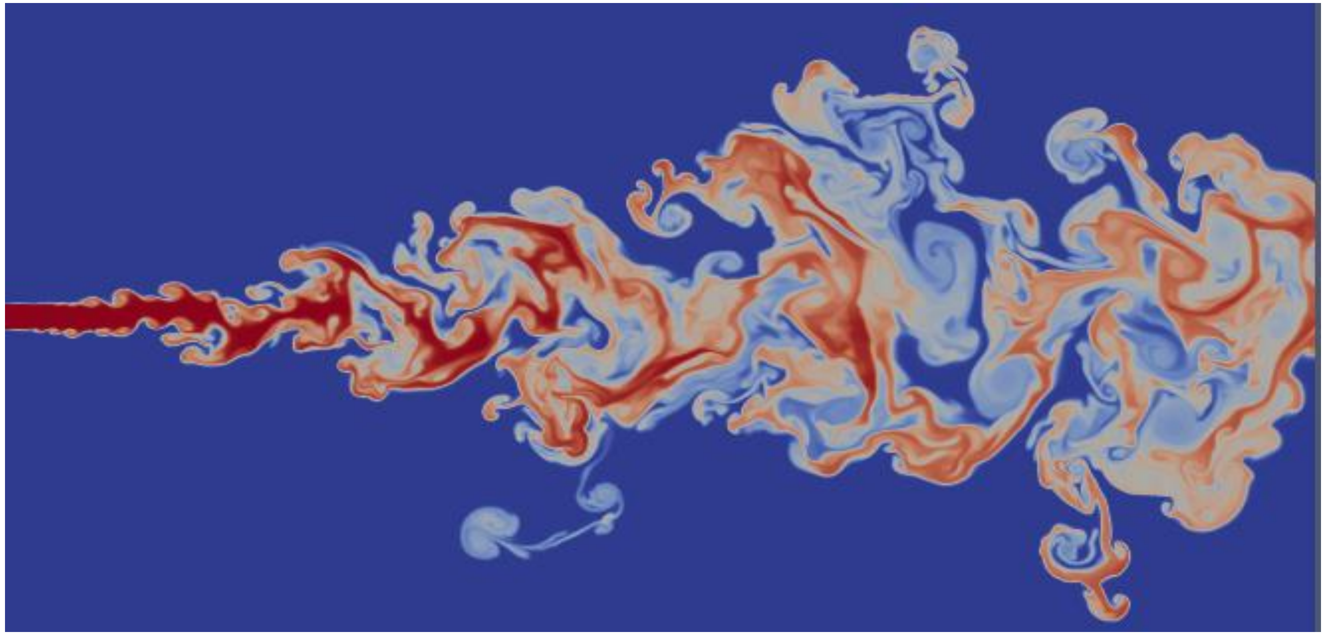
Large Eddy Simulations of Supercritical and Transcritical Jet Flows using Real Fluid Thermophysical Properties



