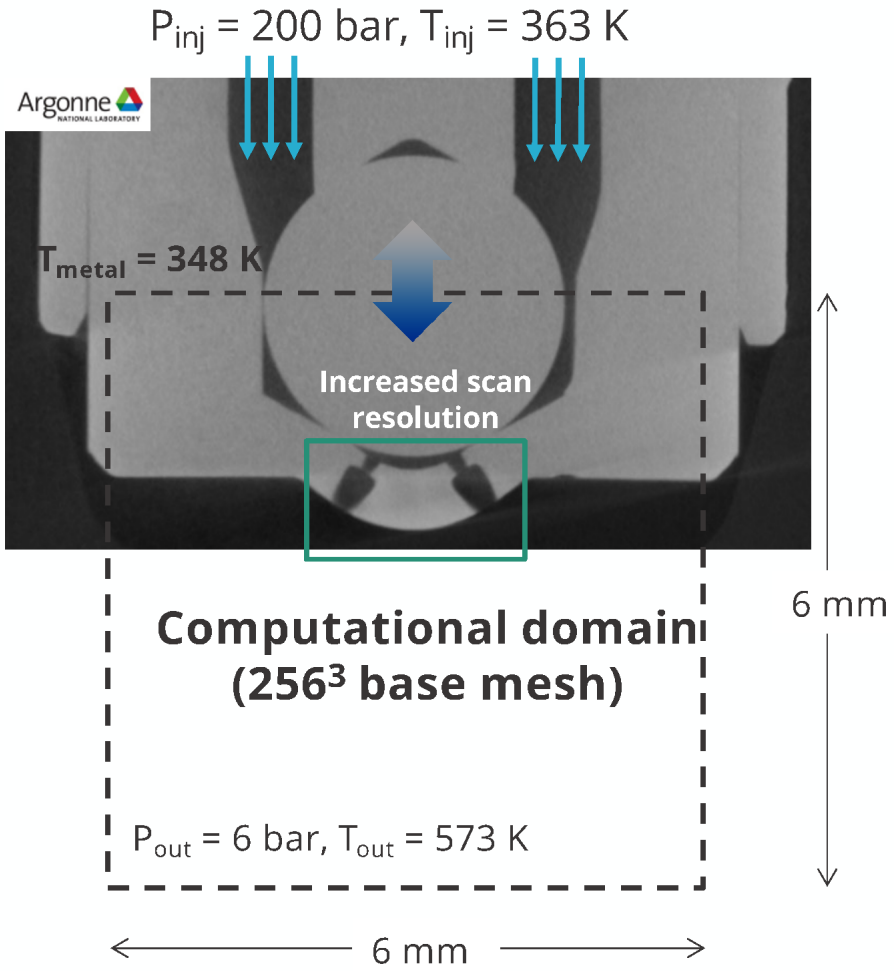
- ECN G1 with up to 450million cells reaching Δx_{min} = 5.86 μm (2 levels of refinement)

