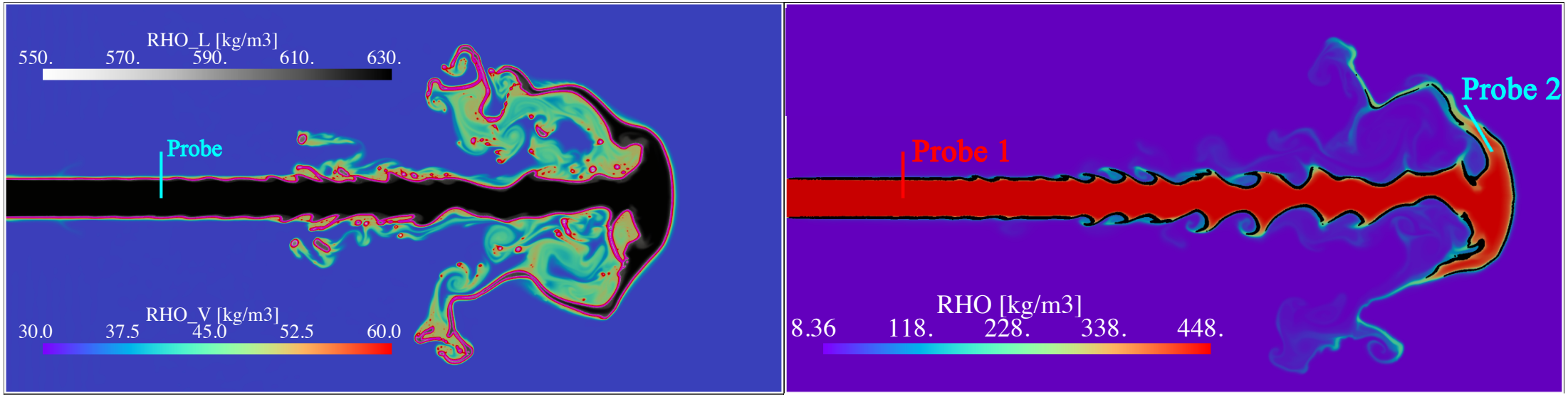
Advanced Modeling & Simulation (AMS) Seminar Series
NASA Ames Research Center, April 18th, 2024

Numerical Modeling of High-Pressure Multi-phase Multi-species Flows



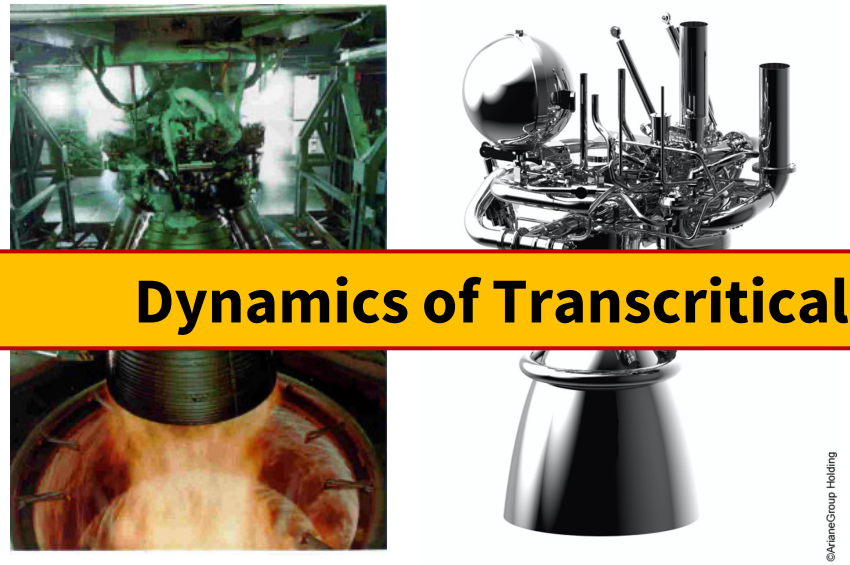
Nguyen Ly, Matthias Ihme
Department of Mechanical Engineering, Stanford University
Mike Hicks, Daniel Dietrich
NASA Glenn Research Center
Uday Hegde
Case Western Reserve University
Jeffrey West
NASA Marshall Space Flight Center

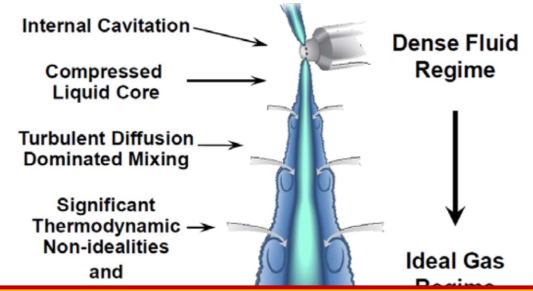
Space Technologies Graduate Research Opportunity Fellowship

Stanford | ENGINEERING

Relevant Applications for Supercritical Fluids

- Supercritical fluids in engineering systems are multi-species





Dynamics of Transcritical Multi-species Flows



Vulcain 1st Stage Rocket Engine for Ariane 5,
H_2/O_2 Injection
Prometheus Reusable Rocket Engine,
CH_4/O_2 Injection

Credit: European Space Agency

Diesel Supercritical Spray Injection
Heavy Hydrocarbon/Air

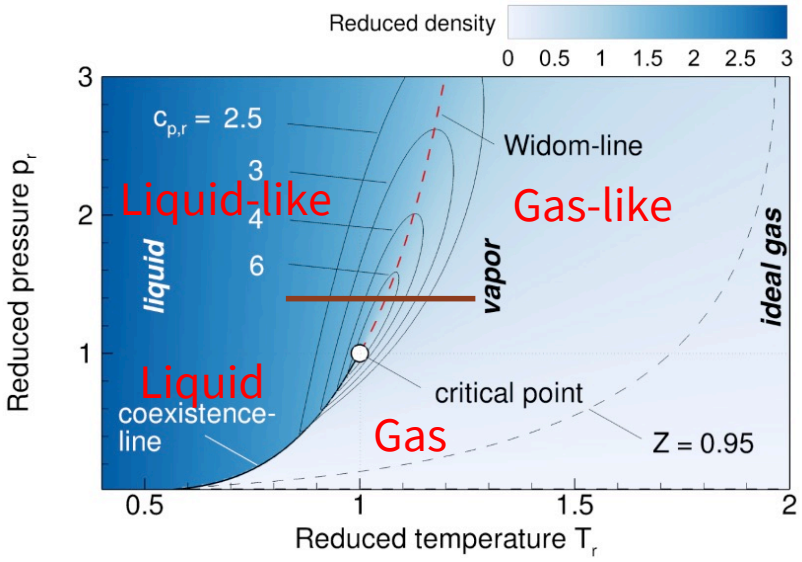
Credit: University of Alabama and DOE

Contents

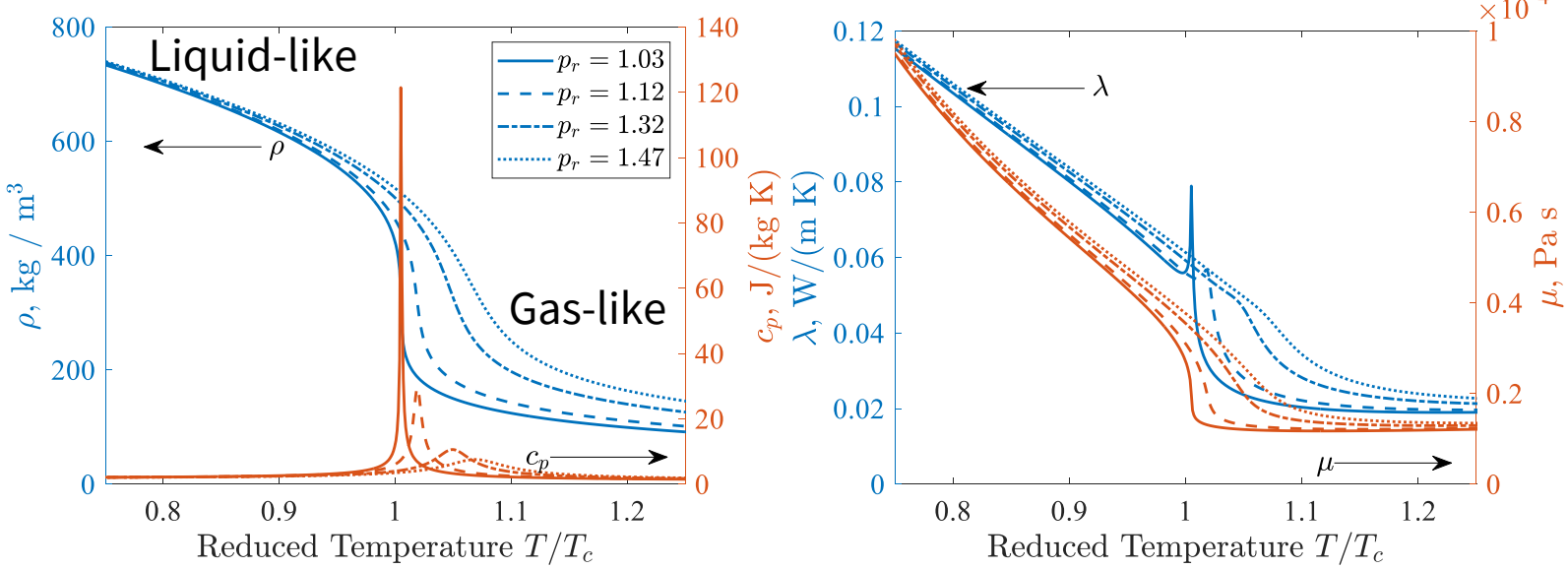
- Theory:
  - Thermodynamics of mixtures
  - Nanoscale interface-resolving formulation
  - Regularized-interface formulation
- Application
  - Transcritical droplet transition
  - High-pressure fuel injection
  - LOX/GH2 mixing layer
  - Transcritical shock/droplet interaction
- Conclusion

Supercritical/Transcritical Flows

- Definition: Fluids crossing to and from subcritical/supercritical temperatures, at supercritical pressures[1]
- Anomalous thermophysical behavior: characteristic peak of c_p at the Widom line, sharp gradients in ρ, μ, λ
- Strong non-linearities and repulsive intermolecular forces (collectively, non-ideal effects)



p_r *vs* T_r Schematic (Widom Line)



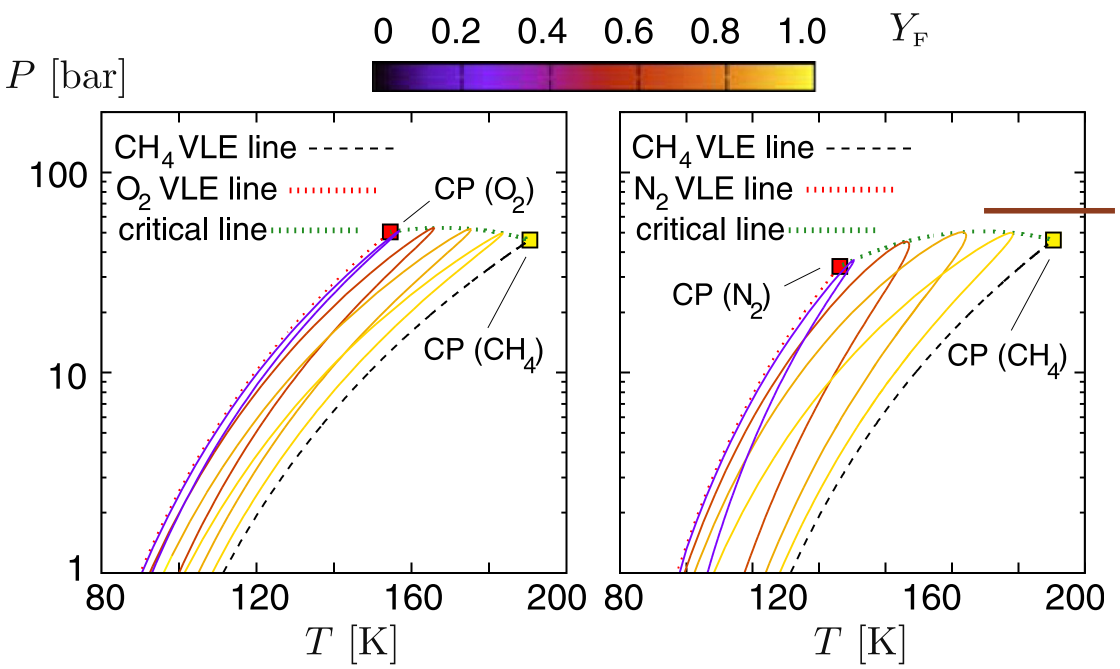
NIST Thermophysical Quantities for N_2

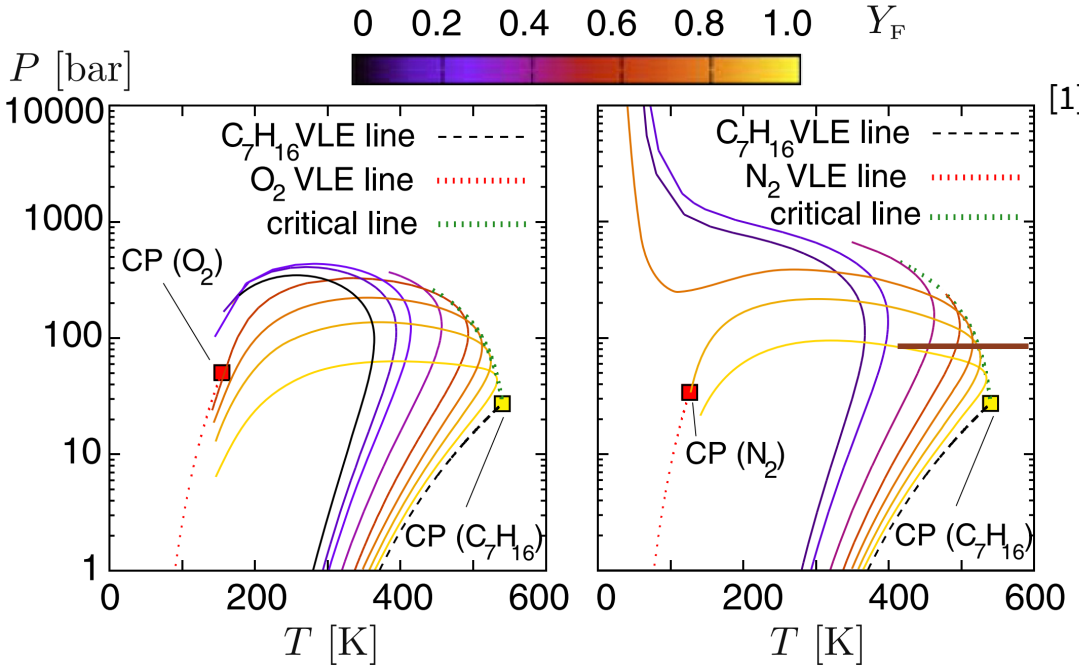
Phase Transfer: Liquid/Gas + Liquid-like/Gas-like

[1] Simeoni, G. G. et. al., *Nat. Phys.* (2010)

[1] Jofre, L. & Urzay, J., 2021. *Progress in Energy and Combustion Science*, *82*, p.100877.
[2] Rowlinson, J.S. & Swinton, F., 2013. *Liquids and liquid mixtures: Butterworths monographs in chemistry.*

Binary mixture thermodynamics

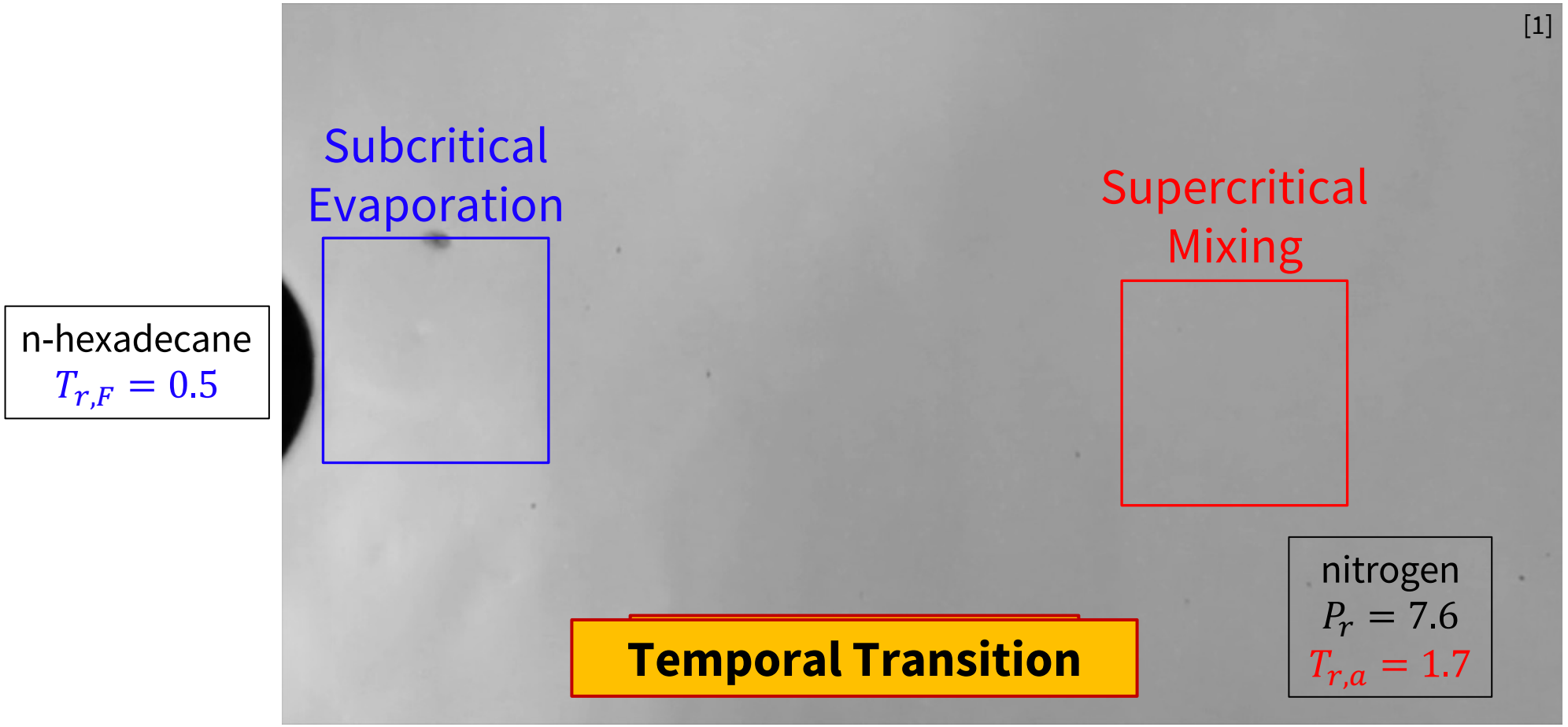




[1]

- For miscible (Type I) mixture: transition depends on pressure, a global parameter.
- For immiscible (Type III) mixture: transition depends on temperature, a local parameter.

Experimental Evidence of High-Pressure Phase Distinction



[1] Crua, C., Manin, J. and Pickett, L.M., 2017. *Fuel*, *208*, pp.535-548.