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Outline

Background and Motivations

Model Presentations

- Validations

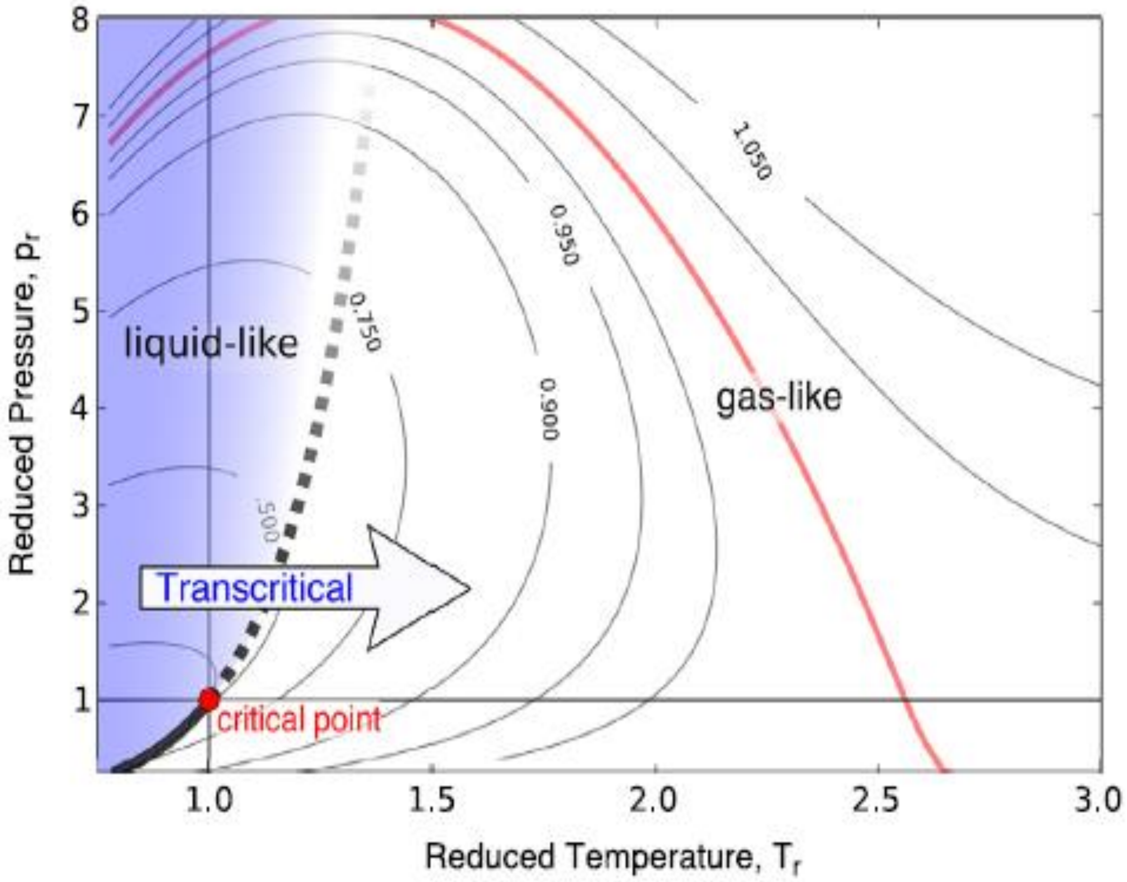
- 2D n-dodecane/nitrogen jet flows

- Conclusions and Work in Progress

Backgrounds and Motivations

- Challenge of emission pollutant control within the regulations which are more and more strict
- Needs for more efficient and cleaner combustion leading to the concept of increasing the operating pressure of combustion chamber
- Transcritical and supercritical jet conditions applied in ICE, gas turbine and rocket engines
- Multi-components *real-fluid* spray in hot turbulent flows are under explored
- Lacks of detailed understandings of the non-linear physics

P.C. Ma et al. / Journal of Computational Physics 340 (2017) 330–357



Model Presentations

- **Governing equations for a two-phase single-fluid compressible flow, in non-reacting conditions**

Mass: $$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0$$

Momentum: $$\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u u) = \nabla \cdot (-pI + \tau)$$

Energy: $$\frac{\partial (\rho h_T)}{\partial t} + \nabla \cdot (\rho h_T u) = \frac{\partial p}{\partial t} + \nabla \cdot (\tau \cdot u) - \nabla \cdot q$$ with $$h_T = h + (1/2)u^2$$

Species: $$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho Y_i u) = \nabla \cdot J_i$$

Model Presentations

- **Equation of State**:

Peng Robinson cubic EoS to model non ideal gas behavior

$$p(v, T, x_i) = \frac{RT}{v - b} - \frac{a\alpha}{v^2 + 2vb - b^2}$$

with a linear average of the critical properties based on mole fraction as mixing rules.

$$a = 0.457236 \frac{R^2 T_c^2}{P_c} \qquad b = 0.077796 \frac{RT_c}{P_c} \qquad \alpha = \left[1 + c_\omega \left(1 - \sqrt{T_r}\right)\right]^2$$

$$c_\omega = \begin{cases} 0.37464 + 1.5422\omega - 0.26992\omega^2, if \omega \leq 0.5 \\ 0.3796 + 1.485\omega - 0.1644\omega^2 + 0.01667\omega^3, \omega > 0.5 \end{cases}$$