Spray G injector



Lift and Wobble for ECN Spray G #28

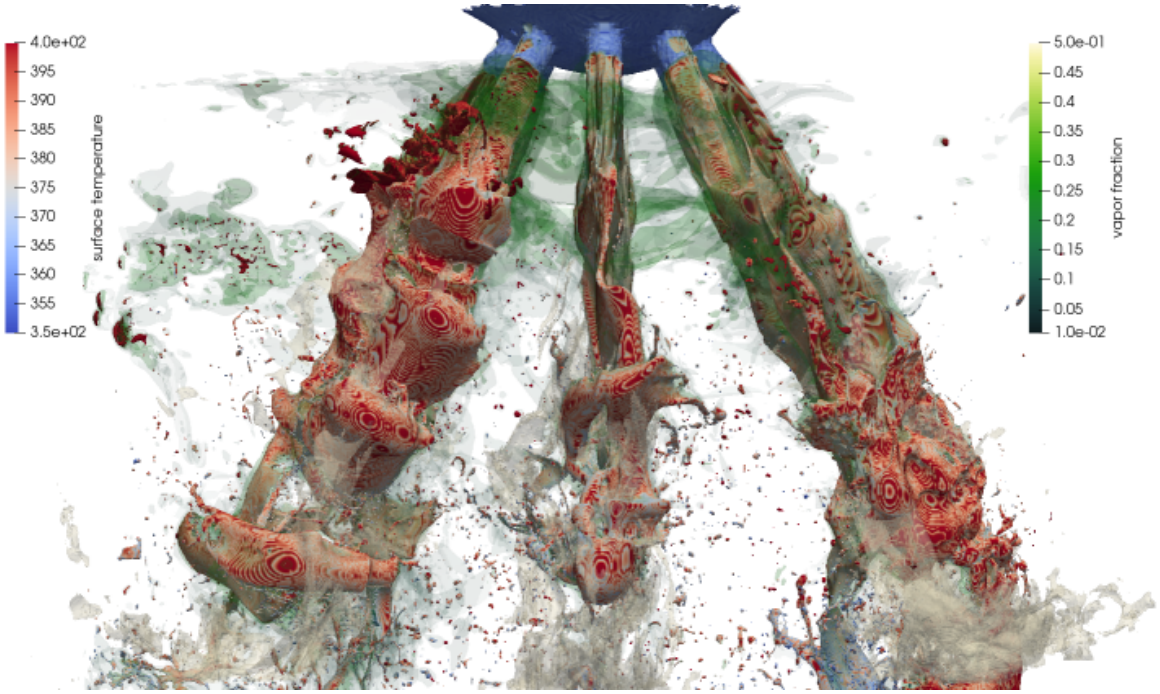




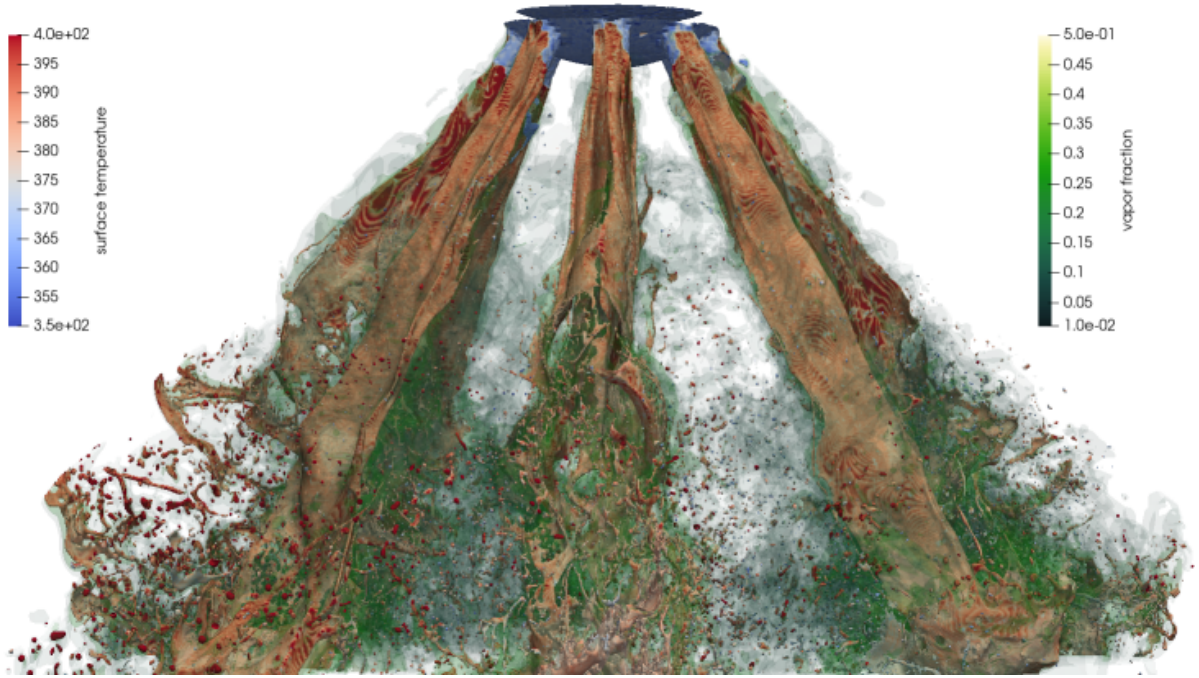
Comparison snapshots with fully open pintle

Observed difference in spray angle and jet structure, with enhanced vaporization for E30

Iso-octane



E30



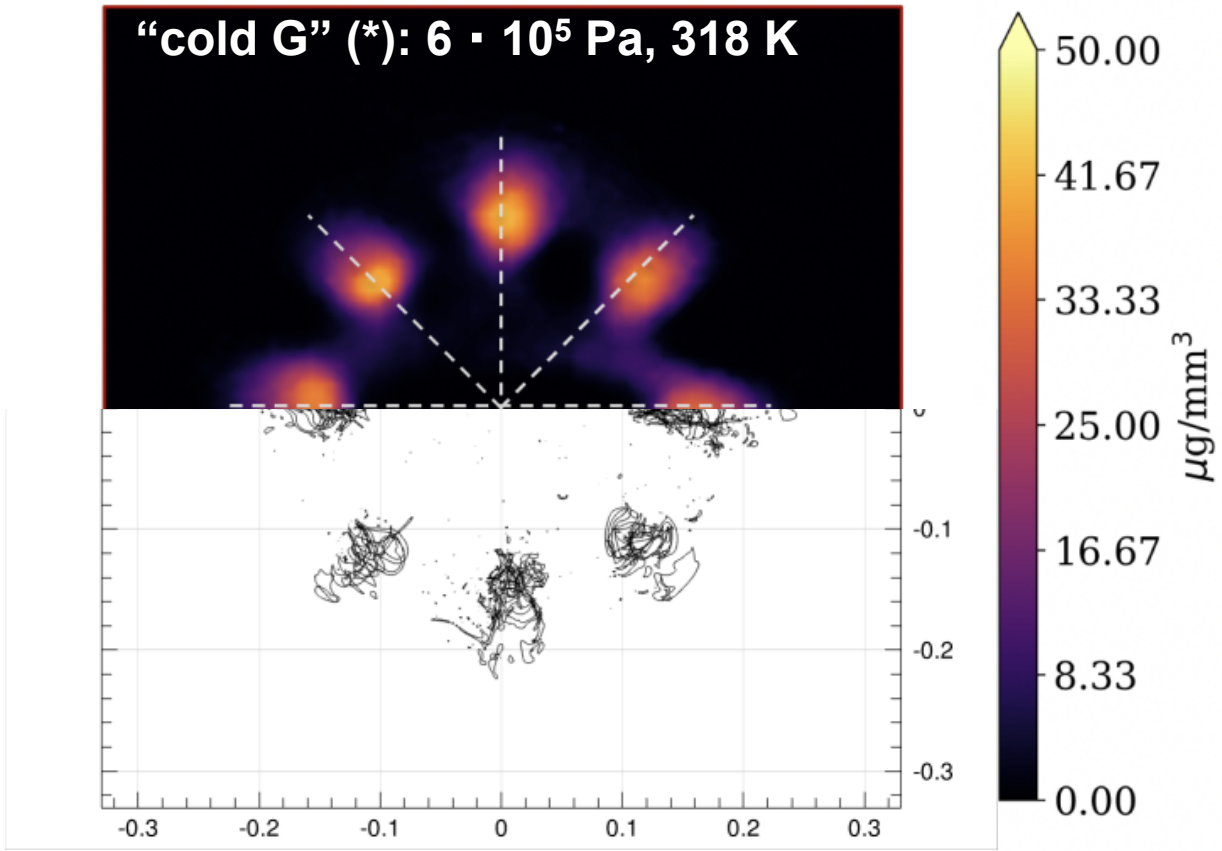
Images obtained by jointly imaging liquid surface (colored by T) and three iso-surfaces for Y_{vapor} = 0.1, 0.25, 0.50