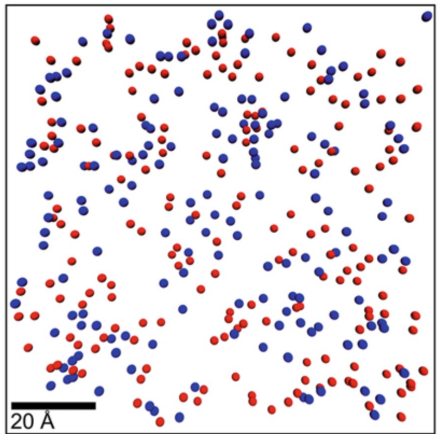
[1] Raju, M. et al., 2017. Scientific reports, 7(1), p.3027.
[2] Mo, G. & Qiao, L., 2017. Combustion and Flame, 176, pp.60-71.
[3] Davis, H.T. & Scriven, L.E., 1982. Adv. in Chemical Physics, 49, pp.357-454.

Linear-Gradient Theory and Interface-Resolving Equations

- Hierarchy of thermodynamic model:

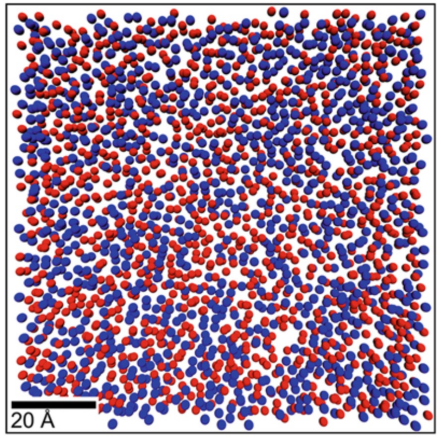
Ideal Gas $P = \rho RT$ —(High-density correction: 0th moment of interaction potential)→ Cubic EOS $P = \frac{RT}{v-b} - \frac{a}{v^2}$ —(High-gradient correction: 1st moment of interaction potential)→ Linear-Gradient Theory [3]

$$f_{GD} = f + \frac{1}{2\rho}\sum_i\sum_j \kappa\nabla(\rho Y_i)\cdot\nabla(\rho Y_j)$$



[1]

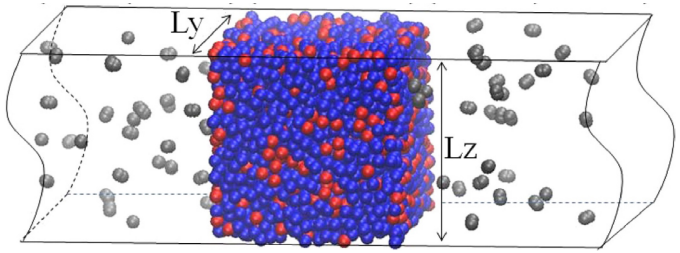
Low density



[1]

High density

[2]

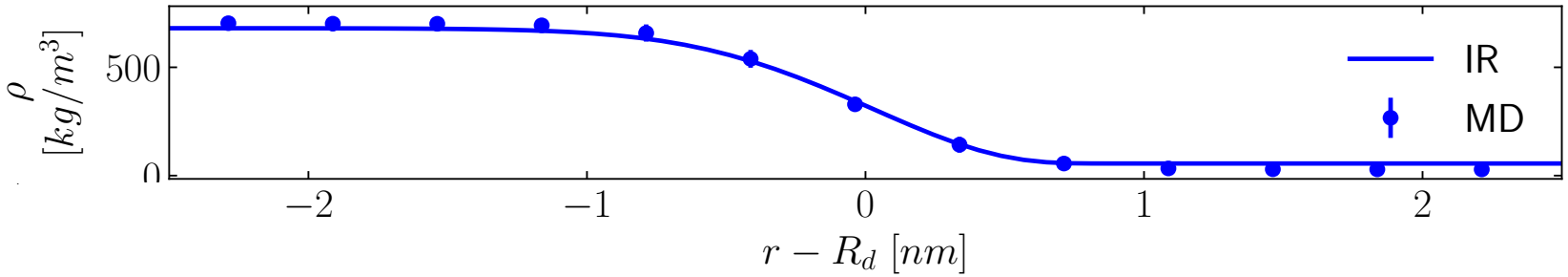


High density gradient

[1] Davis, H.T. & Scriven, L.E., 1982. Adv. in Chemical Physics, 49, pp.357-454.
[2] Gaillard, P. et al., 2016. Combustion Theory and Modelling, 20(3), pp.486-520.
[3] Jofre, L. & Urzay, J., 2021. Prog. in Energy and Comb. Science, 82, p.100877.

Linear-Gradient Theory and Interface-Resolving Equations

- LGT allows for continuum-based construction of the nanoscale interface: [1]



n-dodecane/nitrogen, $P_r = 3.30, T_r = 0.55$

- Couple LGT with Navier-Stokes equations to model dynamics of interfacial regularization [2,3]

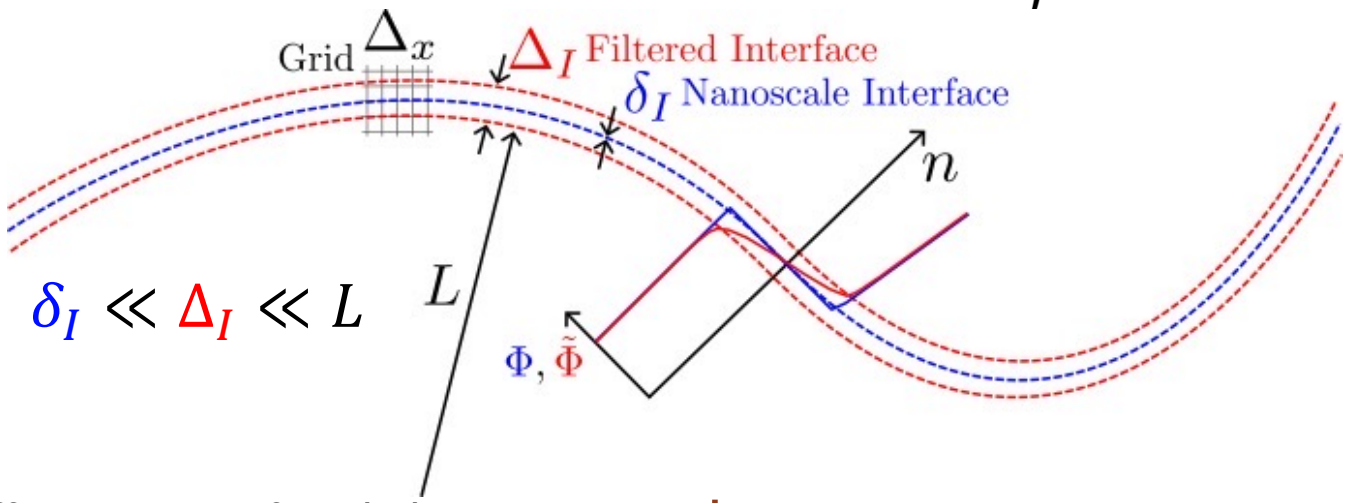
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0,$$
$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = \nabla \cdot (-P_{GD}\boldsymbol{I} + \boldsymbol{\mathcal{K}} + \boldsymbol{\tau}),$$
$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i \mathbf{u}) = -\nabla \cdot (\boldsymbol{J}_i + \boldsymbol{\mathcal{J}}_i),$$
$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E \mathbf{u}) = \nabla \cdot [(-P\boldsymbol{I} + \boldsymbol{\mathcal{K}} + \boldsymbol{\tau}) \cdot \boldsymbol{u}] - \nabla \cdot (\boldsymbol{q} + \boldsymbol{\mathcal{Q}}),$$

- Issues:
  - Nanoscale resolution
  - High-order derivatives

Upscaling the formulation

Apply Gaussian Filter on IR equations

$$\overline{\psi}(\boldsymbol{x},t) \equiv \int \psi(\boldsymbol{\xi},t) G(\boldsymbol{x}-\boldsymbol{\xi};\Delta_I) d\boldsymbol{\xi}$$



$$\delta_I \ll \Delta_I \ll L$$

Standard Species Diffusion + Interfacial Sharpening

$$\boldsymbol{J}_i \xrightarrow{G(\boldsymbol{x}-\boldsymbol{\xi};\Delta_I)} \widehat{\boldsymbol{J}}_i + \overline{J_i^0}\hat{\mathbf{n}},$$ (Resolved + Unresolved Parts)

Resolved: Obtained from filtered flow field

Unresolved: Obtained from reference steady-state IR solution

Interfacial Diffusion

$$\boldsymbol{\mathcal{J}}_i \xrightarrow{G(\boldsymbol{x}-\boldsymbol{\xi};\Delta_I)} -D_i^{\mathrm{reg}} \nabla(\overline{\rho}\tilde{Y}_i)$$ (Unresolved Part)

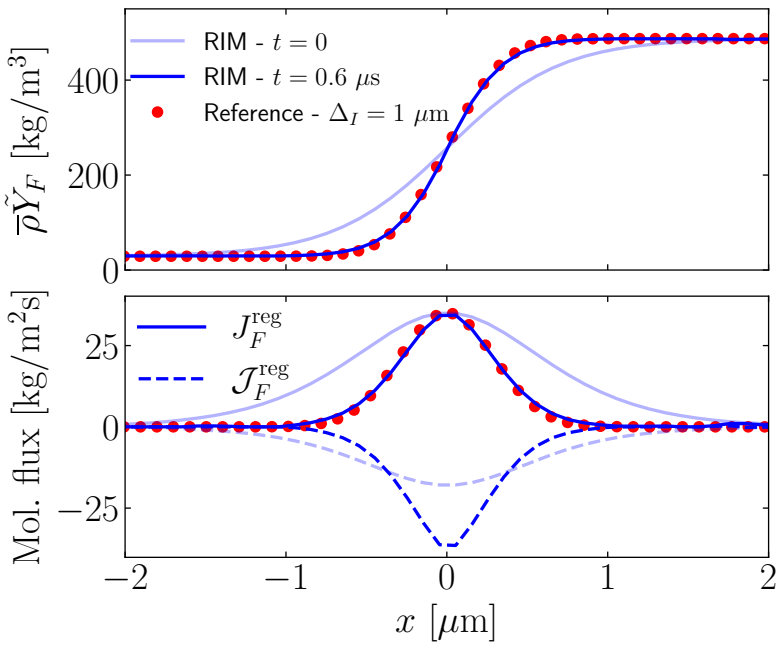
$$D_i^{\mathrm{reg}}(\tilde{\mathbf{Y}};P,T) \equiv \frac{\overline{J_i^0}}{\partial_n(\overline{\rho}\tilde{Y}_i)^0}$$

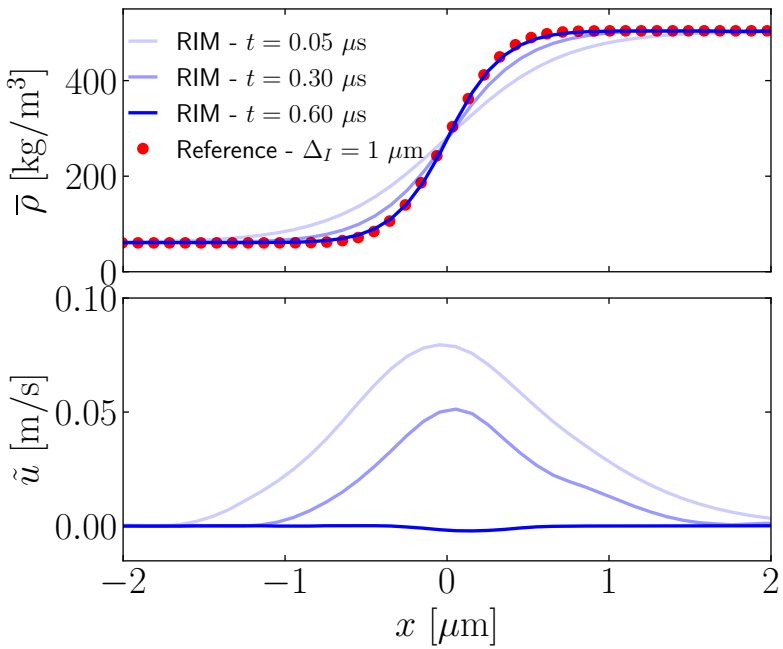
Resolved: Negligible on filtered flow field

Unresolved: Obtained from reference steady-state IR solution

Consistency of SGS model

n-heptane/nitrogen interface, $P_r = 1.85, T_r = 0.66. \Delta_I = 1\mu m$





Steady-state solution to RIM for a planar interface is identical to the filtered profile of the IR solution.

Nanoscale interface regularization dynamics are recovered in filtered scale

Regularized-Interface Method

- Transport equation for filtered flow properties
- Sub-grid-scale terms from filtering of IR equation:
  - Sharpening and diffusion terms of the species composition across the interface
  - Surface tension effects via anisotropic part of Korteweg tensor

$$\frac{\partial \overline{\rho}}{\partial t} + \nabla \cdot (\overline{\rho}\tilde{\mathbf{u}}) = 0,$$

$$\frac{\partial \overline{\rho}\tilde{\mathbf{u}}}{\partial t} + \nabla \cdot (\overline{\rho}\tilde{\mathbf{u}}\tilde{\mathbf{u}}) = \nabla \cdot (-\overline{P}\boldsymbol{I} + \boldsymbol{\mathcal{K}}^{\mathrm{reg}}_{aniso} + \widehat{\boldsymbol{\tau}}),$$

$$\frac{\partial \overline{\rho}\tilde{Y}_i}{\partial t} + \nabla \cdot (\overline{\rho}\tilde{Y}_i\tilde{\mathbf{u}}) = -\nabla \cdot (\widehat{\boldsymbol{J}}_i + \boldsymbol{J}^{\mathrm{reg}}_i - \boldsymbol{\mathcal{J}}^{\mathrm{reg}}_i),$$

$$\frac{\partial \overline{\rho}\tilde{E}}{\partial t} + \nabla \cdot (\overline{\rho}\tilde{E}\tilde{\mathbf{u}}) = \nabla \cdot \left[\left(-\overline{P}\boldsymbol{I} + \boldsymbol{\mathcal{K}}^{\mathrm{reg}}_{aniso} + \widehat{\boldsymbol{\tau}}\right) \cdot \tilde{\mathbf{u}}\right] - \sum_{i=1}^{N-1} \nabla \cdot \left(\overline{(h_i - h_N)}\left(\widehat{\boldsymbol{J}}_i + \boldsymbol{J}^{\mathrm{reg}}_i + \boldsymbol{\mathcal{J}}^{\mathrm{reg}}_i\right)\right) - \nabla \cdot \widehat{\boldsymbol{q}},$$

Resolved diffusion fluxes

$$\widehat{\boldsymbol{J}}_i = -\sum_{j=1}^{N-1} \frac{\overline{L}_{ij}}{\overline{T}} \left[\nabla(\overline{\mu}_j - \overline{\mu}_N) - (\overline{s}_j - \overline{s}_N)\nabla\overline{T}\right]$$

$$\widehat{\boldsymbol{\tau}} = \overline{\eta}\left[\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^T - \frac{2}{3}(\nabla \cdot \tilde{\mathbf{u}})\mathbf{I}\right],$$

$$\widehat{\boldsymbol{q}} = -\overline{\lambda}\nabla\overline{T}.$$

Modeled interfacial fluxes

$$\boldsymbol{\mathcal{K}}^{\mathrm{reg}}_{aniso} = F^{\mathrm{reg}}(\mathbf{I} - \hat{\mathbf{n}} \otimes \hat{\mathbf{n}}),$$

$$\boldsymbol{J}^{\mathrm{reg}}_i = \overline{J^0_i}\hat{\mathbf{n}},$$

$$\boldsymbol{\mathcal{J}}^{\mathrm{reg}}_i = -D^{\mathrm{reg}}_i \nabla(\overline{\rho}\tilde{Y}_i).$$

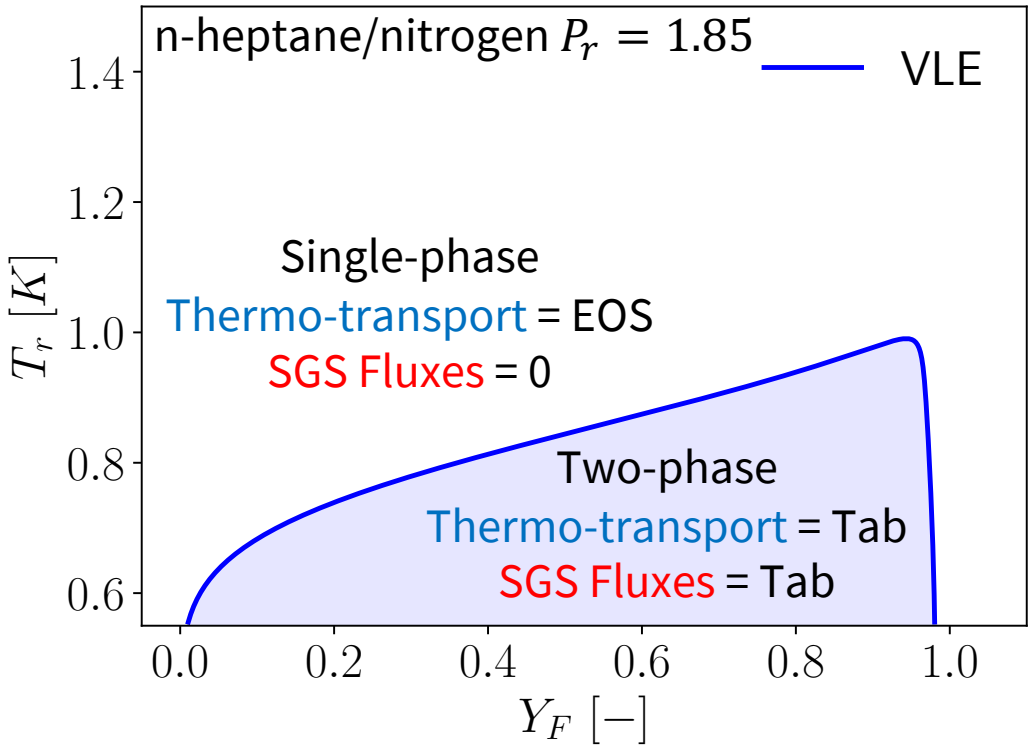
Tabulation

Thermo-transport

$$\{\overline{P}, \overline{e}, \overline{\mu}_i, \overline{s}_i, \overline{h}_i, \overline{\eta}, \overline{L}_{ij}, \overline{\lambda}\} = \begin{cases} \mathrm{EOS}(\overline{\rho}, \tilde{\mathbf{Y}}, \overline{T}) \text{ when } \{\overline{\rho}, \tilde{\mathbf{Y}}\} \notin \mathrm{TwoPhase}(\overline{T}) \\ \mathrm{Tab}(\overline{\rho}, \tilde{\mathbf{Y}}, \overline{T}) \text{ when } \{\overline{\rho}, \tilde{\mathbf{Y}}\} \in \mathrm{TwoPhase}(\overline{T}) \end{cases},$$

SGS Fluxes

$$\left\{F^{\mathrm{reg}}, \overline{J_i^0}, D_i^{\mathrm{reg}}\right\} = \begin{cases} 0 \text{ when } \{\overline{\rho}, \tilde{\mathbf{Y}}\} \notin \mathrm{TwoPhase}(\overline{T}) \\ \mathrm{Tab}(\overline{\rho}, \tilde{\mathbf{Y}}, \overline{T}) \text{ when } \{\overline{\rho}, \tilde{\mathbf{Y}}\} \in \mathrm{TwoPhase}(\overline{T}) \end{cases},$$