Model Presentations

- **Thermodynamics quantities**
  - Caloric properties = ideal gas value + departure function
  - Departure functions are used to account for the deviation from the ideal-gas behavior
  - Example: Sensible enthalpy

$$h(p,T,x_i) = \overbrace{h_0(T,x_i)}^{GivenbyNasapolynamials} + \underbrace{\Delta h(p,T,x_i)}_{RT+\frac{1}{2\sqrt{2}b}ln\left(\frac{v+\left(1-\sqrt{2}b\right)}{v+\left(1+\sqrt{2}b\right)}\right)\left[a-T\left(\frac{\partial a}{\partial T}\right)_{x_i}\right]+pv}$$

Model Presentations

- **Transport properties**

➢ *Chung Method* was implemented to evaluate the dynamic viscosity and the thermal conductivity of real fluids

➢ Straightforward calculation requiring only critical properties

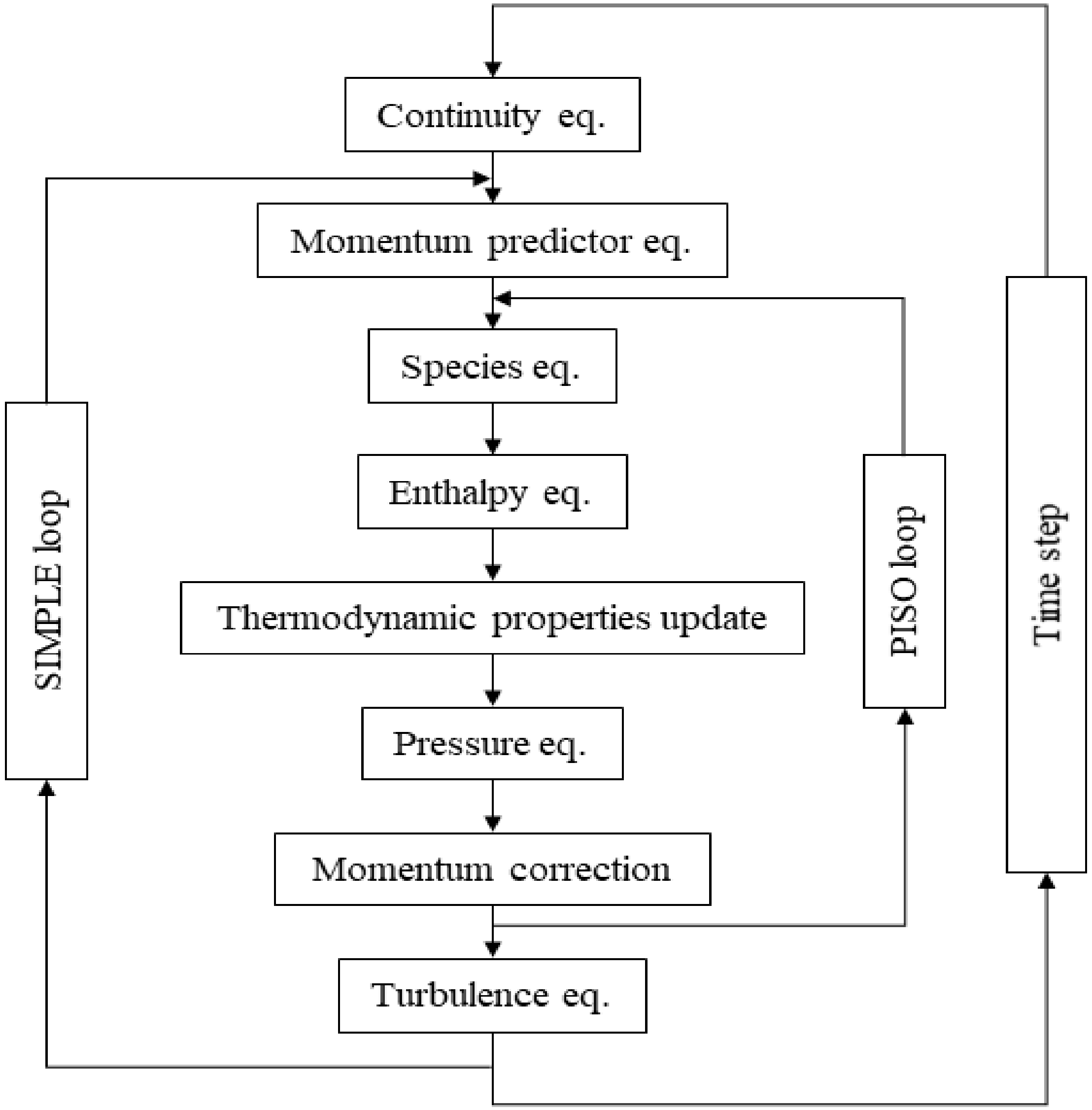
$$\mu(p,T) = \mu^{*}(p,T)\,\frac{36.344(MT_c)^{1/2}}{V_c^{2/3}} \quad ; \quad \mu^{*}(p,T) = \frac{(T^{*})^{1/2}}{\Omega_v} F_c\{[(G_2)^{-1} + E_5 y]\} + \mu^{**}$$