- regression rate: $v_s = \frac{\dot{m}_v}{A_v \rho_l}$ ~ 0.73 cm/s ~ 0.69 cm/s

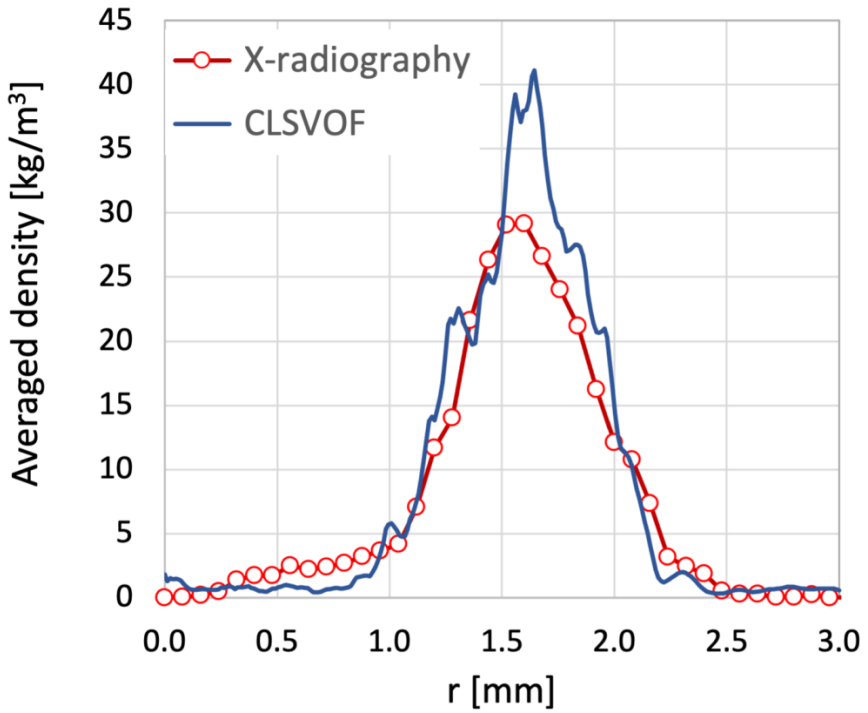
Comparison with data: X-radiography from ANL

Relatively good agreement considering the shorter averaging time of the simulation

Z = 1 mm

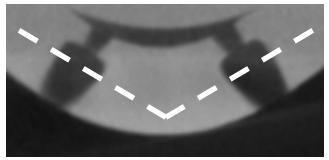


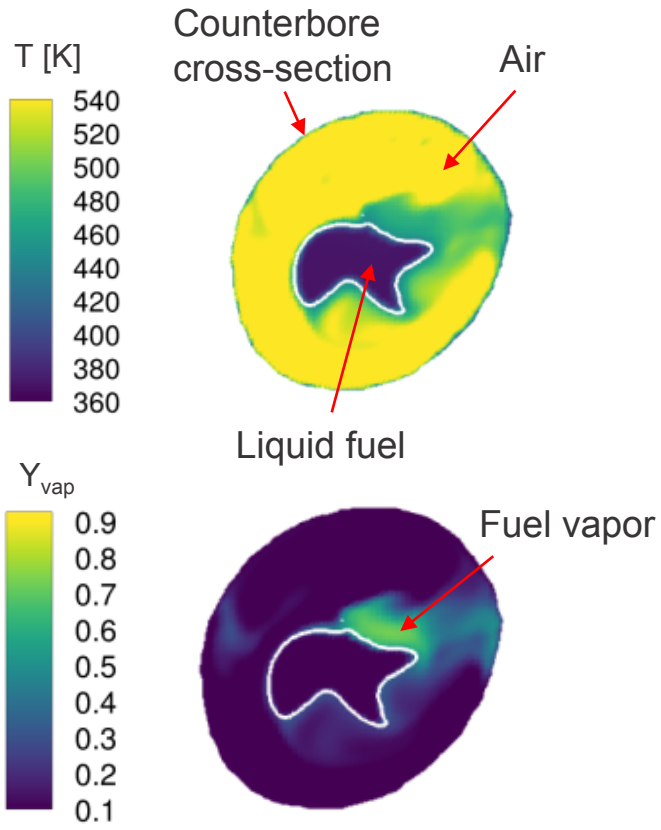
Average of the 8 density profiles passing though the nominal centers of the jets

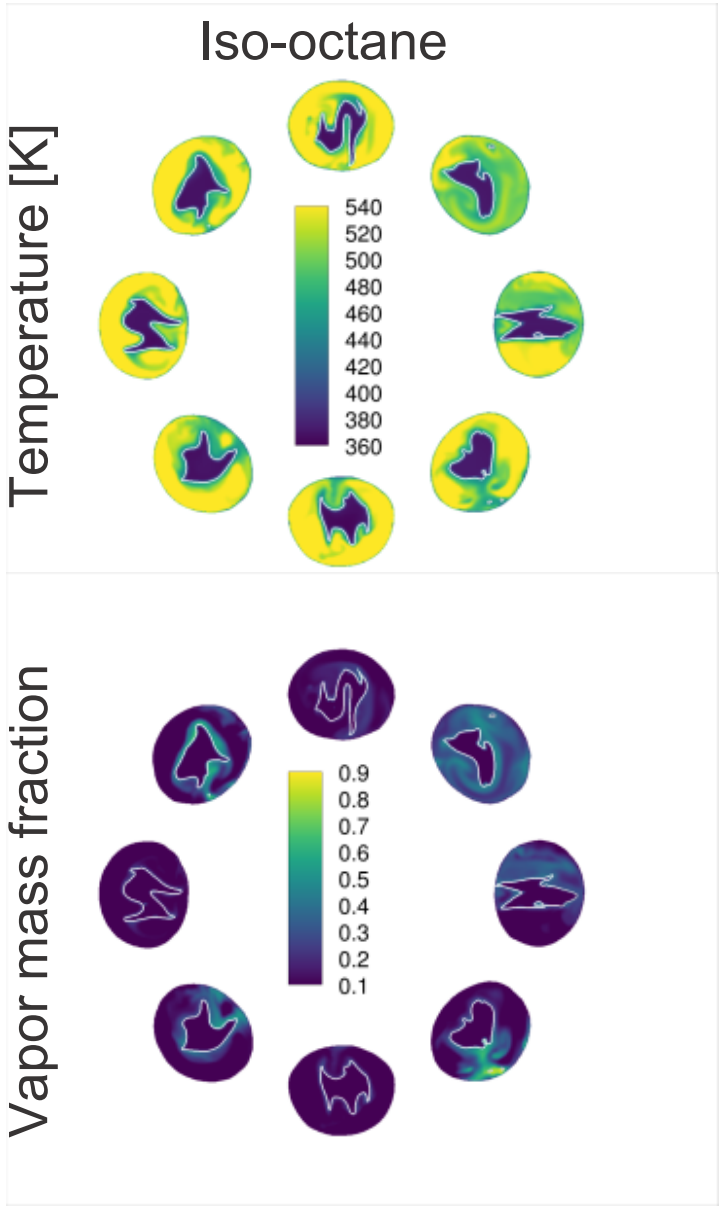


(*) ECN workshops and M. Arienti, E. Wenzel, B.A. Sforzo, C.F. Powell, PCI (2020)