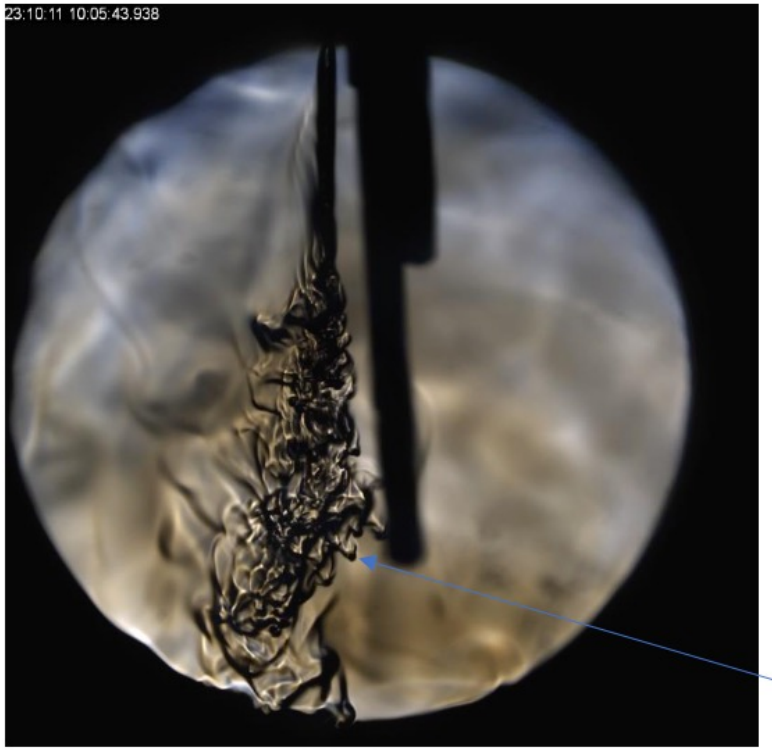
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Numerical Method

- Tabulation via Delaunay triangulation
- EOS/Tabulation inversion via bracketing method
- Fully-hyperbolic formulation using Godunov method:
  - Euler terms discretized via Riemann solver
  - Diffusive and interfacial terms discretized via central scheme
    - At most 2nd order derivatives
  - Reconstruction using WENO scheme
  - RK3 time-stepping

Application: Transcritical fuel droplet

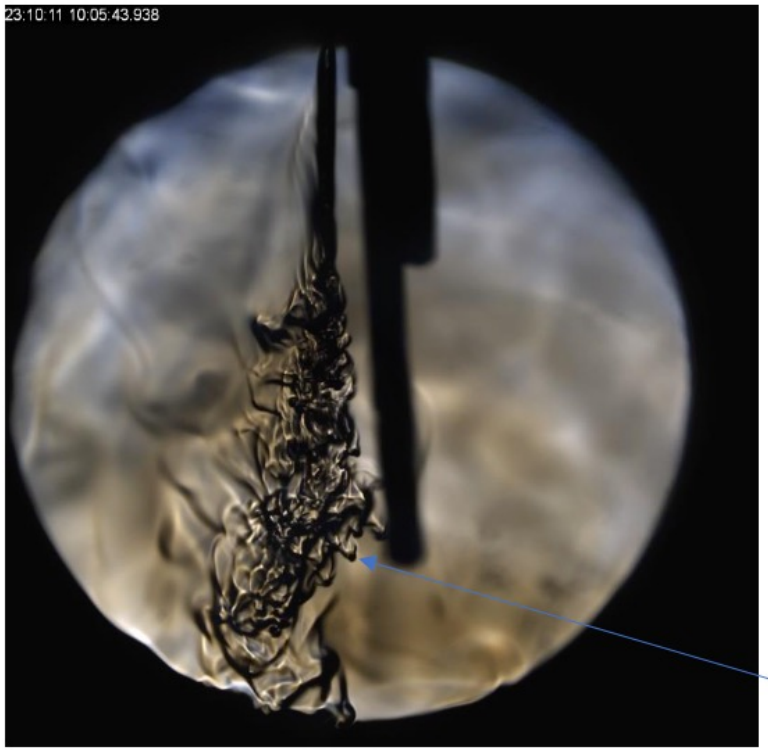


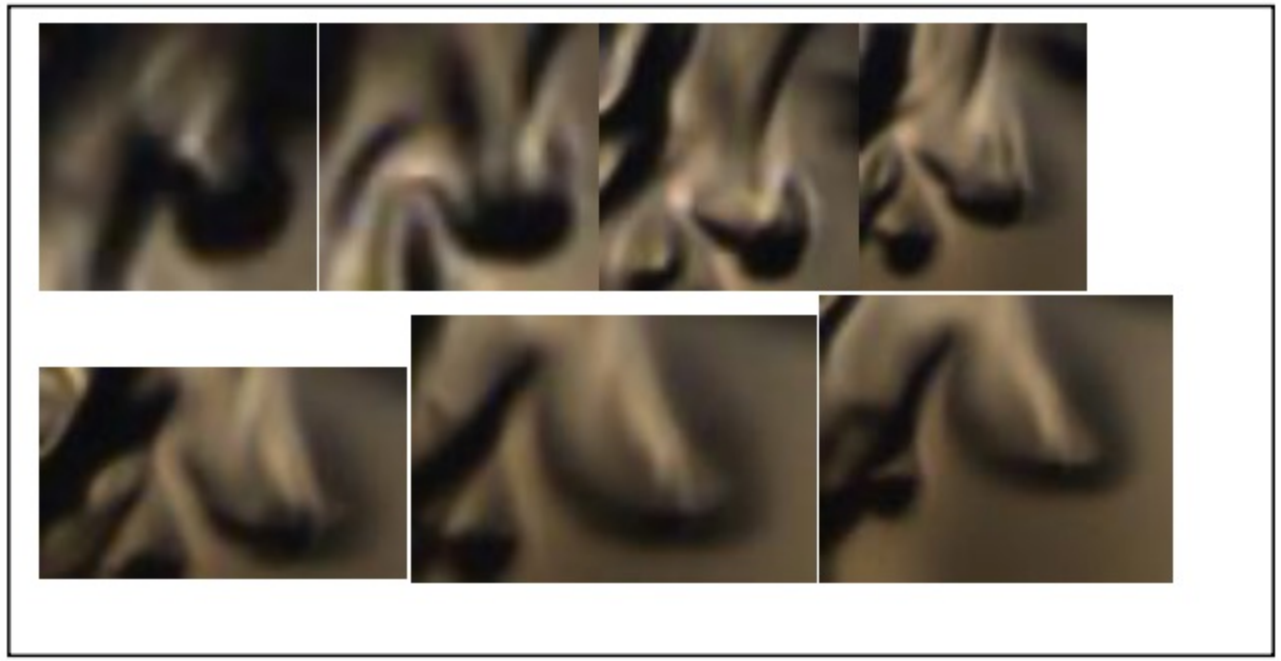
Mike Hicks
NASA Glenn Research Center

Uday Hegde
Case Western Reserve University

Transcritical Droplet: Experiment (GRC)

- Heptane/Nitrogen system
- Slow jet injection in microgravity (8cm/s)
- High pressure condition ($P_r = 3.7$)
- Near-critical temperature ($T_{r,F} = 0.99$, $T_{r,a} = 1.16$)



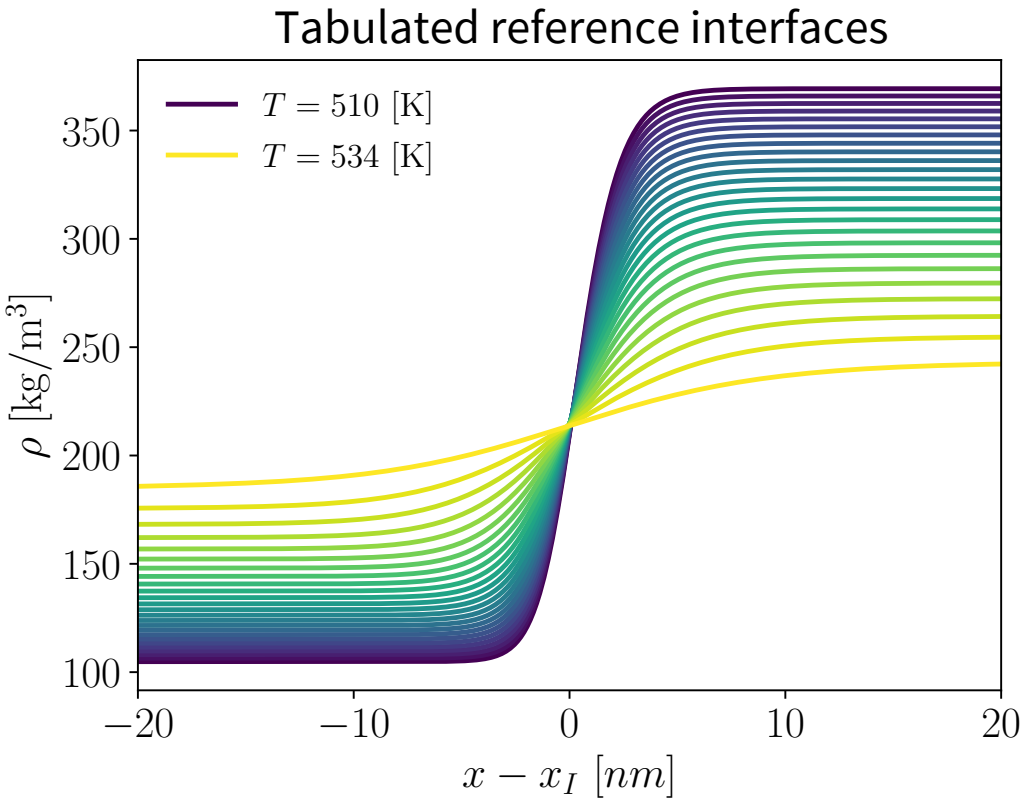


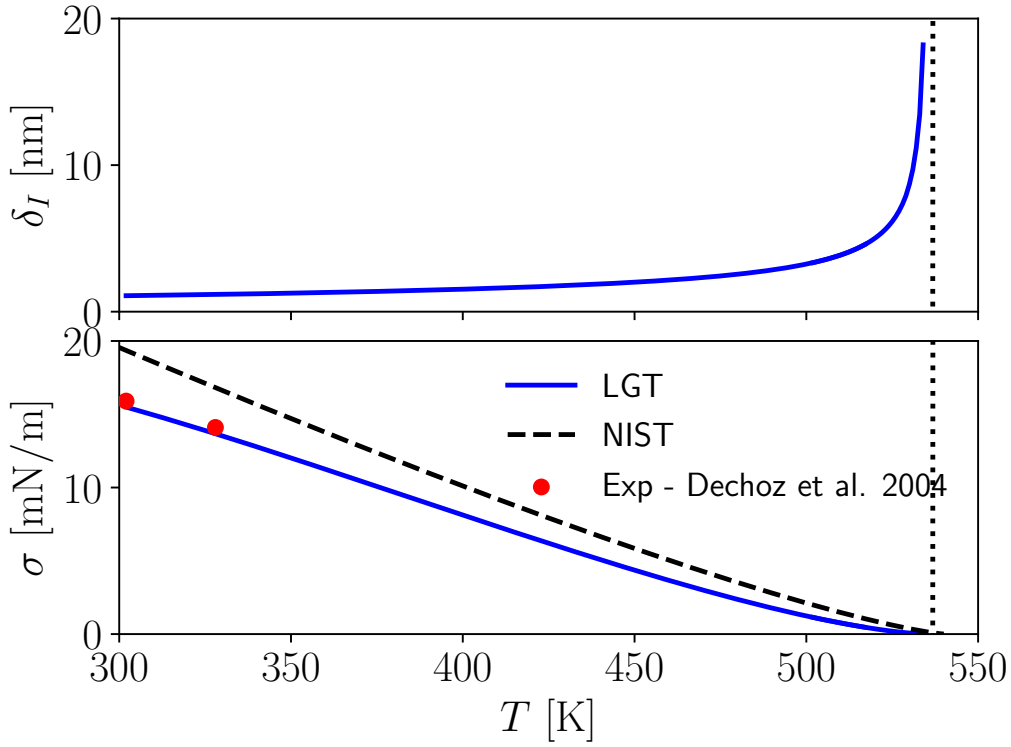
Follow this droplet

Follow the droplet which is surrounded by the hot N2.

Modeling

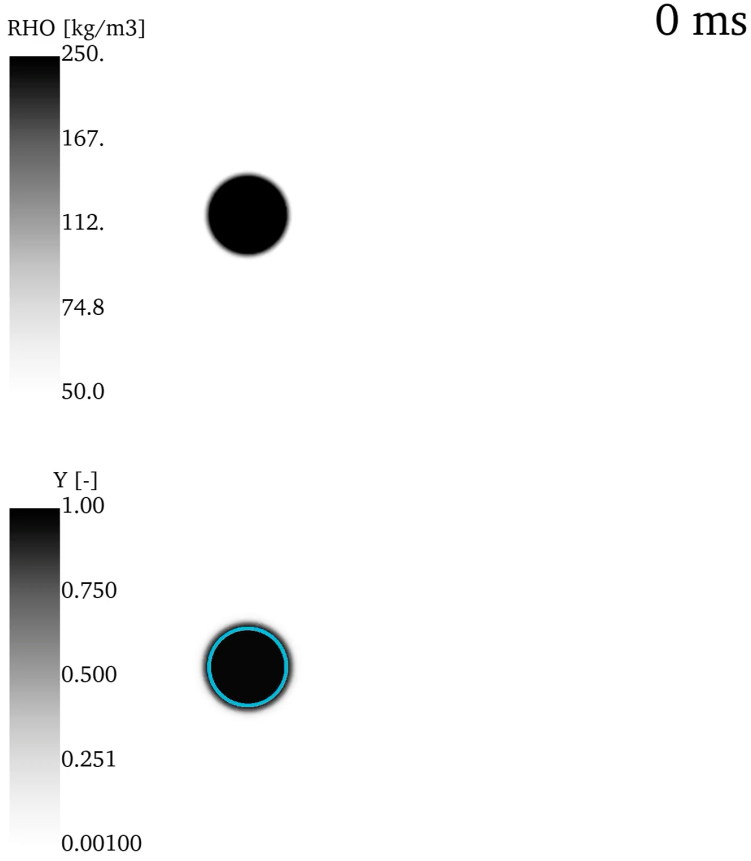
- 2D simulation
- Initially stationary droplet placed in flow
- $D/\Delta_I = 40, D/\Delta_x = 100$

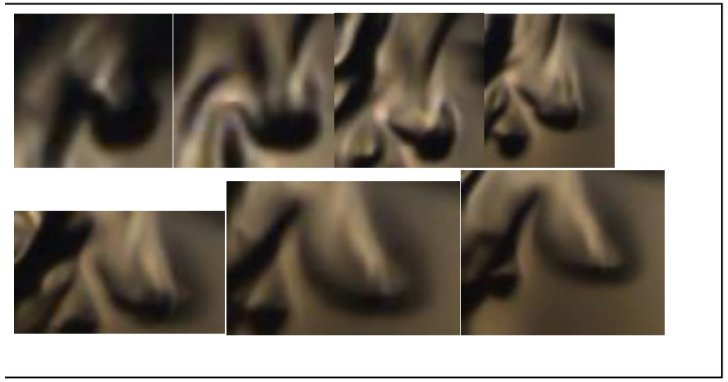




Results

- First, spherical droplet under surface tension ($We = 1.0$) evaporating, leading to dense tails of evaporated vapor.
- Then, local vanishing of interface, leading to the deformation of the droplet into a bag shape after the complete transition to supercritical mixing.





A question arises…

- What causes the sudden change in droplet shape even at very low flow (8 cm/s)?