(E_0 to E_9 are linear functions of ω)

➢ Better prediction for a wide range of fluid states accounting for shapes and polarities of fluids

$$F_c = 1 - 0.2756\omega + 0.059035{\eta_r}^{4} + c$$

- **Solver: Modified reactingFoam**
  - Pressure based solver
  - Update of species, enthalpy and thermodynamic properties at each PISO loop

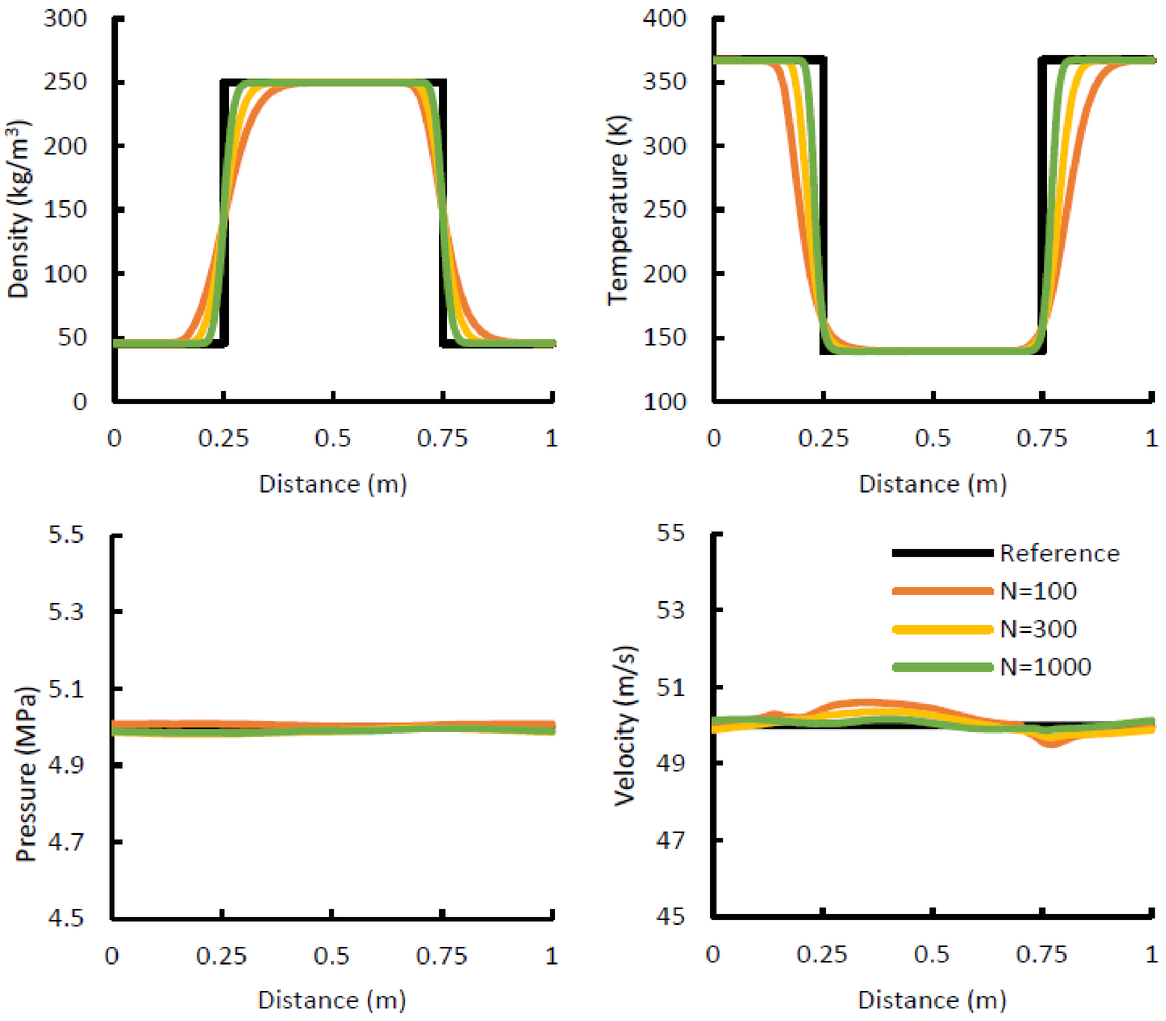


- **Implicit LES**
  - No SGS model used in the current simulations
  - Laminar on fine grids

Verification of the schemes on 1D test case

- Temporal discretisation: 1 order Euler