Flow passing through the counterbores at fully open conditions



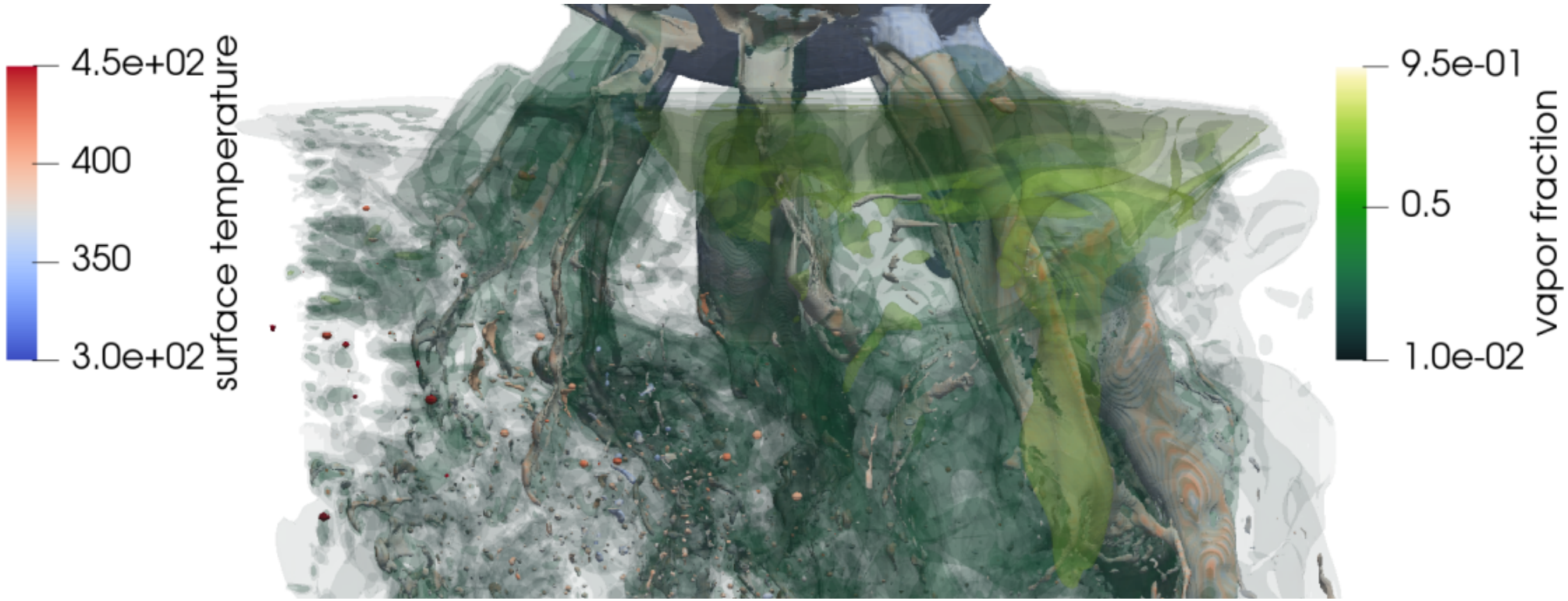




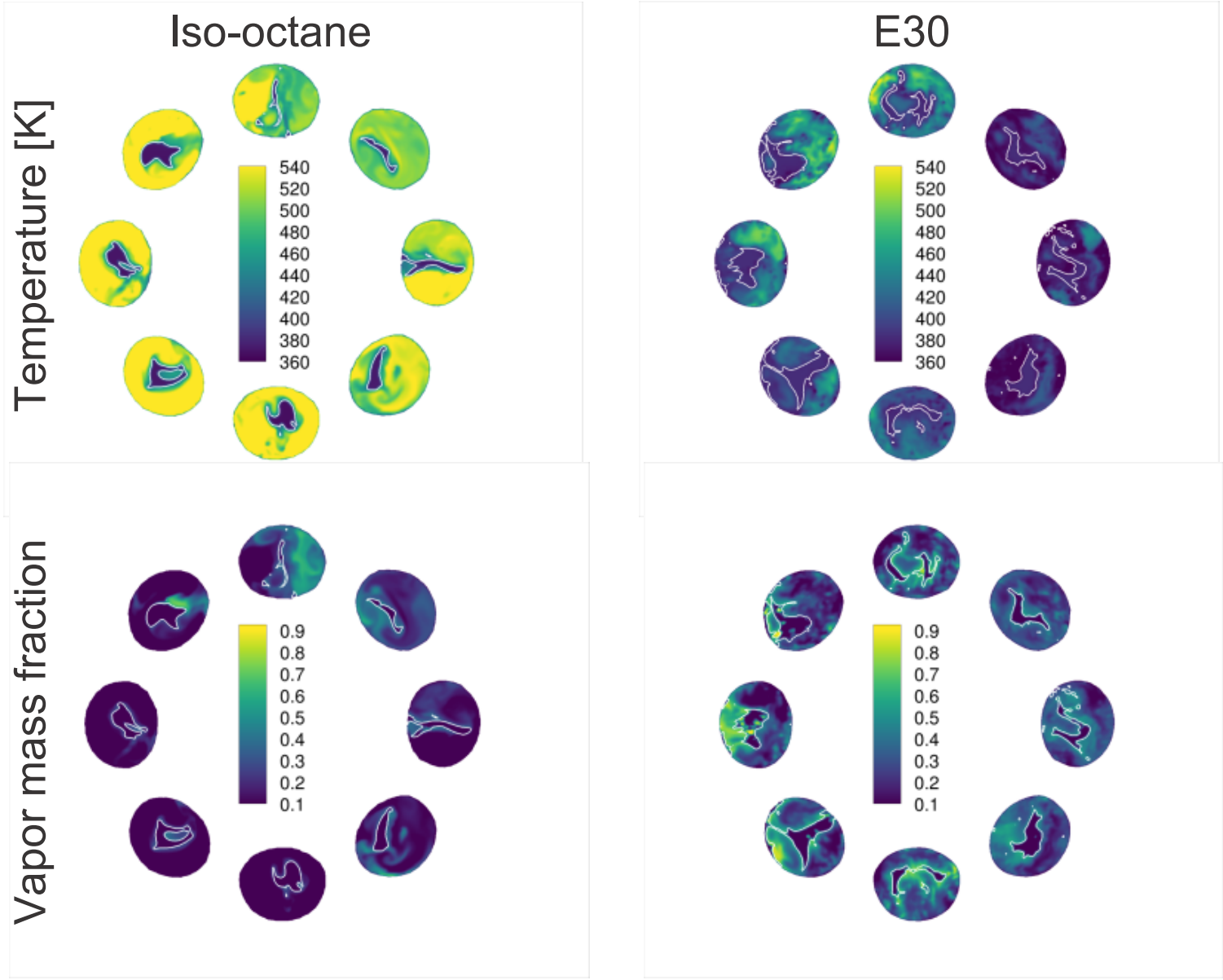
Toward end of injection for iso-octane

Increased amount of vapor – no evidence of boiling

Iso-octane 9 μm gap



Entrainment of hot gas is counterbalanced by cooling effect of E30



Conclusions

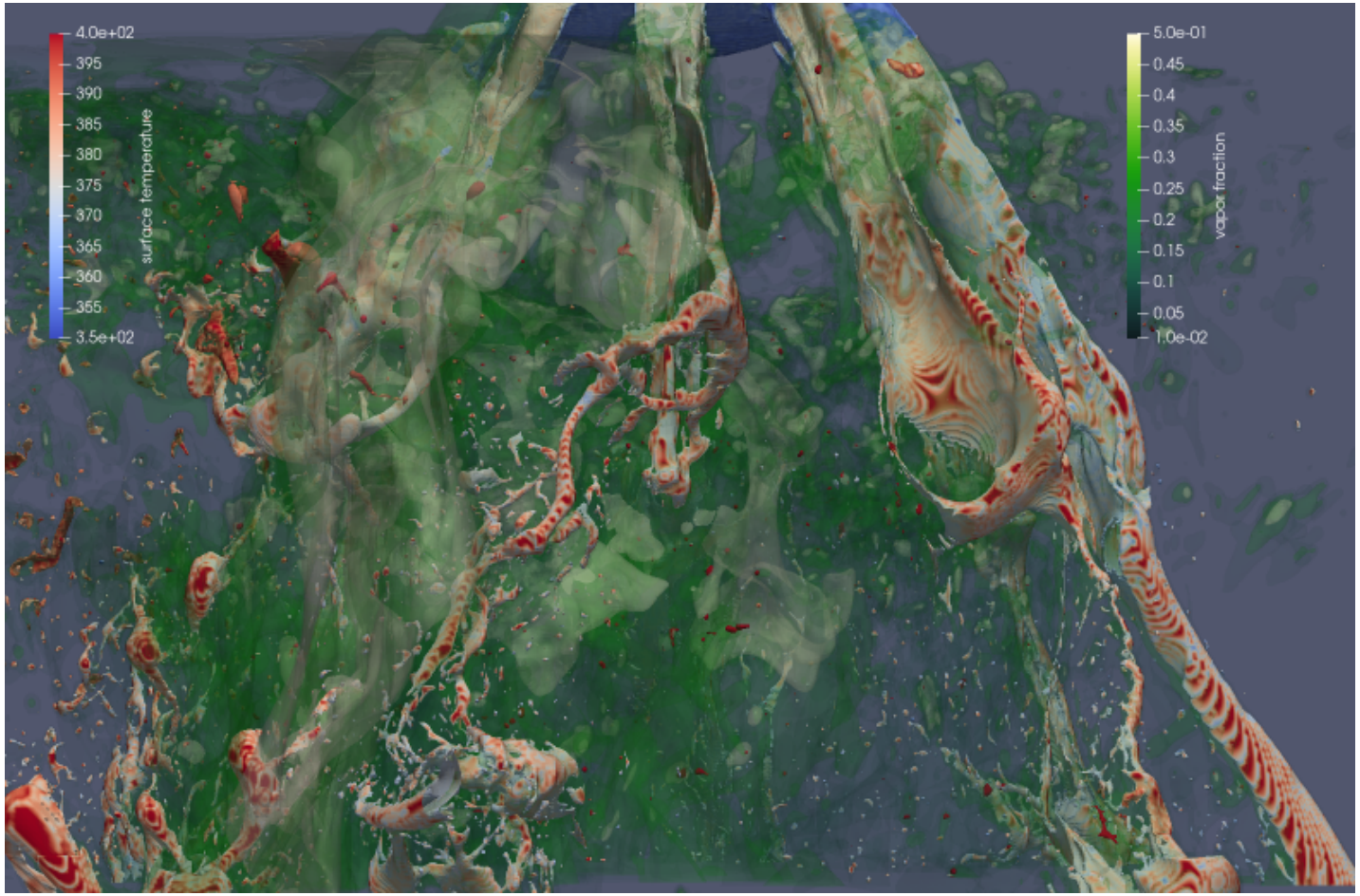
- A sharp-interface method for the multiphase Navier-Stokes equations is applied to calculate the vapor concentration in the counterbores of a gasoline injector
- Pe ~ 3 $\Longrightarrow$ co-evaporation model – but it is only an average value for specific injection conditions
- Differences between neat iso-octane and E30 are particularly clear toward the end of injection
  - The simulation shows that gas stops being entrained in the counterbores during the closing transient;
  - It also shows that the temperature increase at the liquid surface is mitigated by the cooling effect of evaporation only in the case of E30
- Work is in progress to analyze the CFD results and provide further insight into the primary atomization processes