$t = 15$ ms

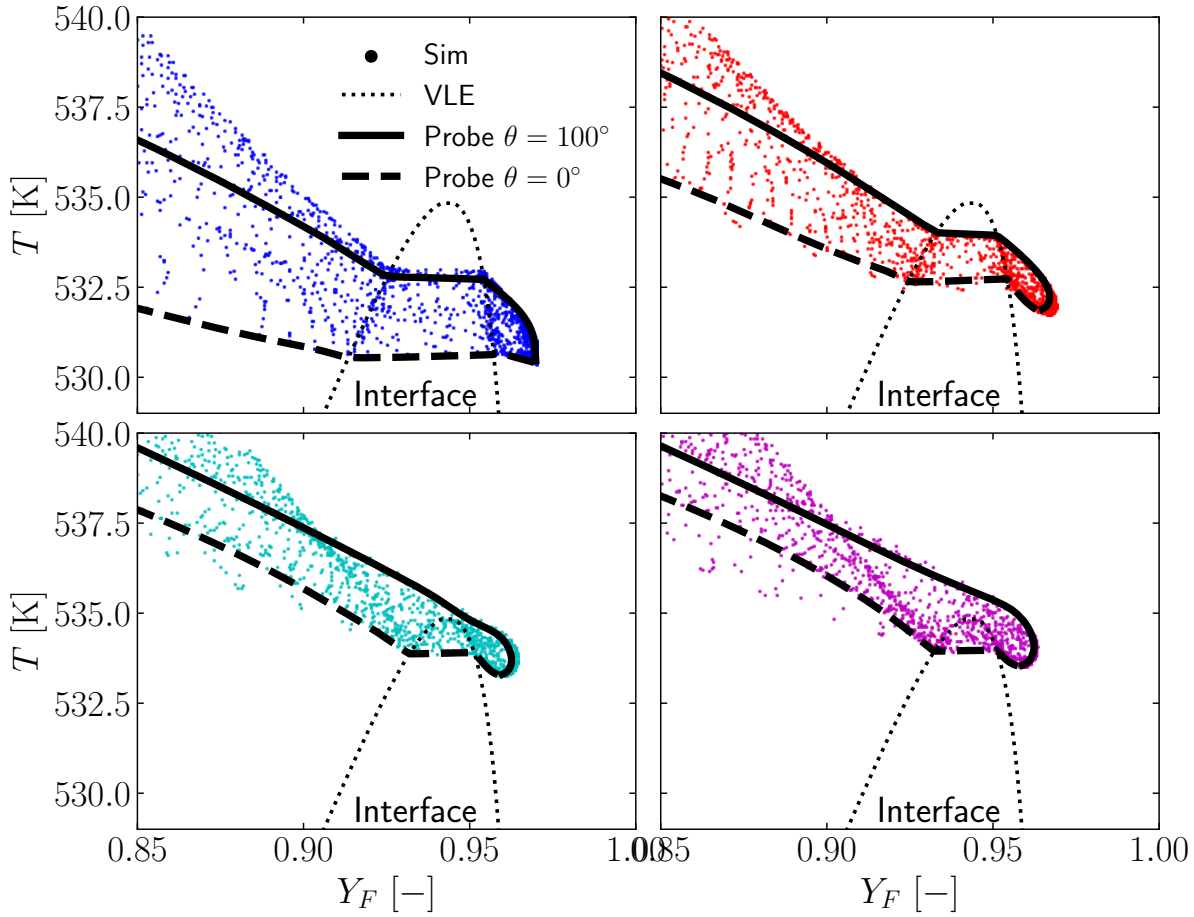


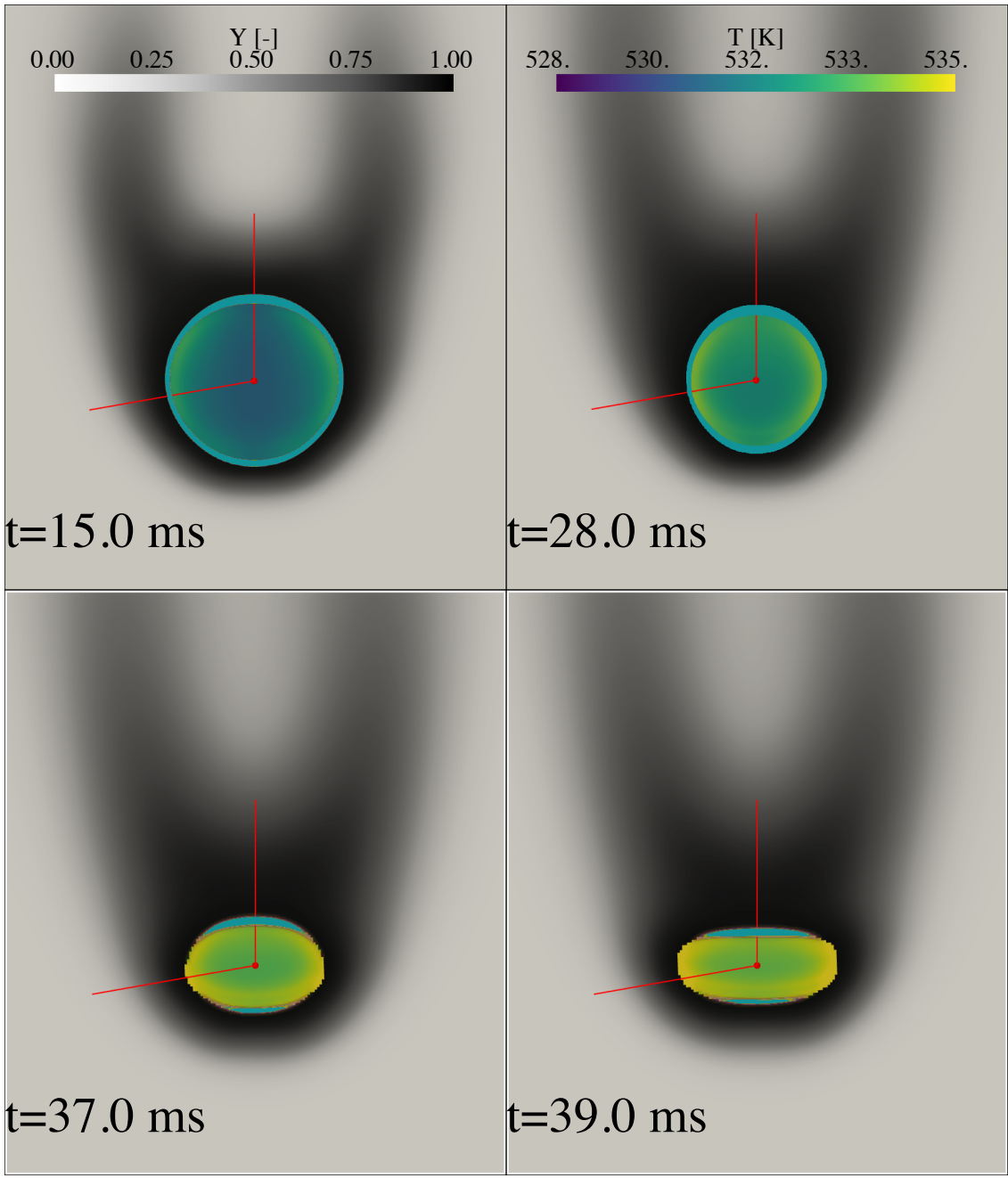
$t = 52$ ms



The Spatial Transition

- Transition to supercritical is not uniform since there is temperature variation along the droplet surface.
- Flattening of the droplet is due to the disconnected interfaces



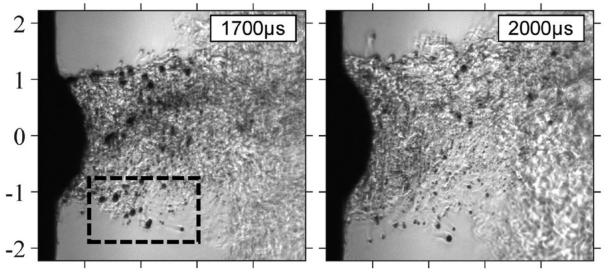


Application: High-pressure fuel injection

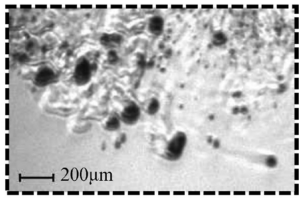
[1] Jofre, L et al., 2015. Center Turbul. Res. Ann. Res. Briefs, 2015, pp.55-64.
[2] Poursadegh, F. et al., 2017. Energy & Fuels, 31(6), pp.6445-6454.
[3] Mayer, W.O. et al., 2001. *Journal of Propulsion and Power*, *17*(4), pp.794-799.
[4] Crua, C. et al., 2017. Fuel, 208, pp.535-548.

Liquid Injection Dynamics: Background

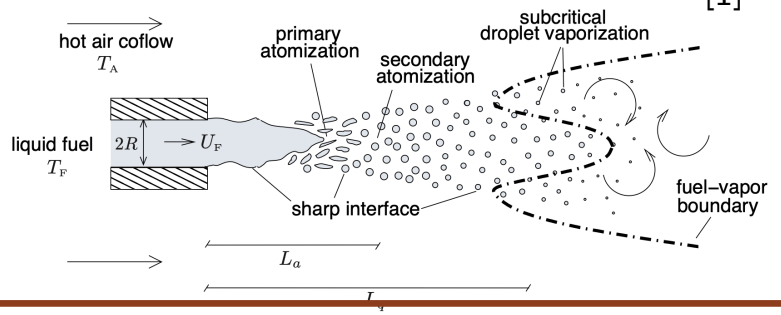
Propane/N2: $T_{F,r} = 0.9; P_r = 0.7, T_r = 0.9$



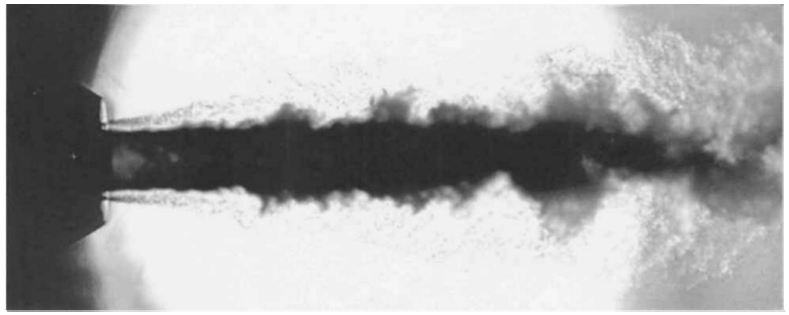
[2]



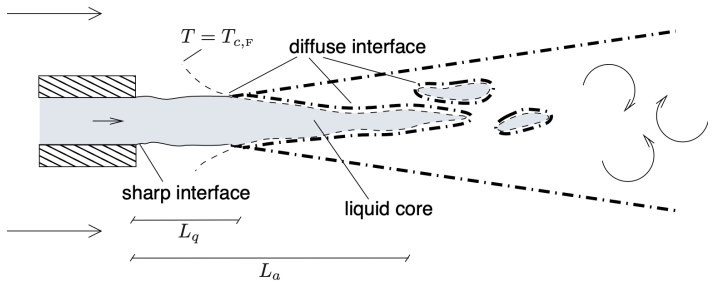
[1]



LN2/He: $T_{F,r} = 0.77; P_r = 1.76, T_r = 2.2$



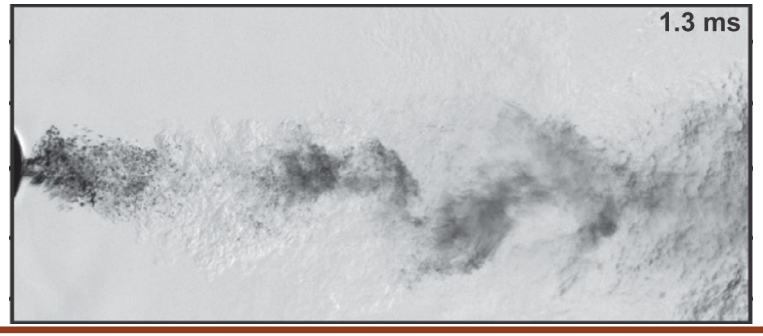
[3]

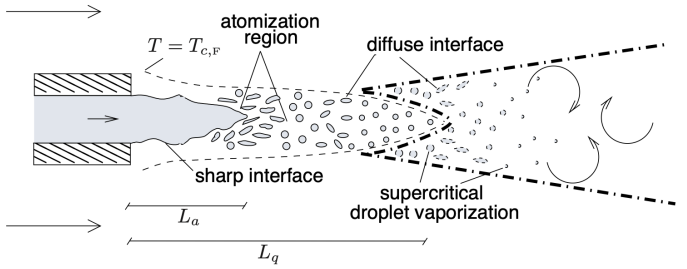


(a) subcritical

(b) transcritical $(L_q/L_a < 1)$

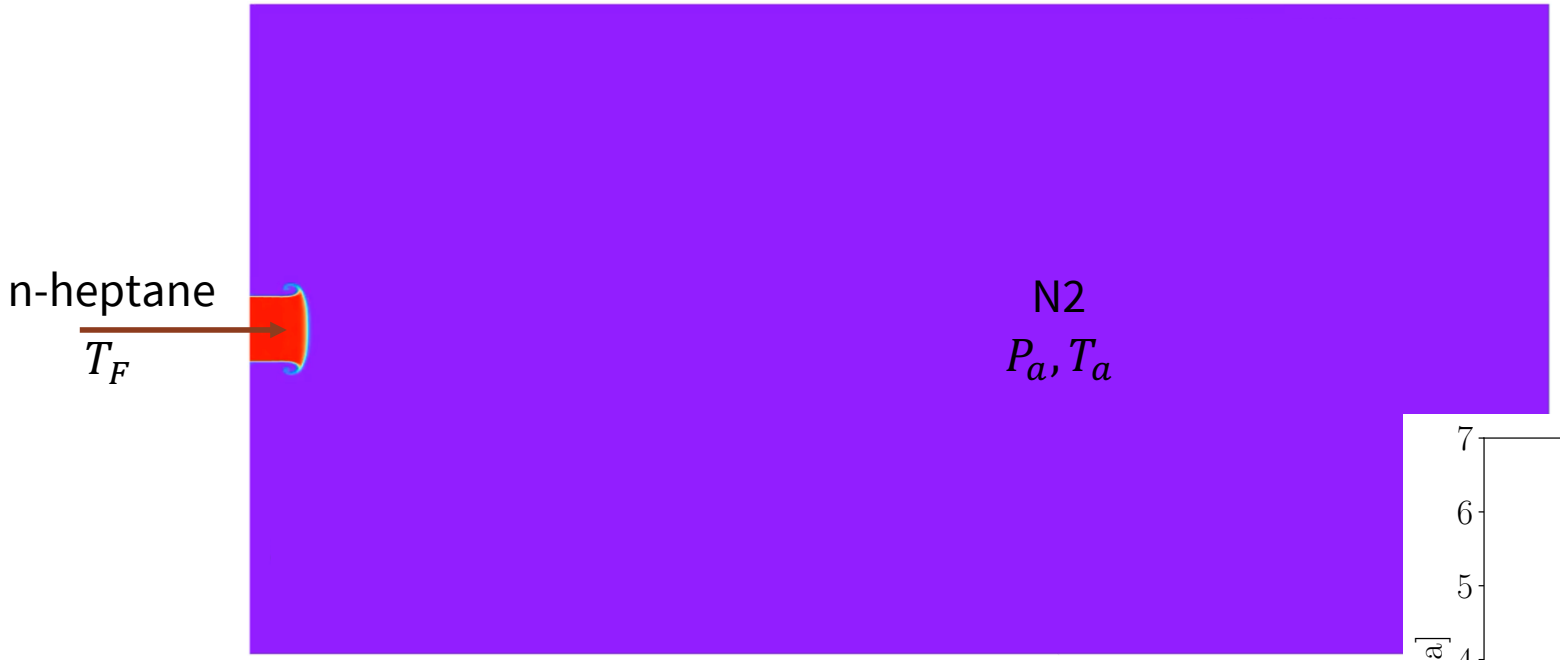
nC16/N2: $T_{F,r} = 0.5; P_r = 7.6, T_r = 1.7$ [4]



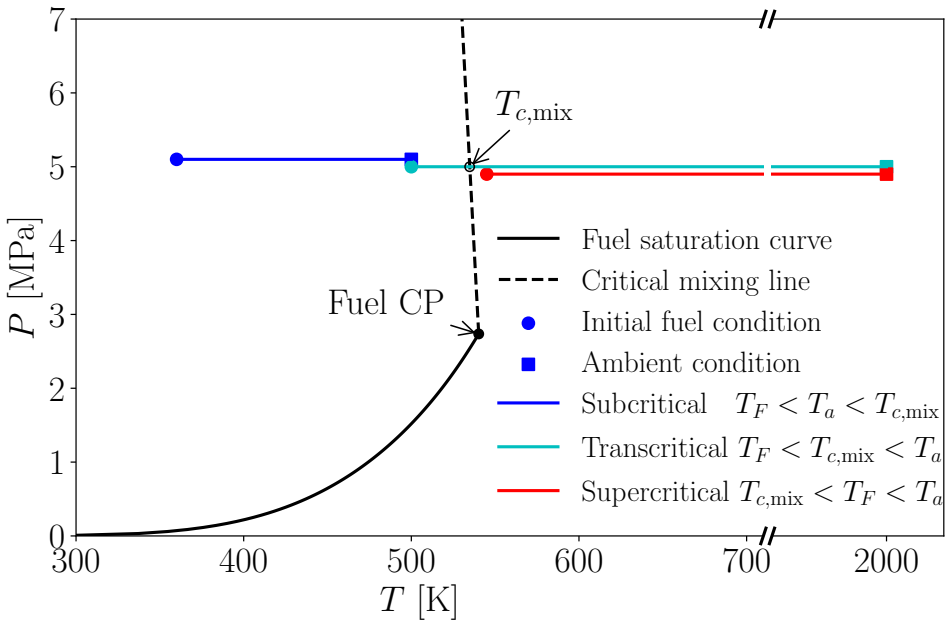


(c) transcritical $(L_q/L_a > 1)$

Liquid Injection Dynamics: Configuration



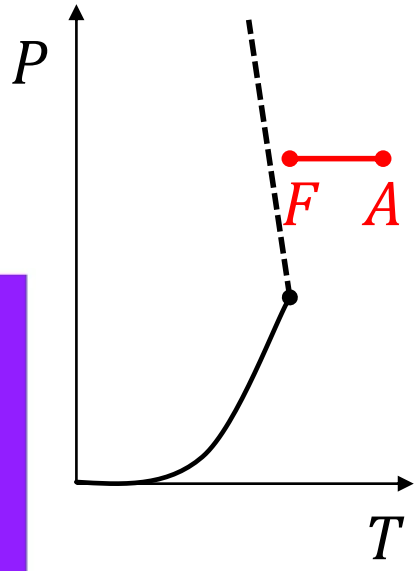
Thermodynamic Condition	P_a [MPa]	$T_{c,\mathrm{mix}}$ [K]	T_F [K]	T_a [K]
Subcritical	5.0	534.8	360	500
Transcritical	5.0	534.8	500	2000
Supercritical	5.0	534.8	540	2000

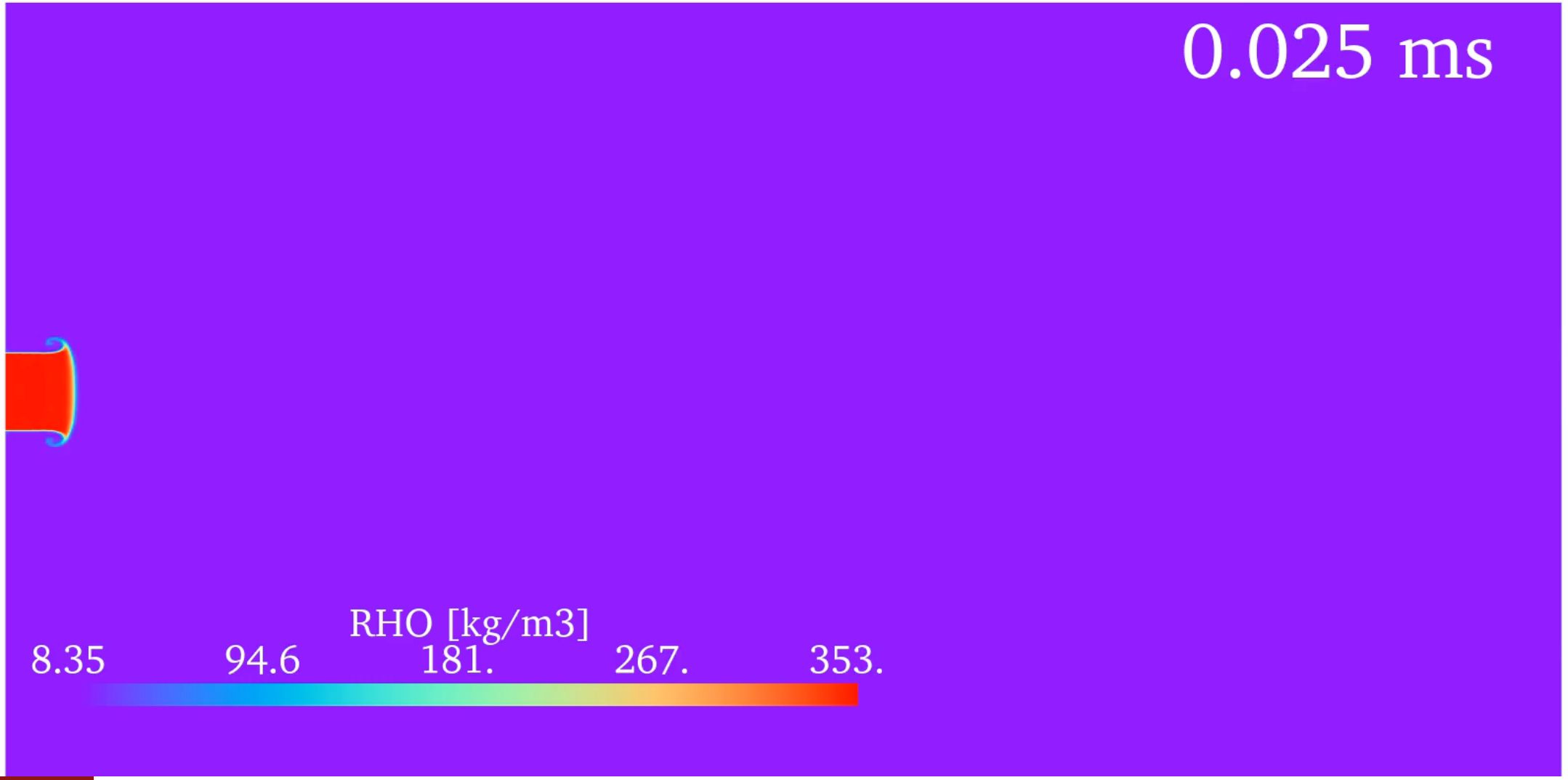


- Jet Injection of n-heptane into gaseous N2 environment.
- Jet parameters:
  - D = 0.5 mm
  - U = 20 m/s
- $D/\Delta_I = 40, D/\Delta_x = 100$
- Focus on the near-injection region at three conditions:
  - Transition from atomization to mixing layer