- Advection & Diffusion: 2 order Gauss limited-linear Schemes
- Verification:

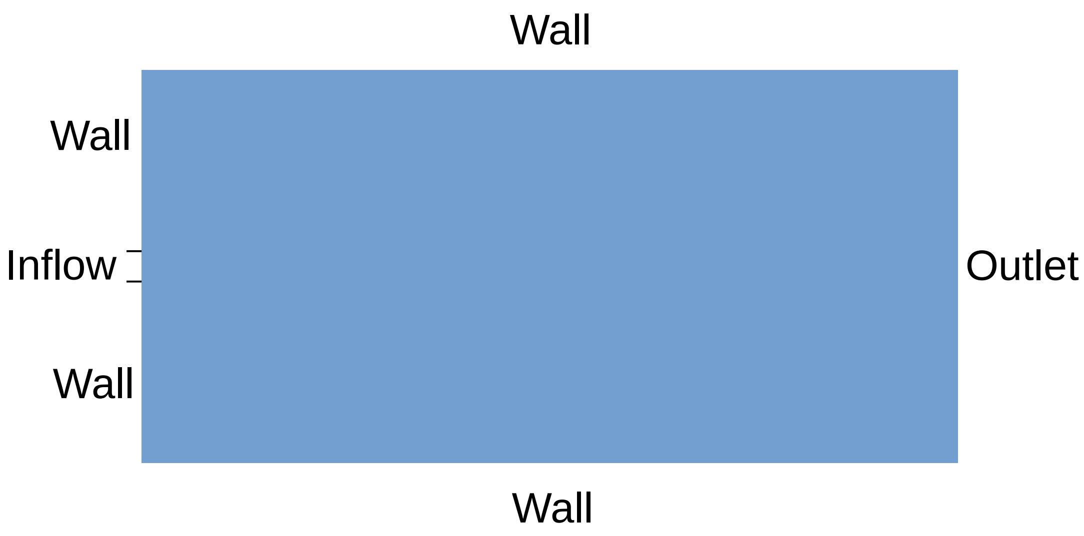
Fluid	N_2	N_2
Domain [m]	0.25 < x < 0.75	0.25 > x or x > 0.75
Pressure [MPa]	5	5
Temperature [K]	139.4	367.4



Validations

2D Mayer et al. 2003 exp. test case with cryogenic L-N_2 jet into warm G-N_2

Injected liquid	cryogenic nitrogen
Computational domain, $54d \times 27d$	120 mm × 60 mm
Diameter of nozzle jet, d	2.2 mm
Jet inlet velocity, u_{inj}	4.9 m/s (uniform)
Chamber pressure, p_{amb}	4 MPa
Chamber temperature, T_{amb}	298 K
Jet temperature, T_{inj}	128.5 K