THANK YOU

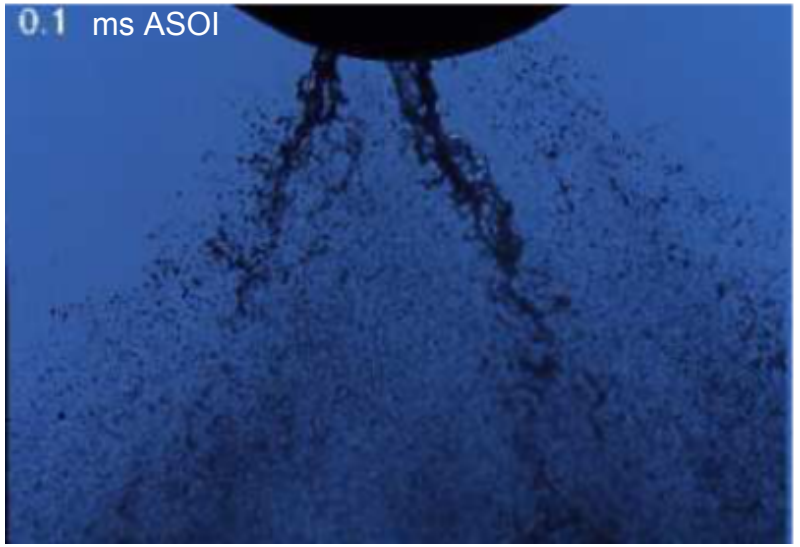
Questions?

Close-up showing evidence of dribbling at end of injection

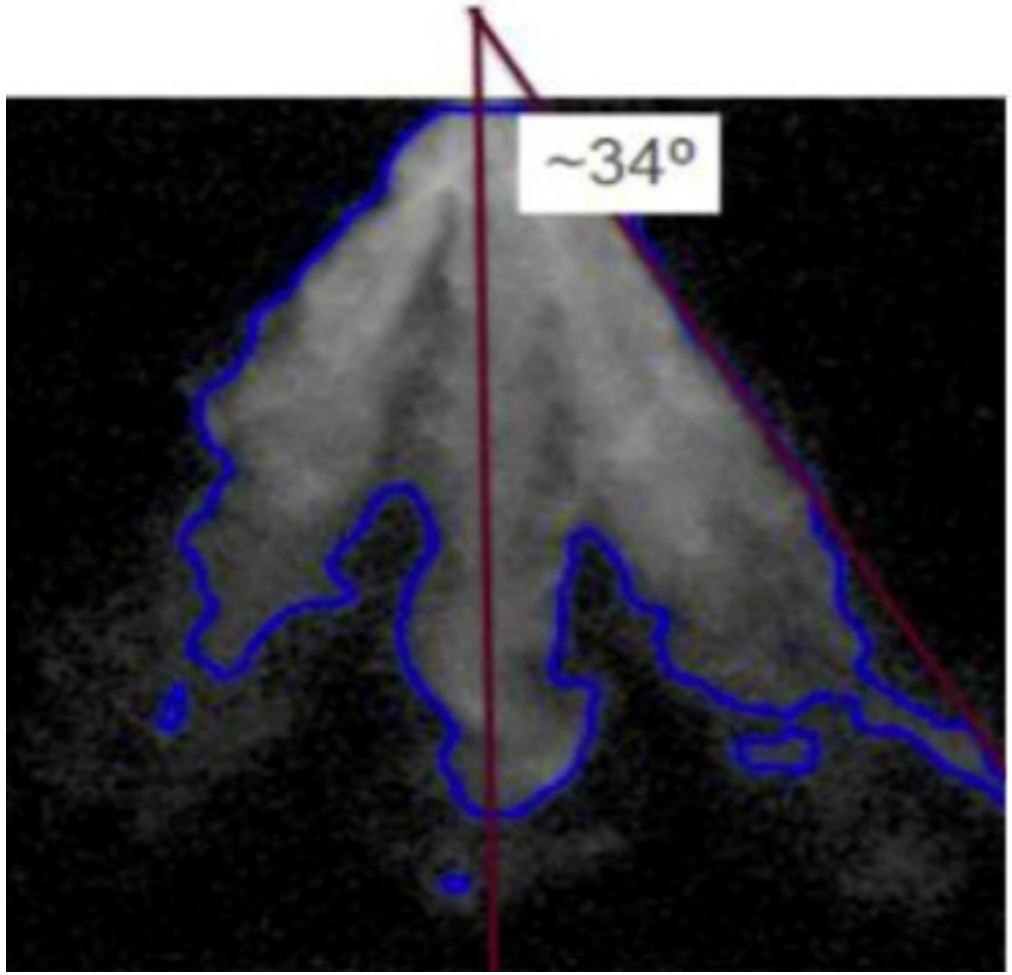
Iso-octane 9 μm gap



commercial gasoline with 5% ethanol



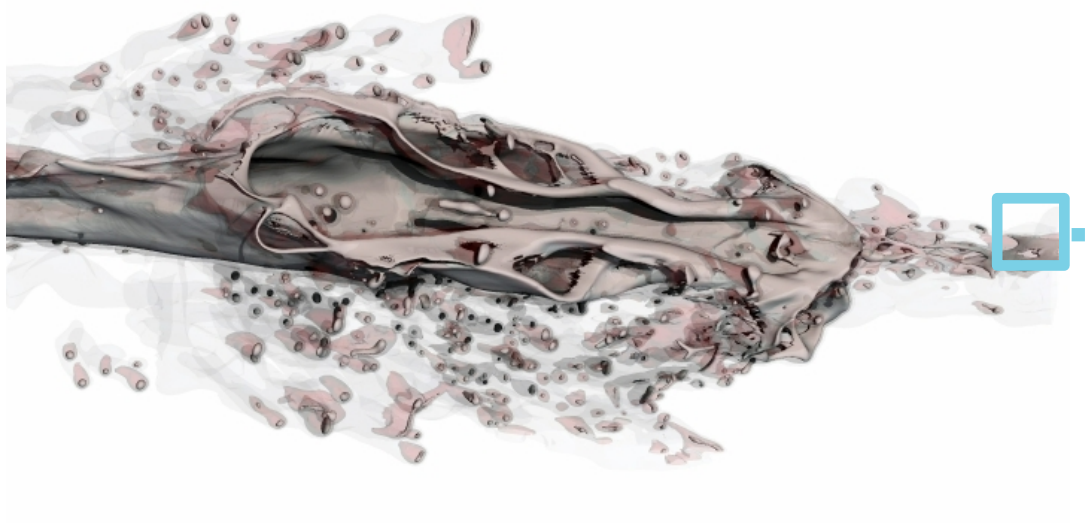
Six-hole injector at ambient conditions Hélie, et al., International Journal of Engine Research 22.1 (2021): 125-139.