Fuel Injection: Supercritical

$P_a = 50$ bar
$T_{c,mix} = 532$ K
$T_l = 540$ K
$T_a = 2000$ K

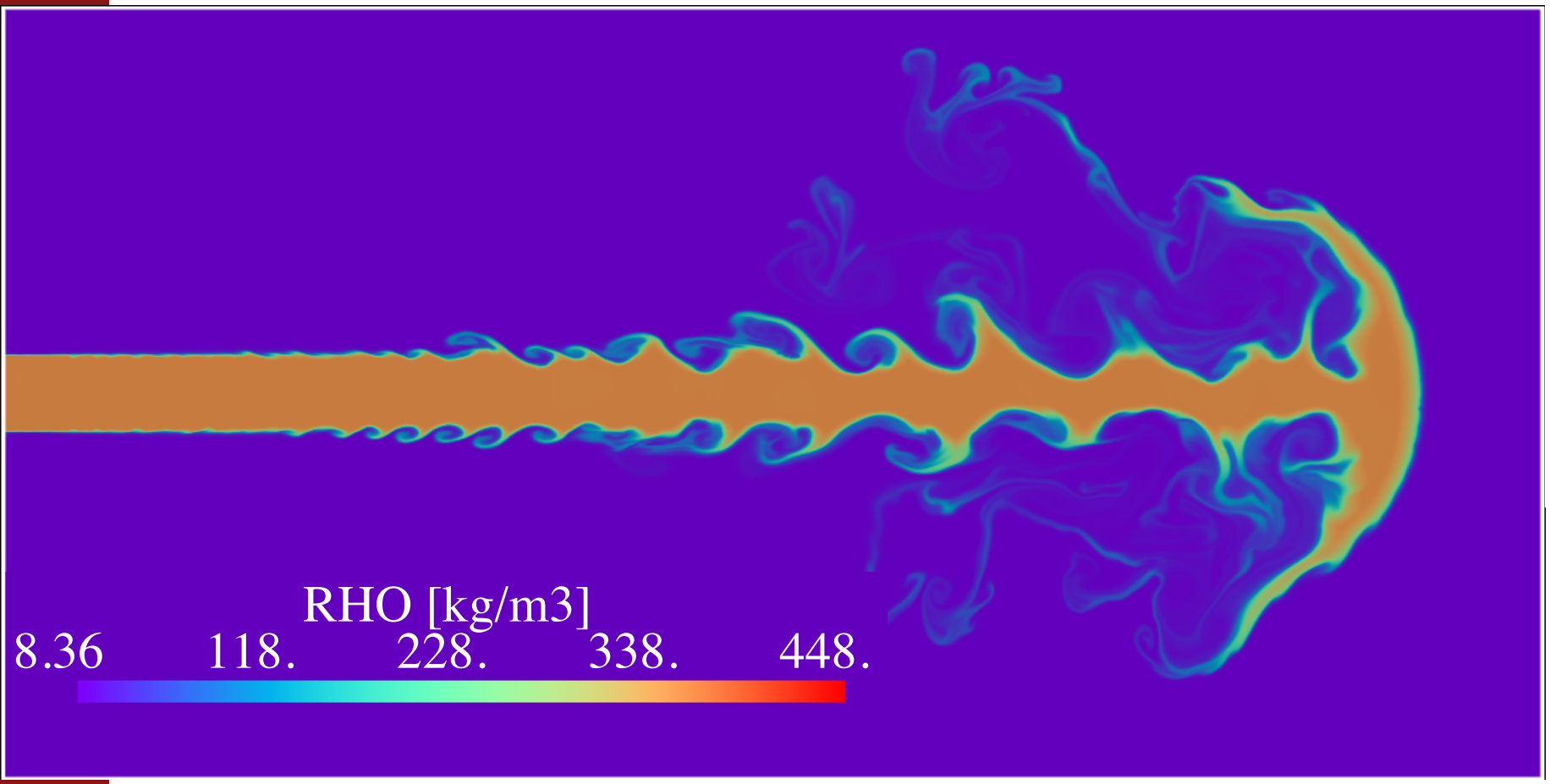


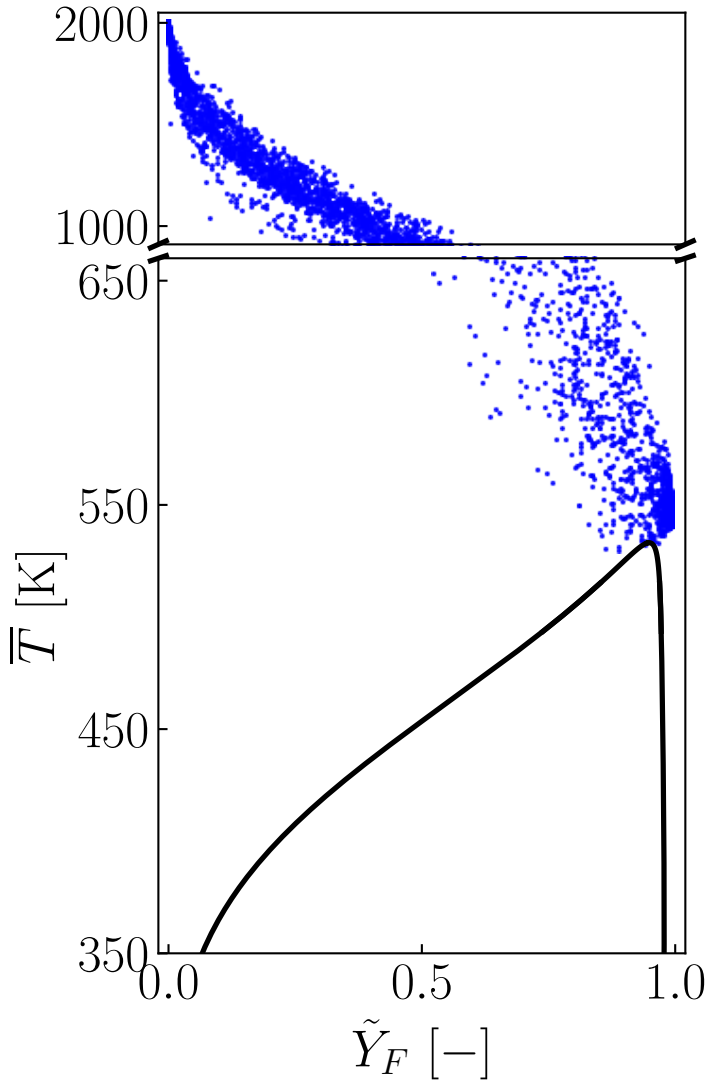


Fuel Injection: Supercritical

- Monolithic supercritical mixing condition
- No subcritical interfacial dynamics
- Density contrast due to Widom-line transition!

$t = 0.6$ ms

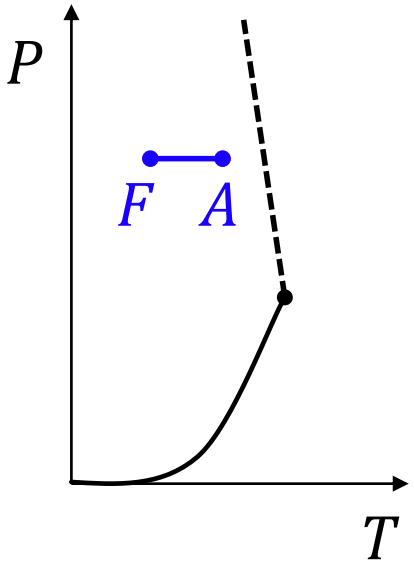


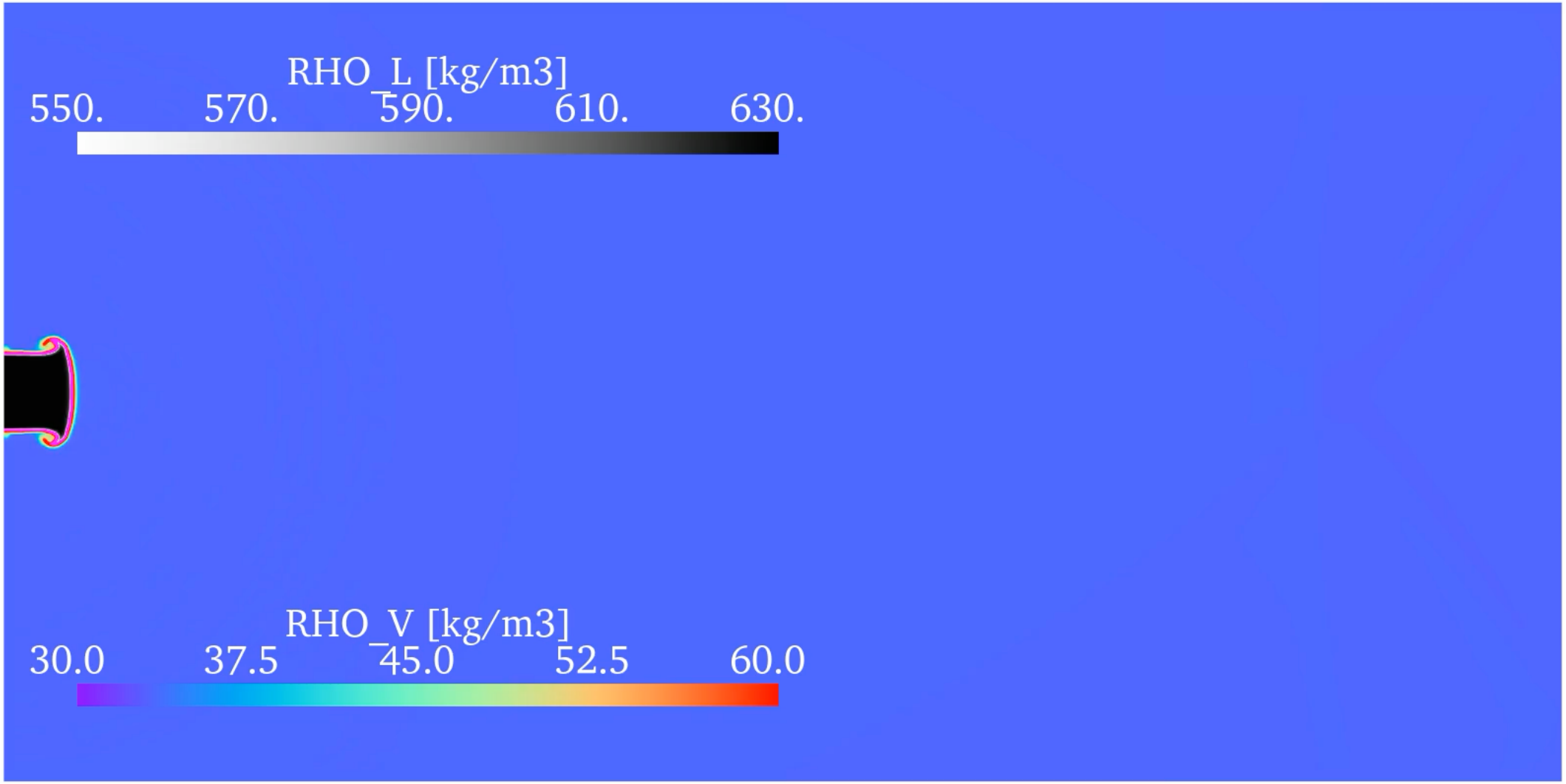


Fuel Injection: Subcritical

- Injection of n-heptane into nitrogen with $U_0 = 20$ m/s and $h = 0.5$ mm

$P_a = 50$ bar
$T_{c,mix} = 532$ K
$T_l = 360$ K
$T_a = 500$ K

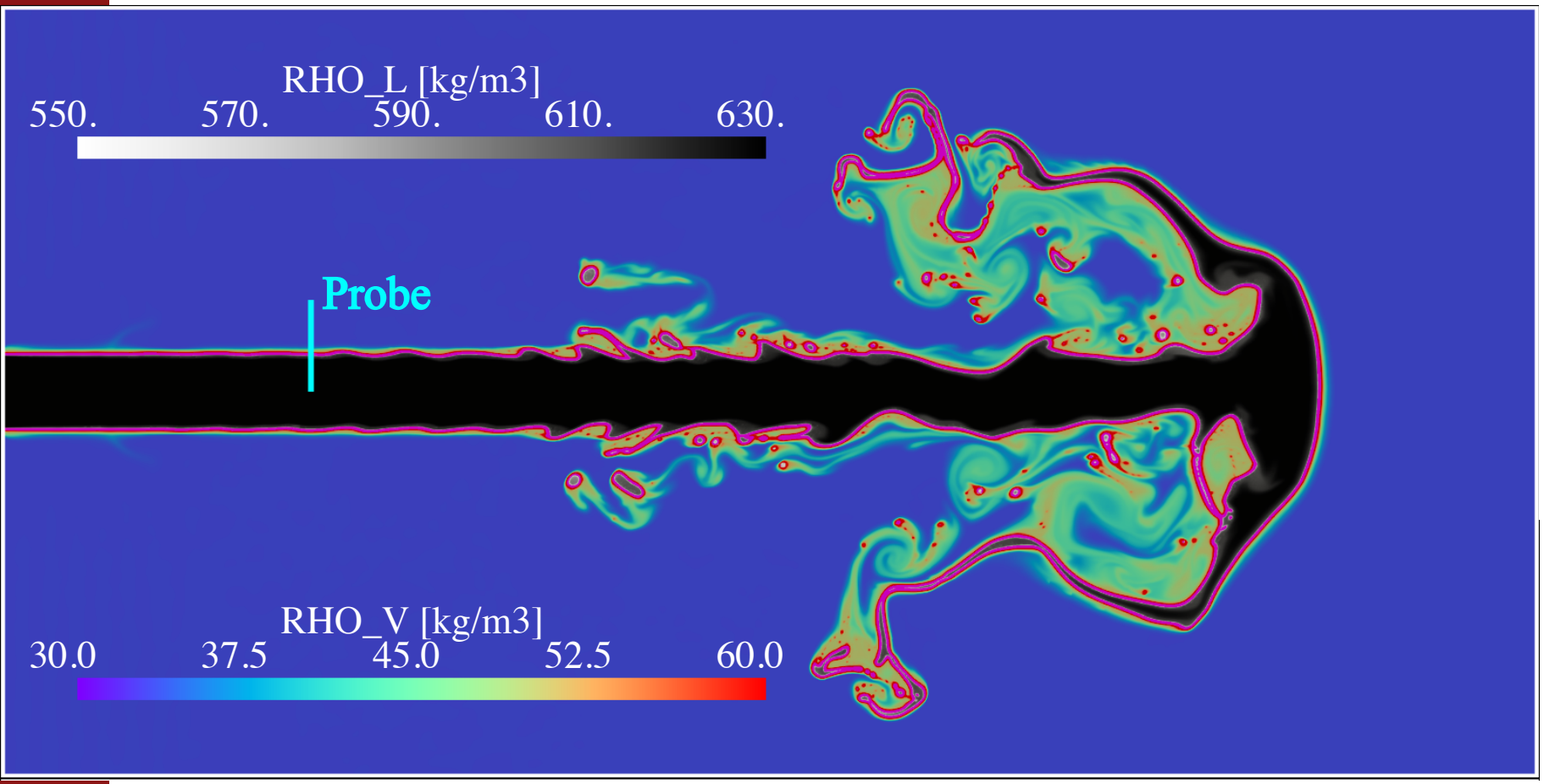


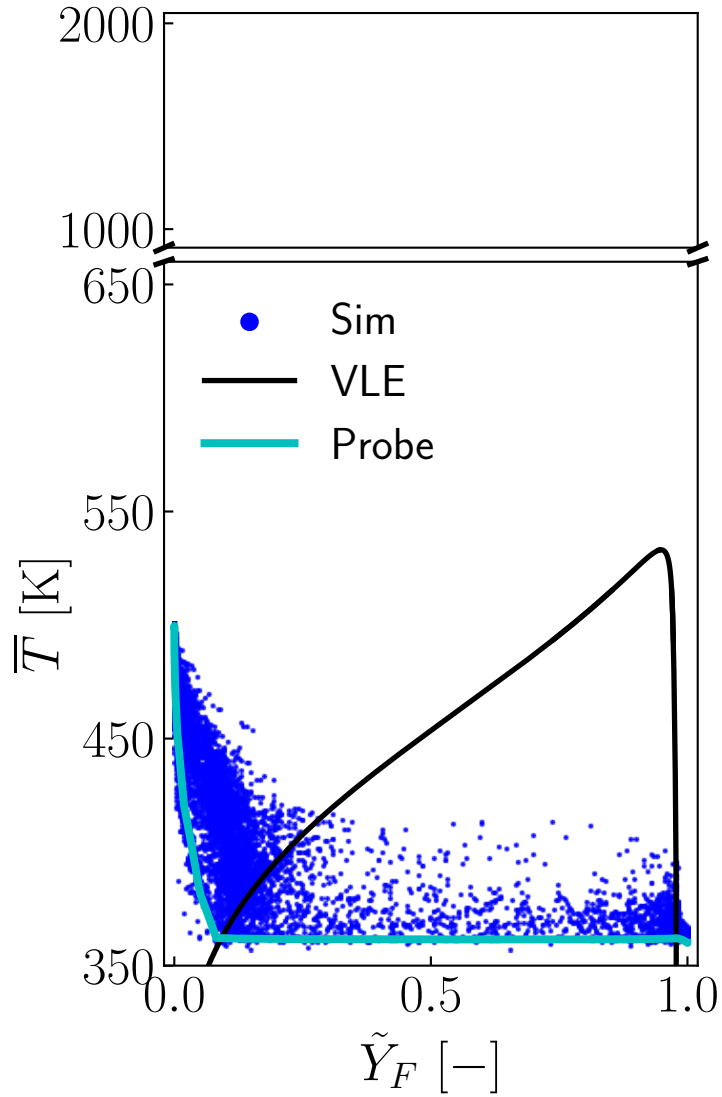


Fuel Injection: Subcritical

- Monolithic subcritical interfacial process
- Evaporation across jump condition of VLE (Stefan Flow)
- Internal-phase convection/mixing