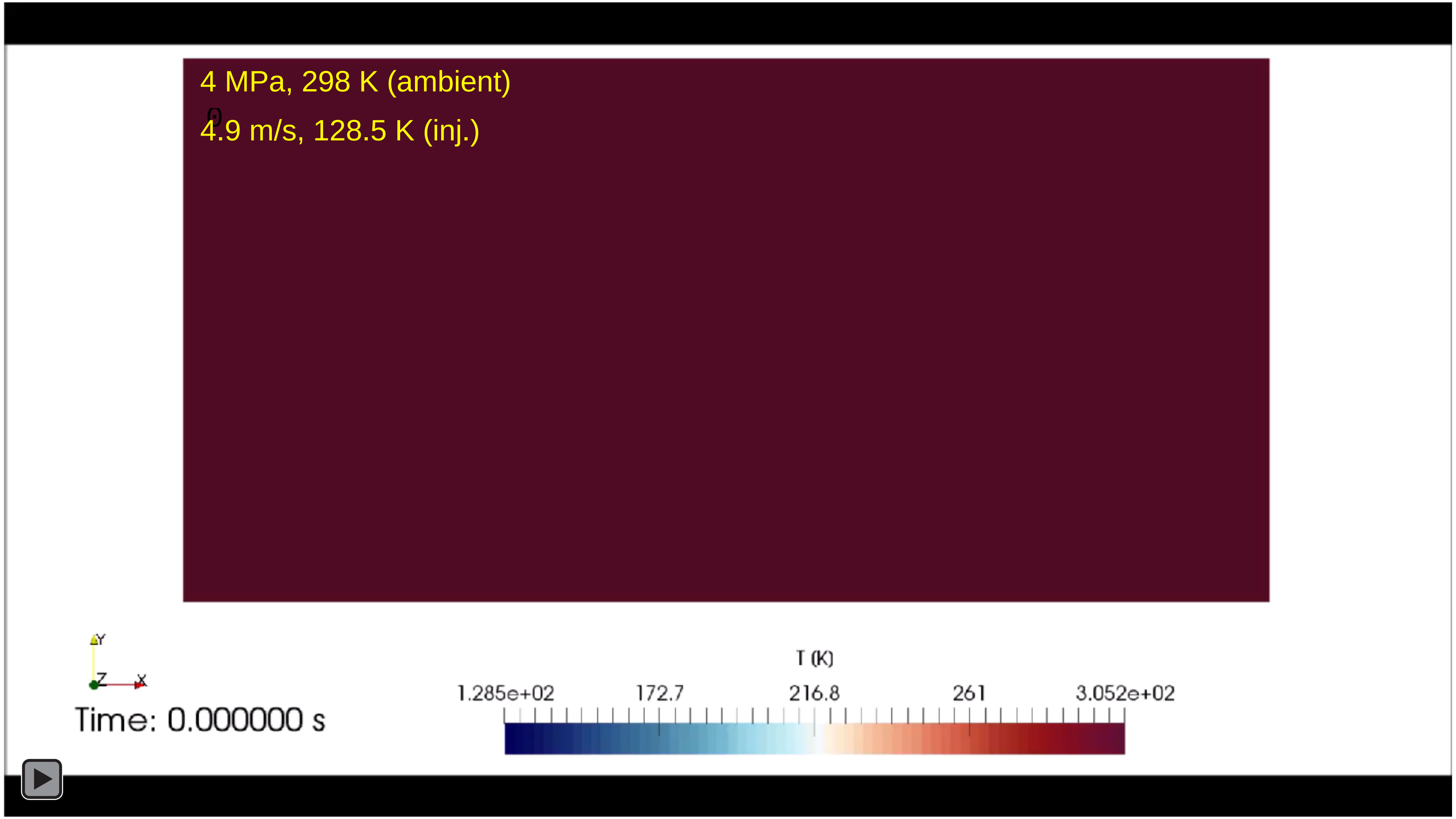


Critical properties of N_2 :