~34°

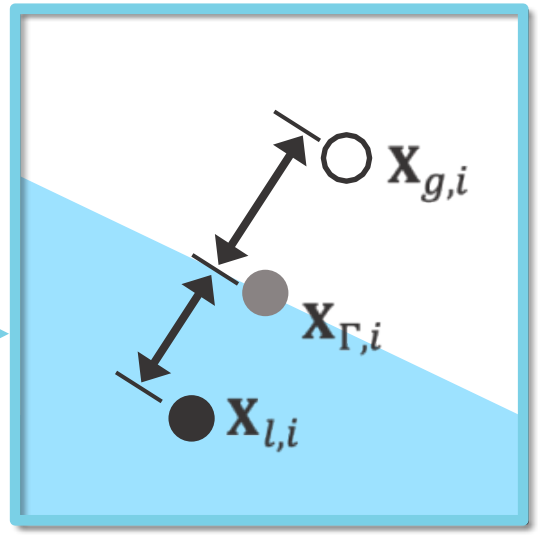
Numerical discretization of evaporating fuel sprays

- Sharp-interface discretization (no Lagrangian droplets or associated models)
- Liquid and gas treated as compressible
- Conserved quantities stored at liquid/gas center of mass in each computational cell
- Diffusion and phase change defined by a novel, operator-split methodology that is consistent and conservative

Windowed view of full-scale spray simulation



Interface reconstruction in computational cell i



Navier-Stokes equations solved at Liquid/Gas centers-of-mass $\mathbf{X}_{l,i}$ and $\mathbf{X}_{g,i}$

Interfacial quantities required at $\mathbf{X}_{\Gamma,i}$ to quantify heat/mass transfer

Operator-split, mixed-time level integration approach

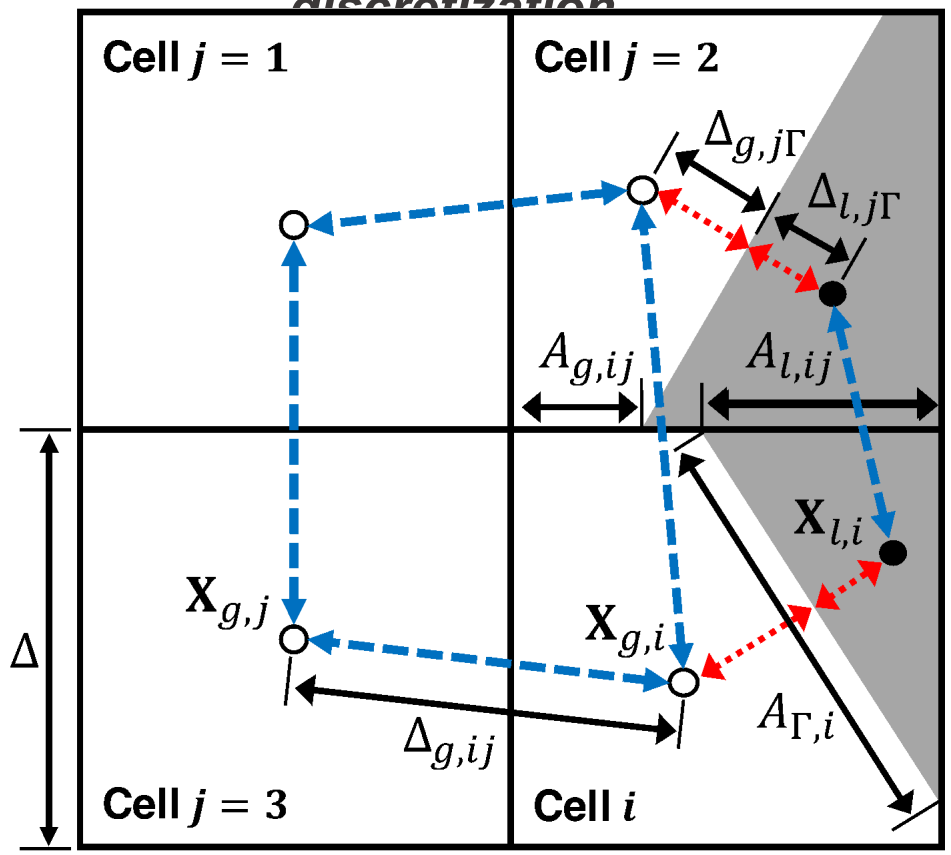
- Sharp interfaces require implicit time integration
- Capillary dynamics require small time steps
- Phase change systems are tightly-coupled

Solution:

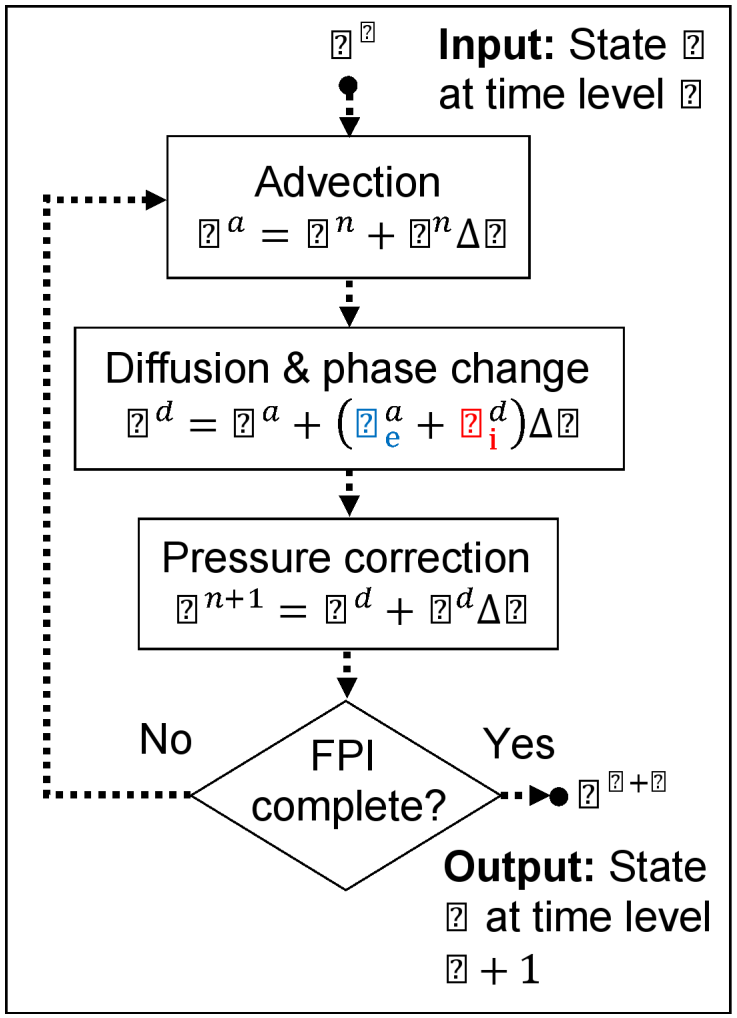
Implicit intra-cell fluxes

Explicit inter-cell fluxes

Spatial discretization

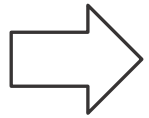


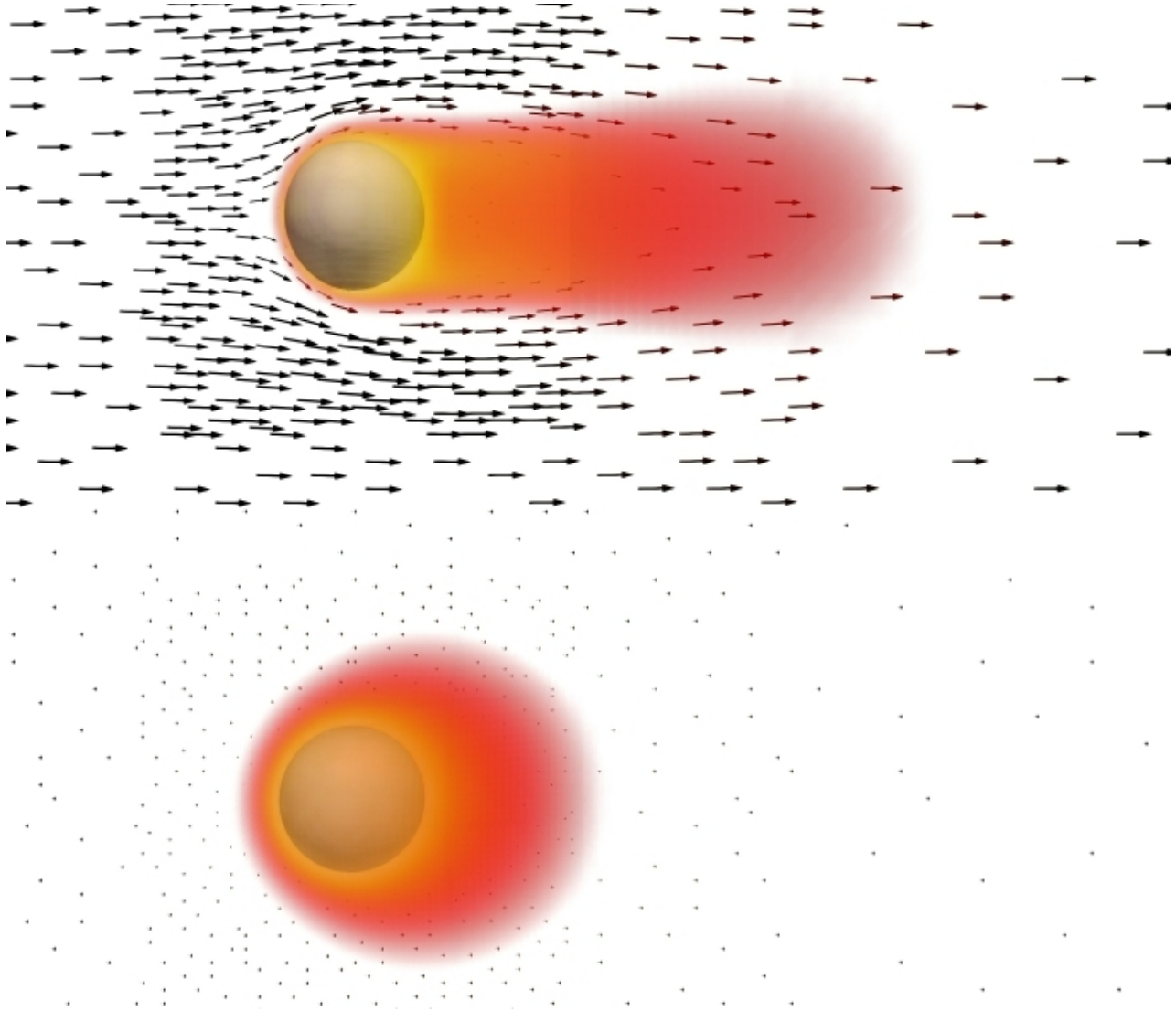
Temporal discretization



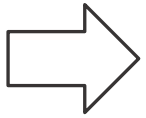
200 µm diameter iso-octane droplets evaporating

U_{cross} = 500 cm/s





U_{cross} = 62.5 cm/s



P_g = 3 bar
T_g = 573 K
T_l = 362 K