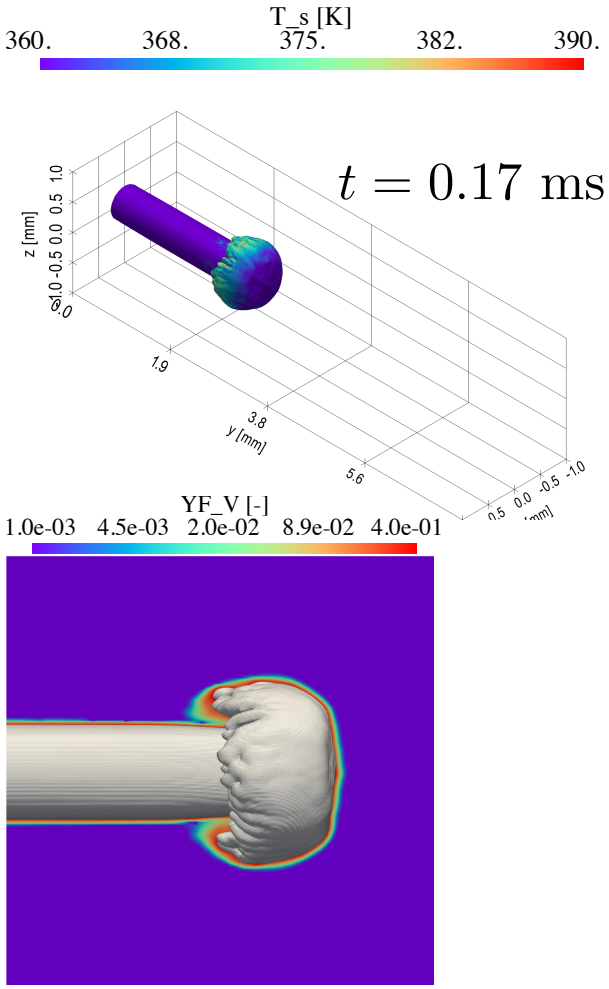
$t = 0.6$ ms

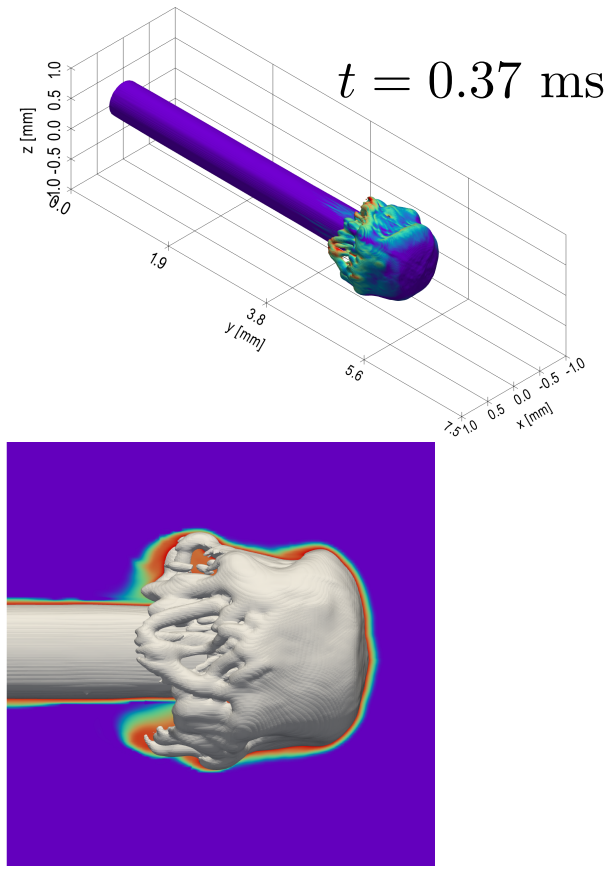


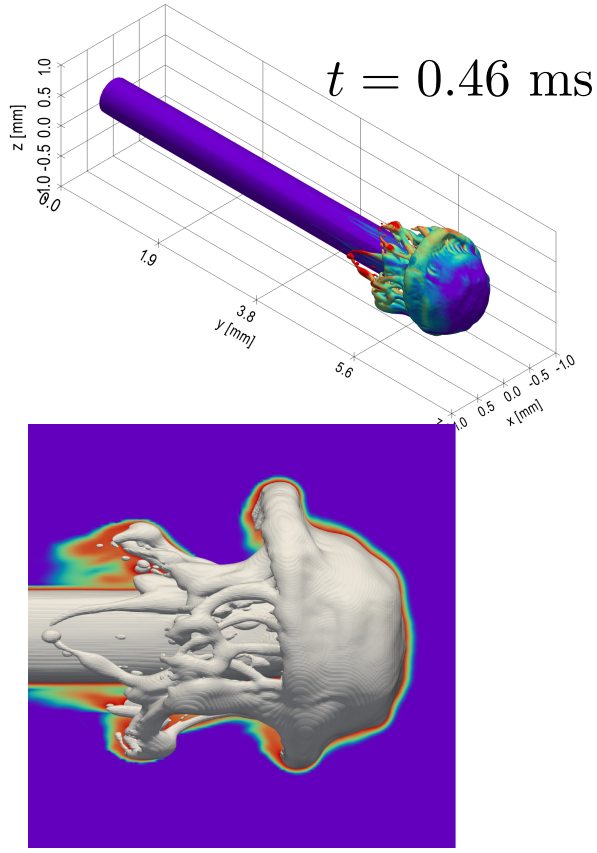


Fuel Injection: Subcritical

- 3D Simulation:
  - Atomization: Added Rayleigh-Plateau instability.
  - Heat-up of fuel surface along leading edge and ligaments.
  - Mixing of evaporation fuel vapor along the fuel surface.

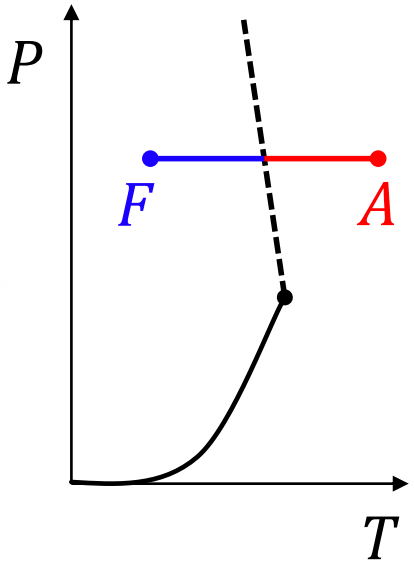


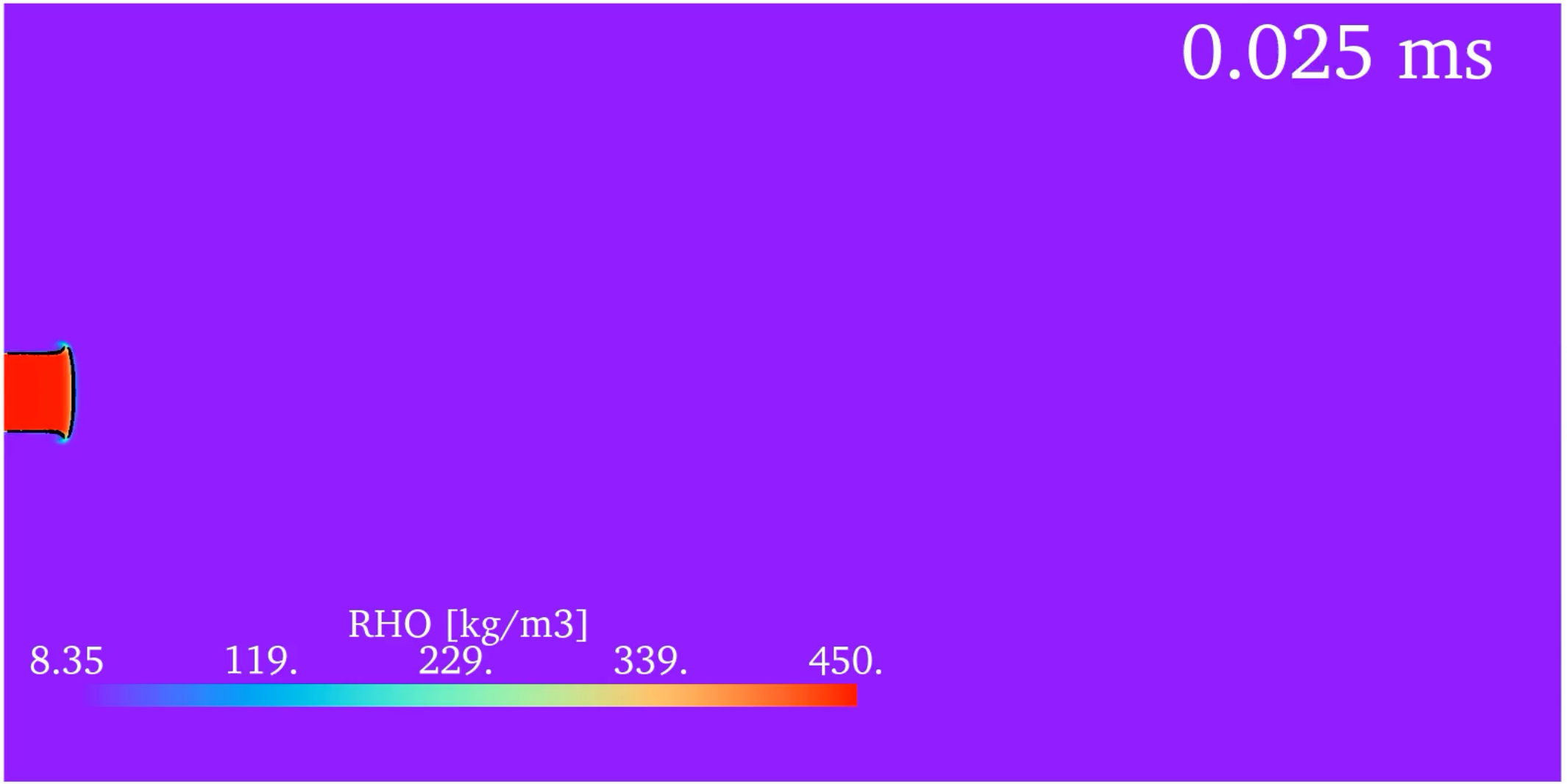




Fuel Injection: Transcritical

$P_a = 50$ bar
$T_{c,mix} = 532$ K
$T_l = 500$ K
$T_a = 2000$ K

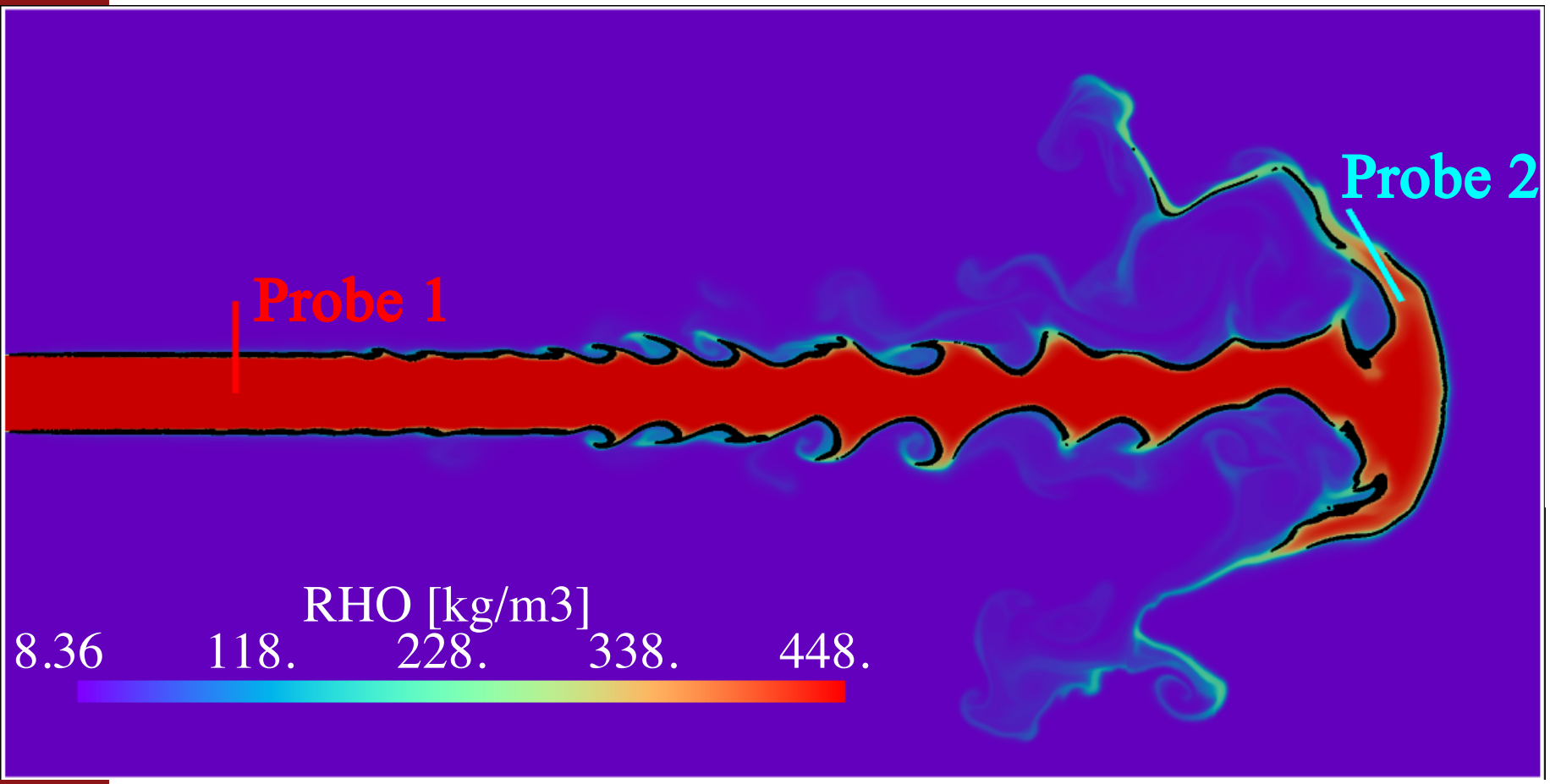


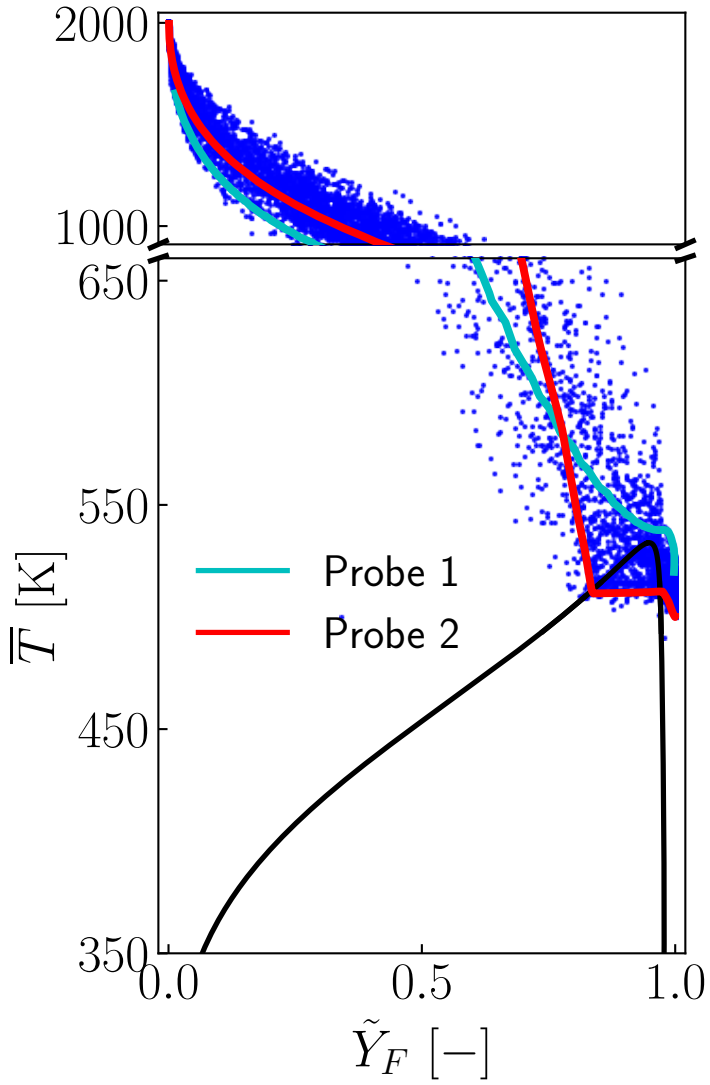


Fuel Injection: Transcritical

- **Coexistence of both sub and supercritical dynamics**
- Surface tension + evaporation near nozzle
- Supercritical mixing at ligaments

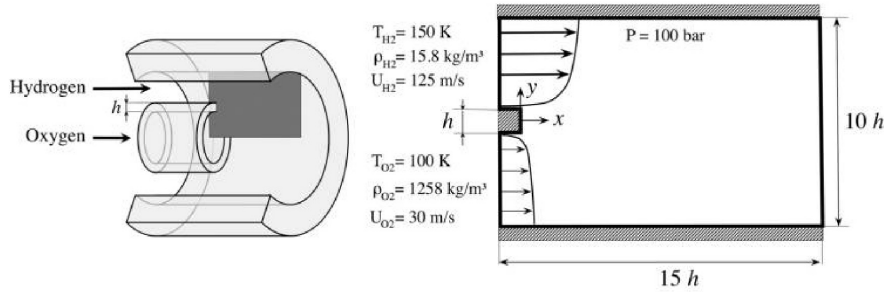
$t = 0.6$ ms





Application: LOX/GH2 mixing layer

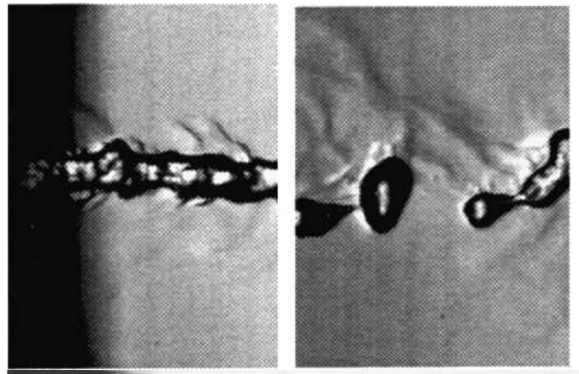
Mixing Layer Dynamics: LOX/GH2



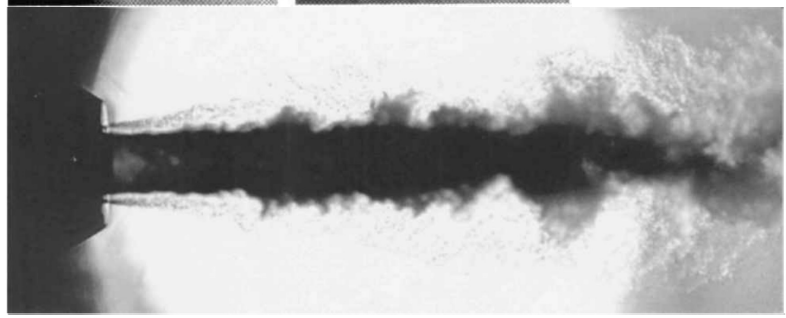
- Motivation:
  - Application of RIM to high-speed flow
  - Investigate impact of resolving capillarity on mixing layer dynamics
- Background:
  - Focus on cold-flow conditions (before ignition)
  - Experiment: LN2/GHe
    - $T_{r,F} = 0.77; P_r = 1.76, T_{r,a} = 2.2$
    - Evidence of surface tension
  - Simulation: LOX/GH2
    - $T_{r,F} = 0.65; P_r = 2.00, T_{r,a} = 0.97$
    - DIM formulation, no interface

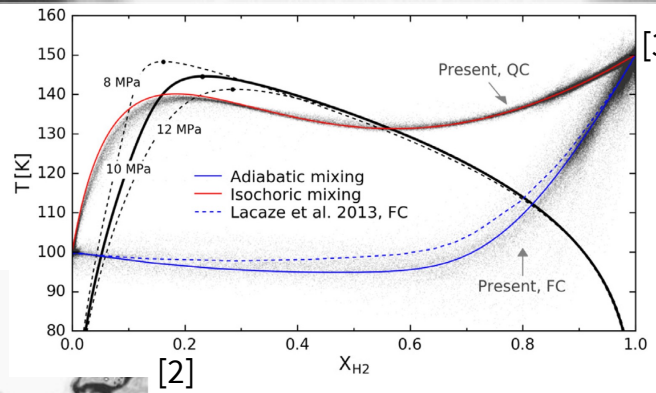
Effect of neglecting interface? [4]

[1] Mayer, W.O. et al., 1998. Journal of Propulsion and Power, 14(5), pp.835-842.
[2] Ruiz, A.M. et al., 2016. *AIAA Journal*, *54*(5), pp.1445-1460.
[3] Ma, P.C. et al., 2019. International Journal of Multiphase Flow, 113, pp.231-249.
[4] Biancofiore, L. & Gallaire, F., 2010. *Physics of Fluids*, *22*(1).



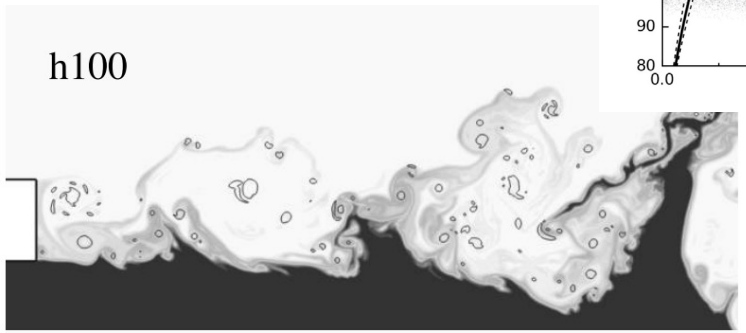
[1]





[3]

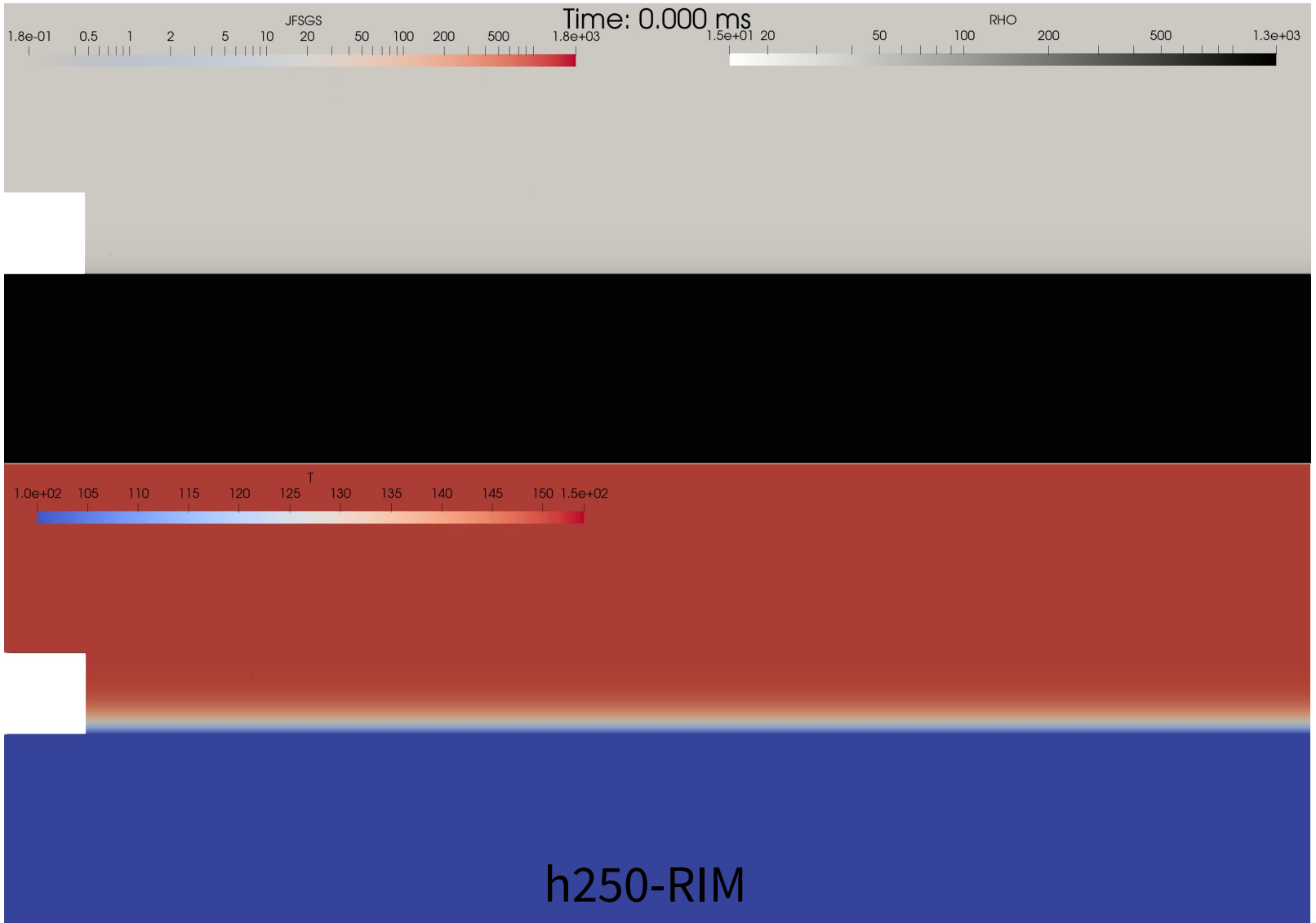
[2]



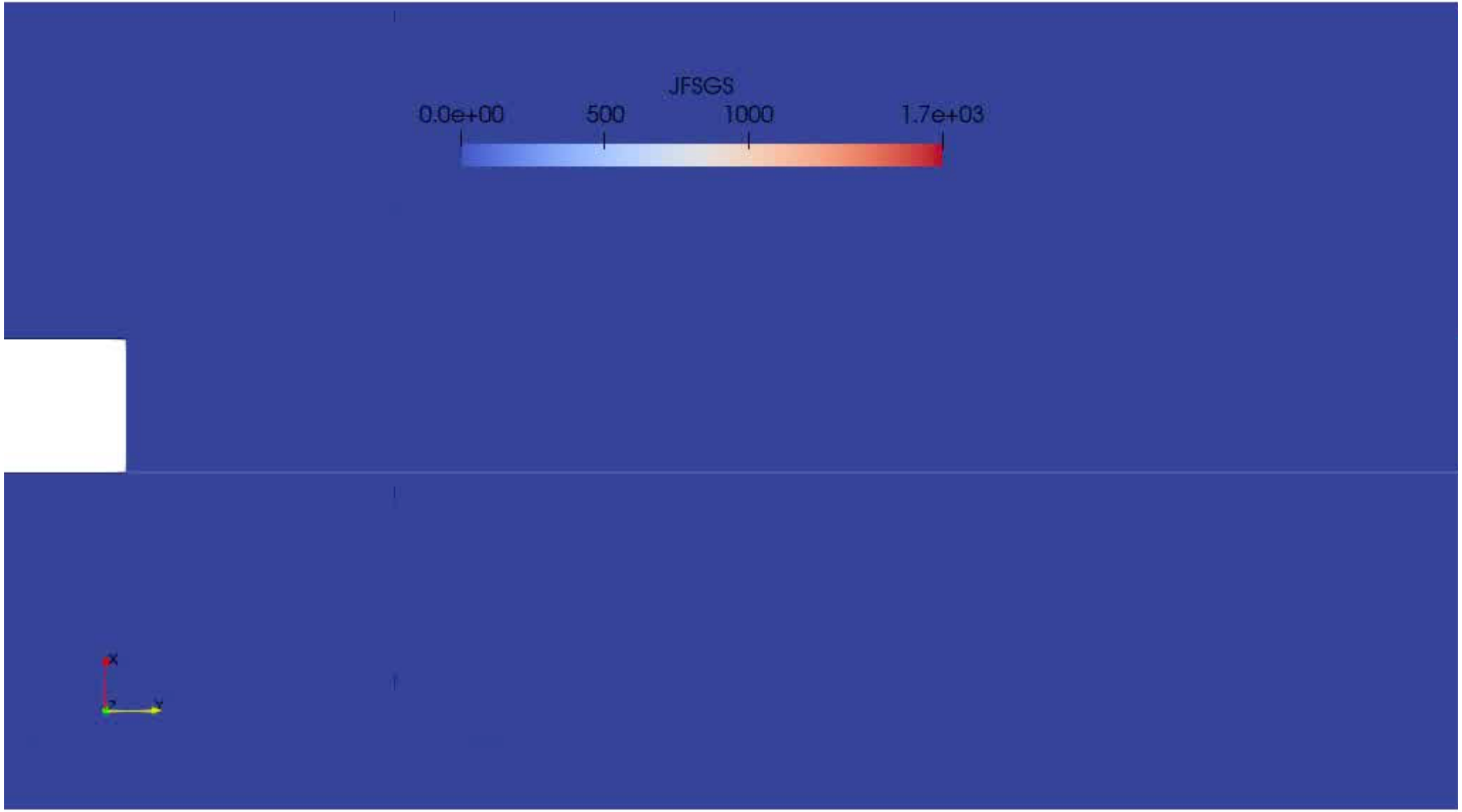
Stanford University

RIM simulation

- Interaction between atomization and dual sheal layers



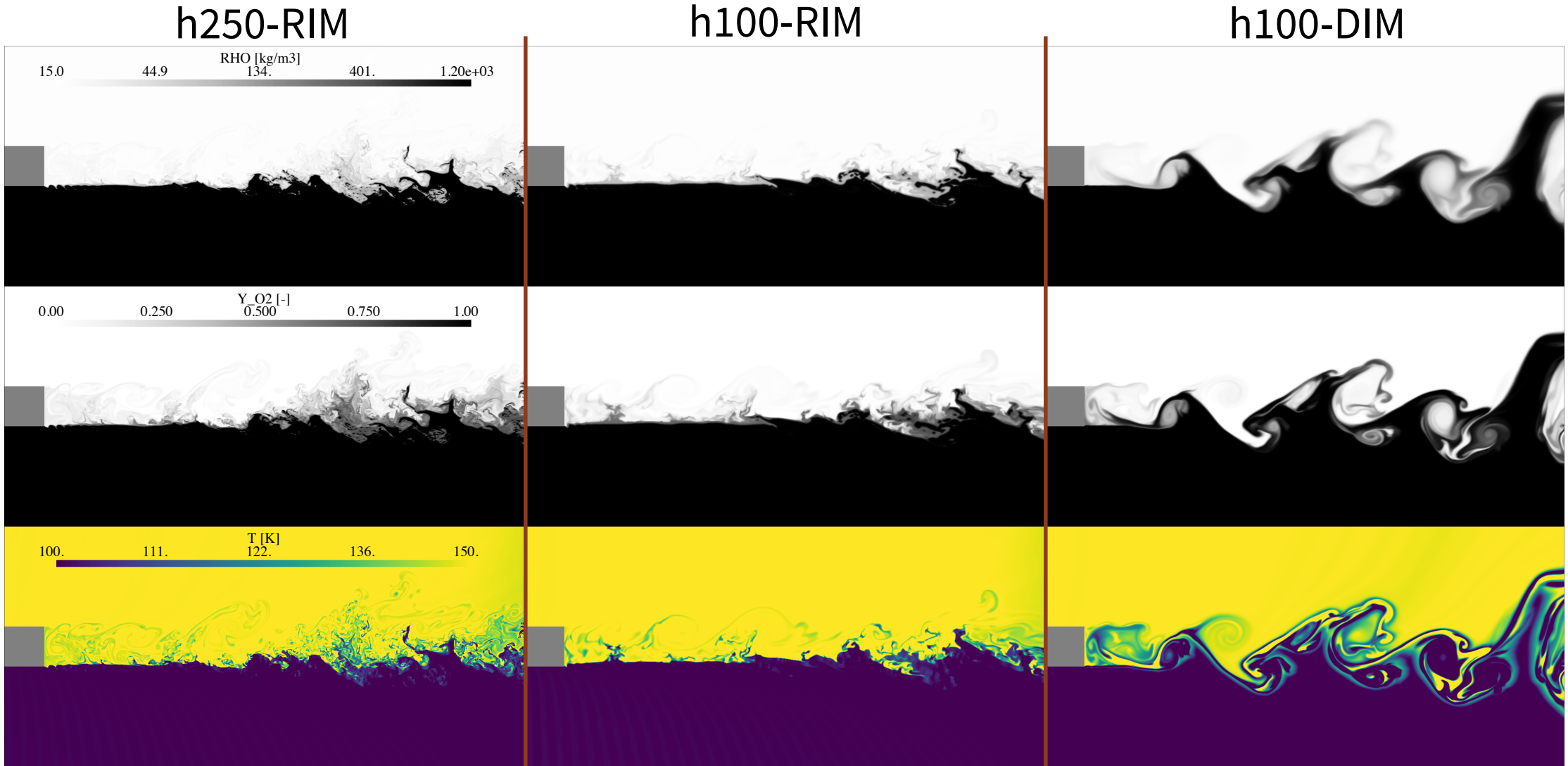
RIM simulation: Coupling with dual shear layers



h100-RIM

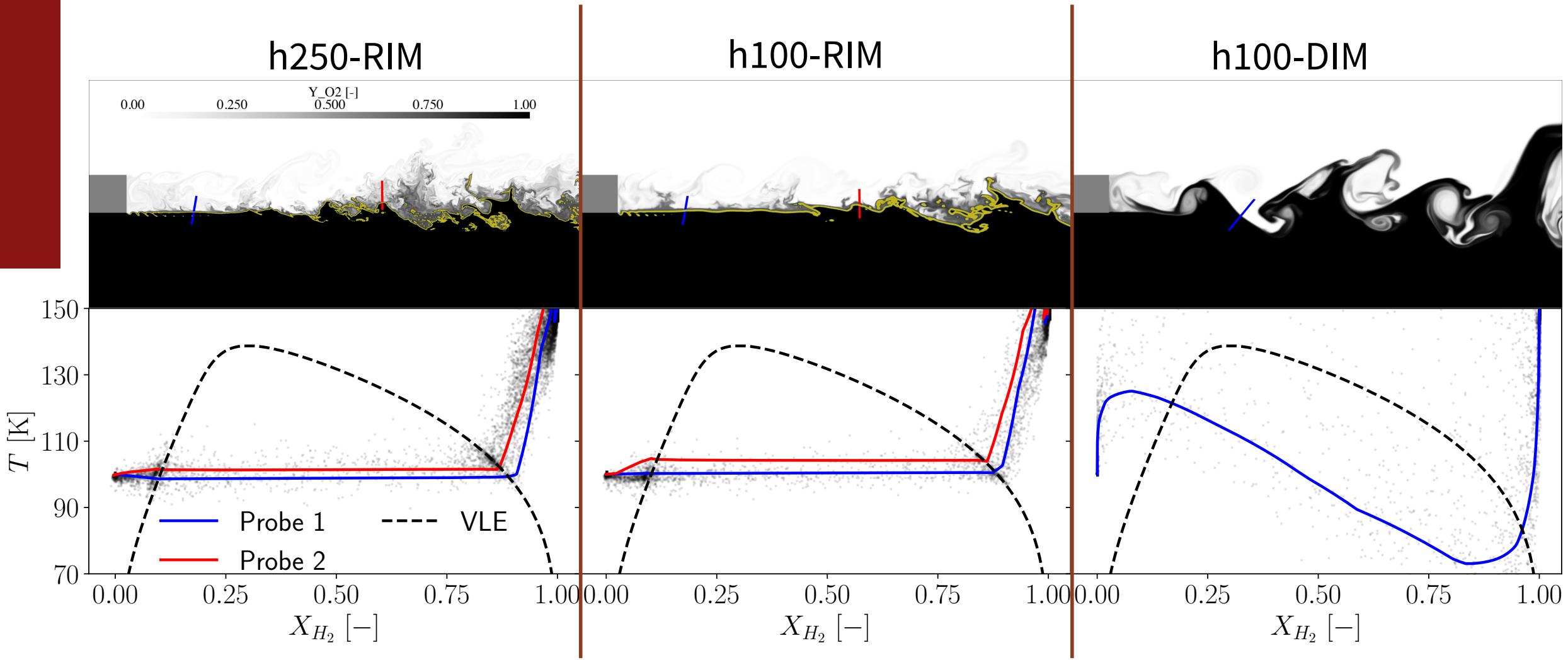
Comparison with DIM: Atomization Dynamics

- DIM simulation:
  - Stronger surface deformation due to neglected surface tension
  - Diffusion instead of atomization and evaporation



Comparison with DIM: Phase-Exchange Dynamics

- Thermal and compositional mixing is strongly influenced by the capturing of the interface

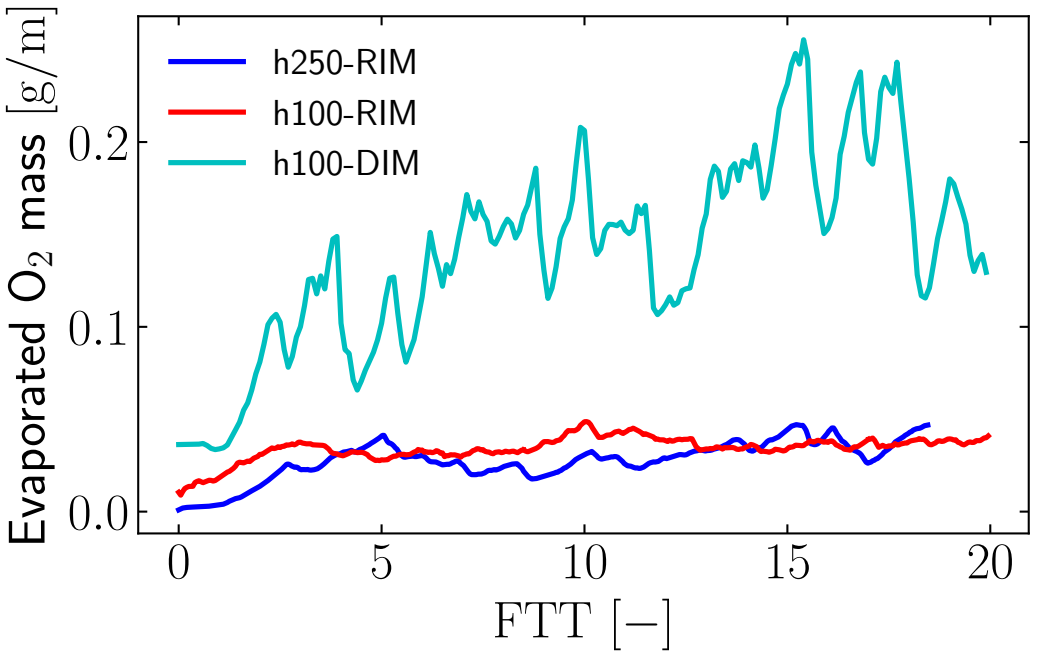


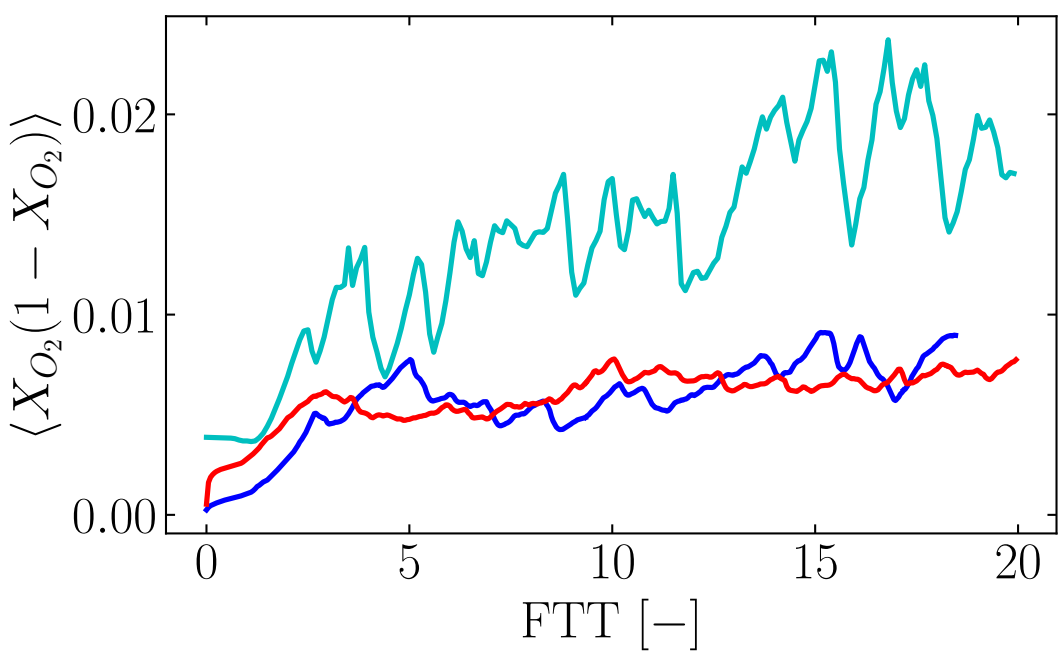
Comparison with DIM: LOX/GH2 mixing

- Thermal and compositional mixing is strongly influenced by the resolution of the interface
  - There is a strong difference in the mixedness predicted by RIM and DIM

$$\text{Evaporated O2 mass} = \int_{\Omega:\rho<250\ kg/m^3} \rho Y_{O_2} dV$$

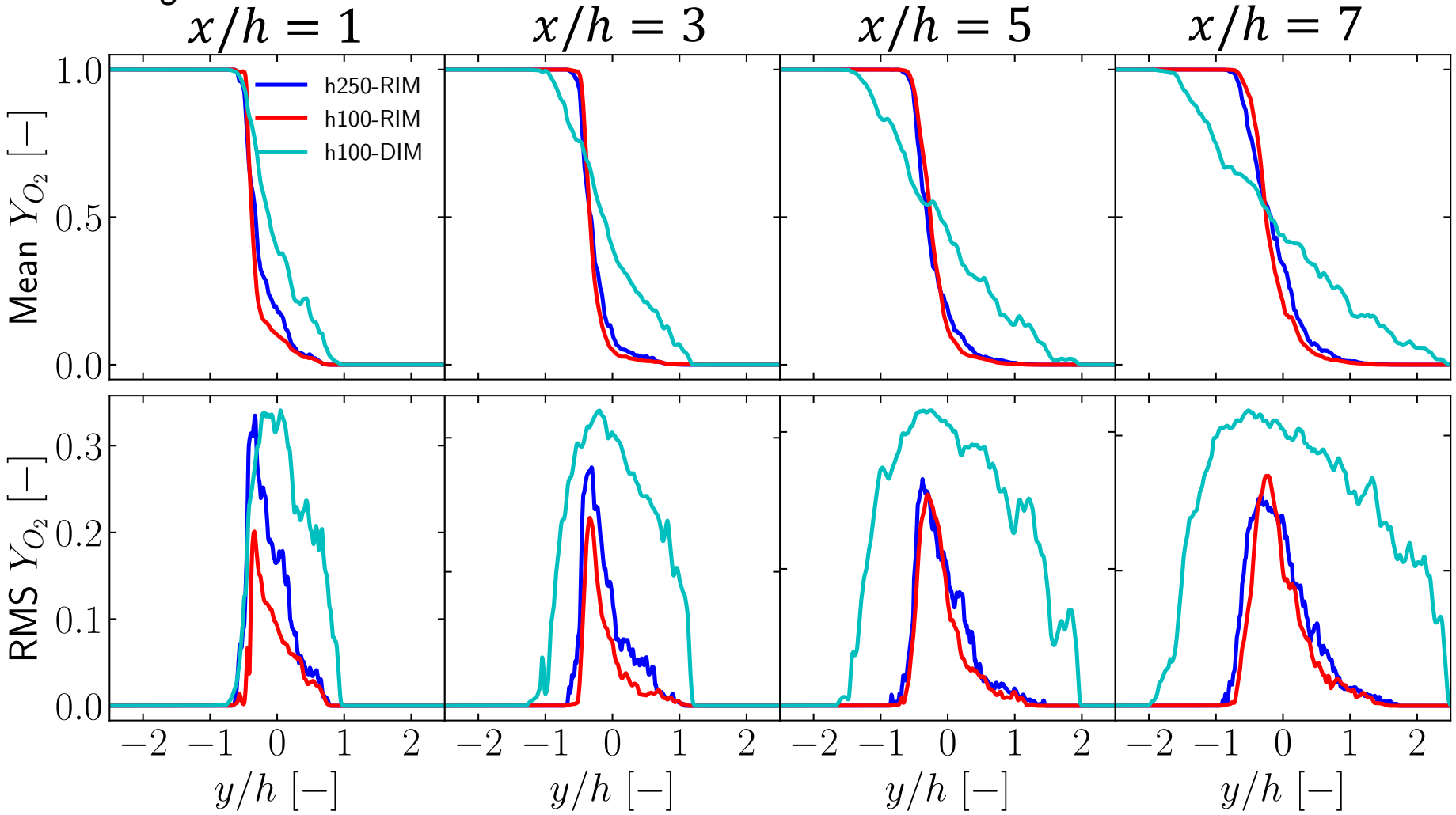
$$\langle X_{O_2}(1-X_{O_2})\rangle = \frac{1}{\Omega}\int_{\Omega} X_{O_2}(1-X_{O_2})dV$$





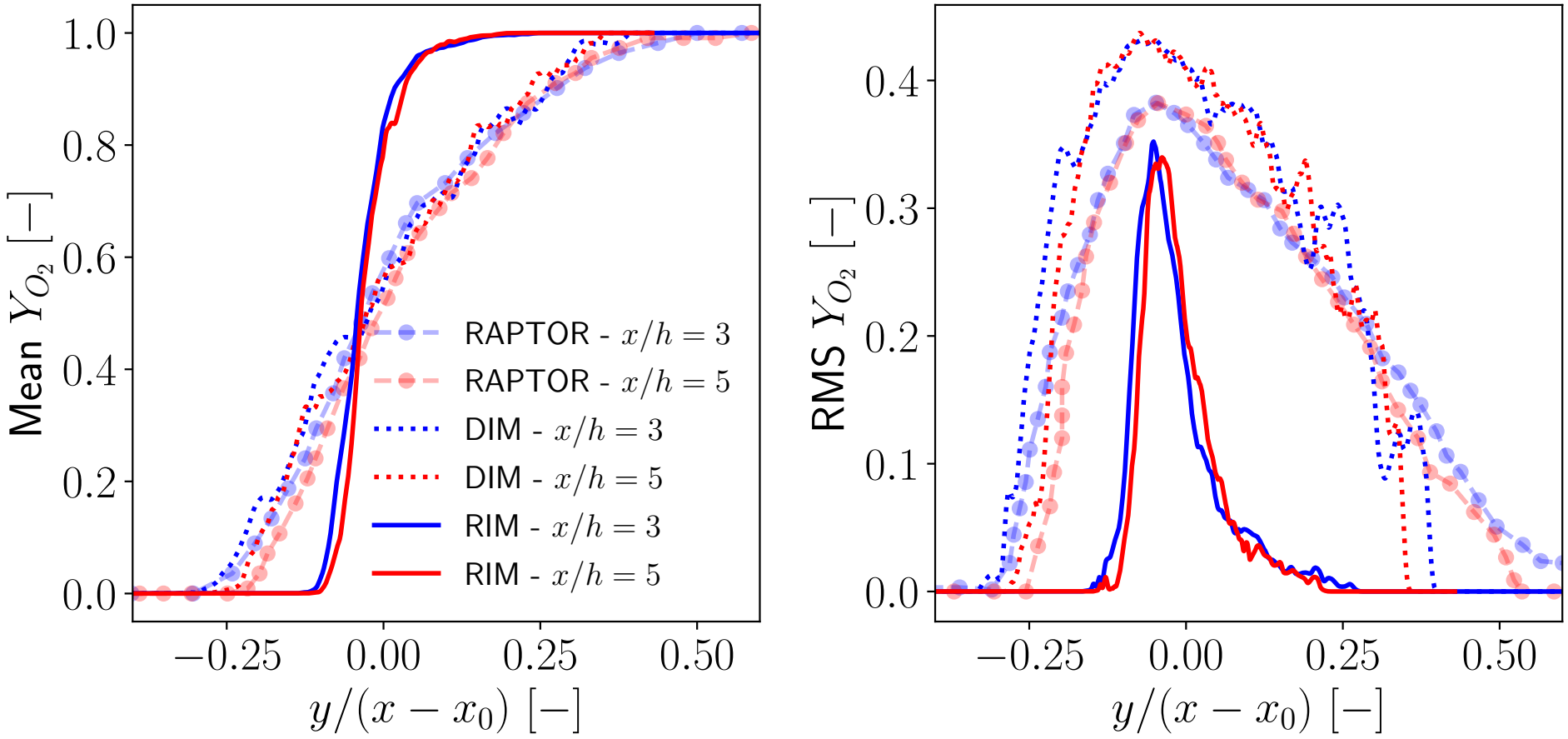
Comparison with DIM: Temporal averaged mixing

- Temporal-averaged mixing is a combination of diffusion + large-scale convection
  - DIM overpredicts mixing of the LOX and GH2 streams
  - Good convergence between h100 and h250



Comparison with DIM: Temporal averaged mixing

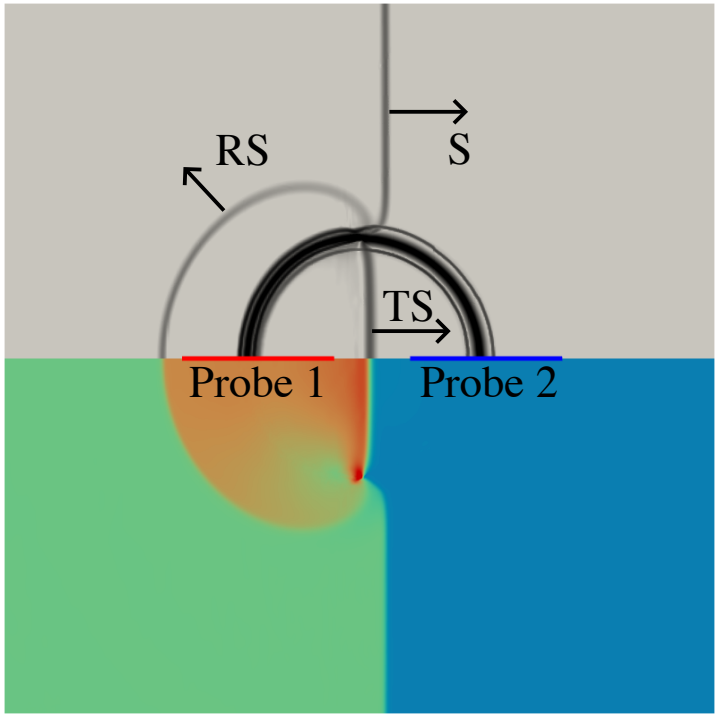
- Theory: Mixing layer grows with axial distance
  - DIM: Good comparison against RAPTOR benchmark results
  - RIM also obeys linear growth rate, but with a lower spread angle



Application: Shock-droplet interaction

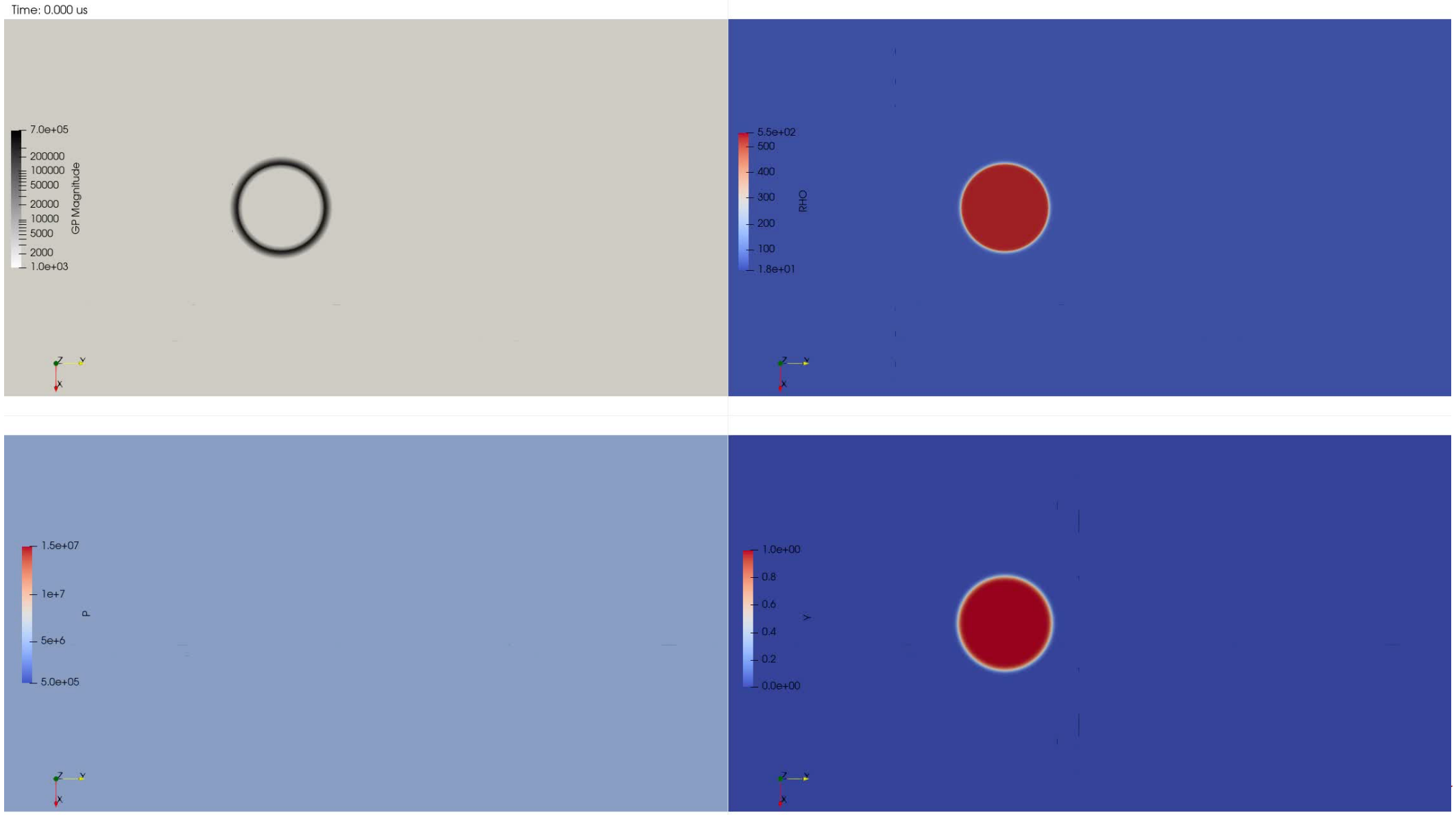
Shock-droplet interaction: Near-critical condition

- n-heptane/air system
- Initial condition: subcritical temperature with liquid/vapor interface.
- Post-shock conditions: transcritical condition
  - Is interfacial dynamics still important?



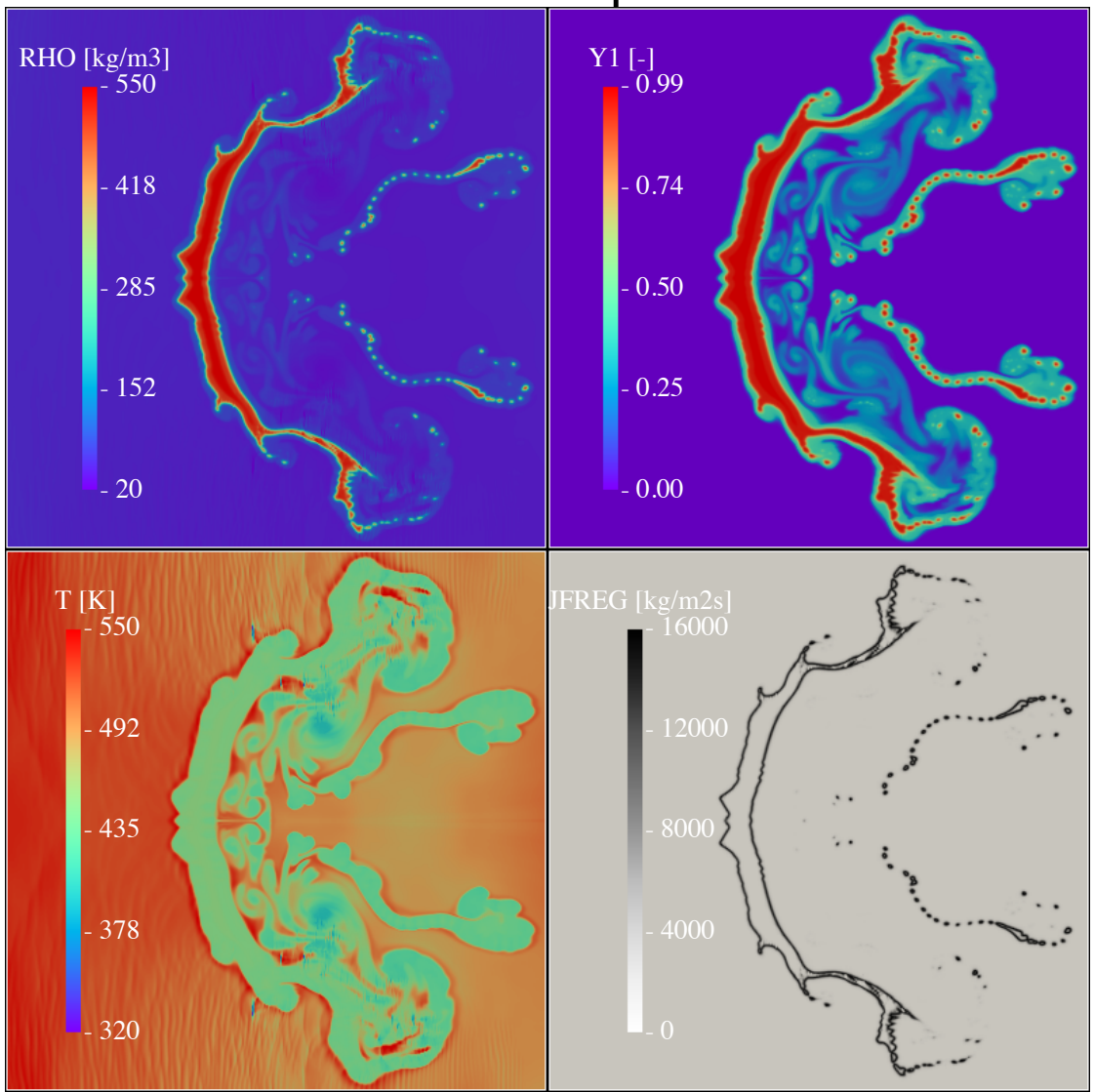
	Condition	Y_1 [−]	P [MPa]	T [K]	U [m/s]
Ambience	Pre-S	0.001	5	450	0
	Post-S	0.001	11	560	250
	Post-RS	0.001	15	620	150
Droplet	Pre-S	0.99	5	450	0
	Post-TS	0.99	15	456	36

Shock-droplet interaction: Results



Shock-droplet interaction: Aerobreakup

- Surface-tension induced atomization + Evaporation



Conclusion

- Fluid dynamics at transcritical conditions are fascinating:
  - Fundamental interfacial questions: What happens to the interface at very near the critical point?
- Application to engineering systems: Emergent of complex multi-mode phase-transfer behaviors
  - Spatio-temporal transitions between sub- and supercritical regimes

- RIM: an effective model for systematic investigation of these dynamics:
  - Resolves evaporation and interfacial flows without external models
  - Reverts to Navier-Stokes at conditions where interfaces do not manifest

- Many high-pressure engineering flows requires interfacial modeling:
  - Jet injection: Atomization + Surface tension modulates jet instability
  - Shock-droplet interaction: Atomization of the post-shock droplet