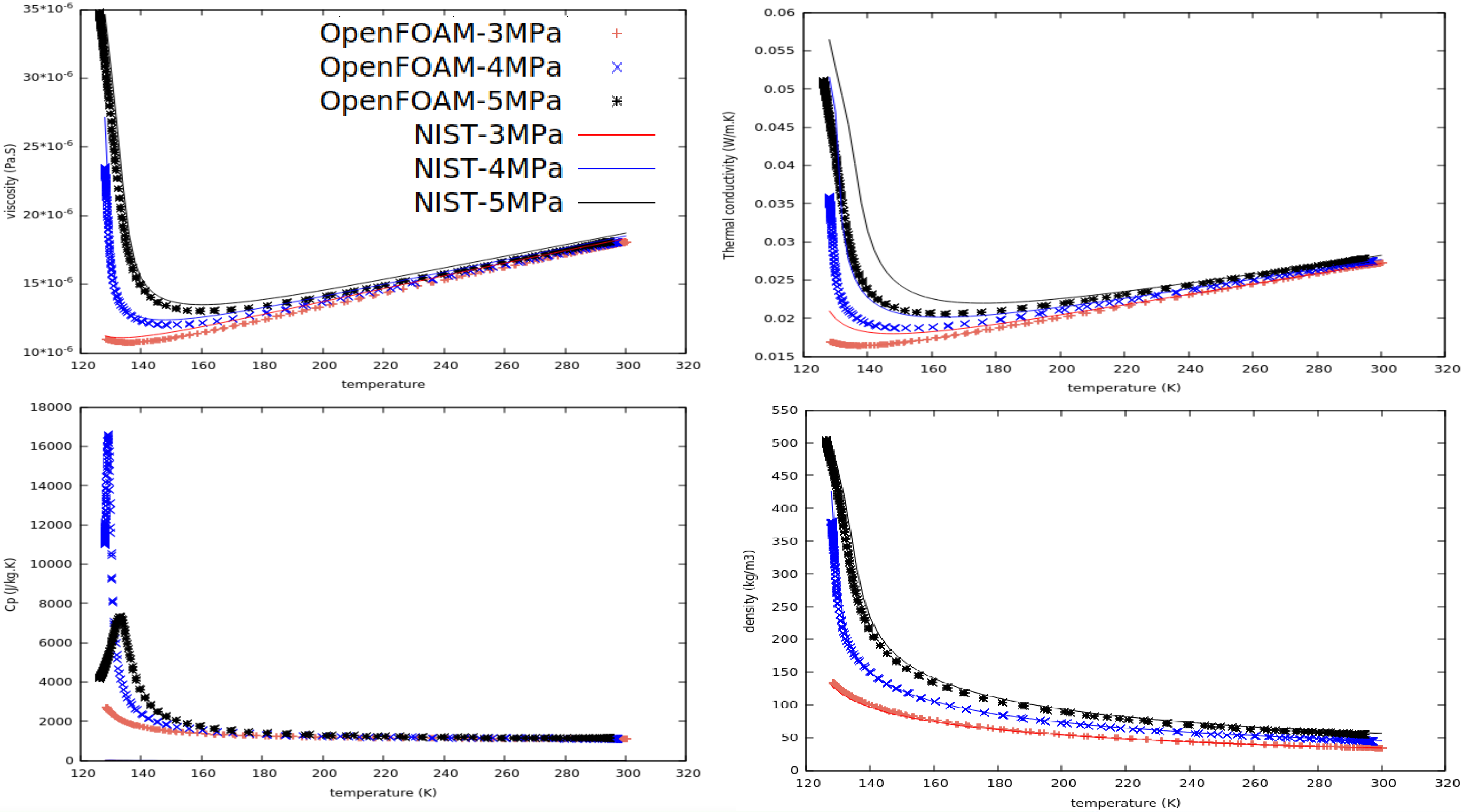
- P_{cr} = 3.39 MPa
- T_{cr} = 126.2 K

Mayer, W., Telaar, J., Branam, R., Schneider, G., & Hussong, J., "Raman measurements of cryogenic injection at supercritical pressure." Heat and Mass Transfer 39(8): 709-719, 2003.

Example of simulation results



- **Variations of thermophysical quantities of N_2 with different conditions**



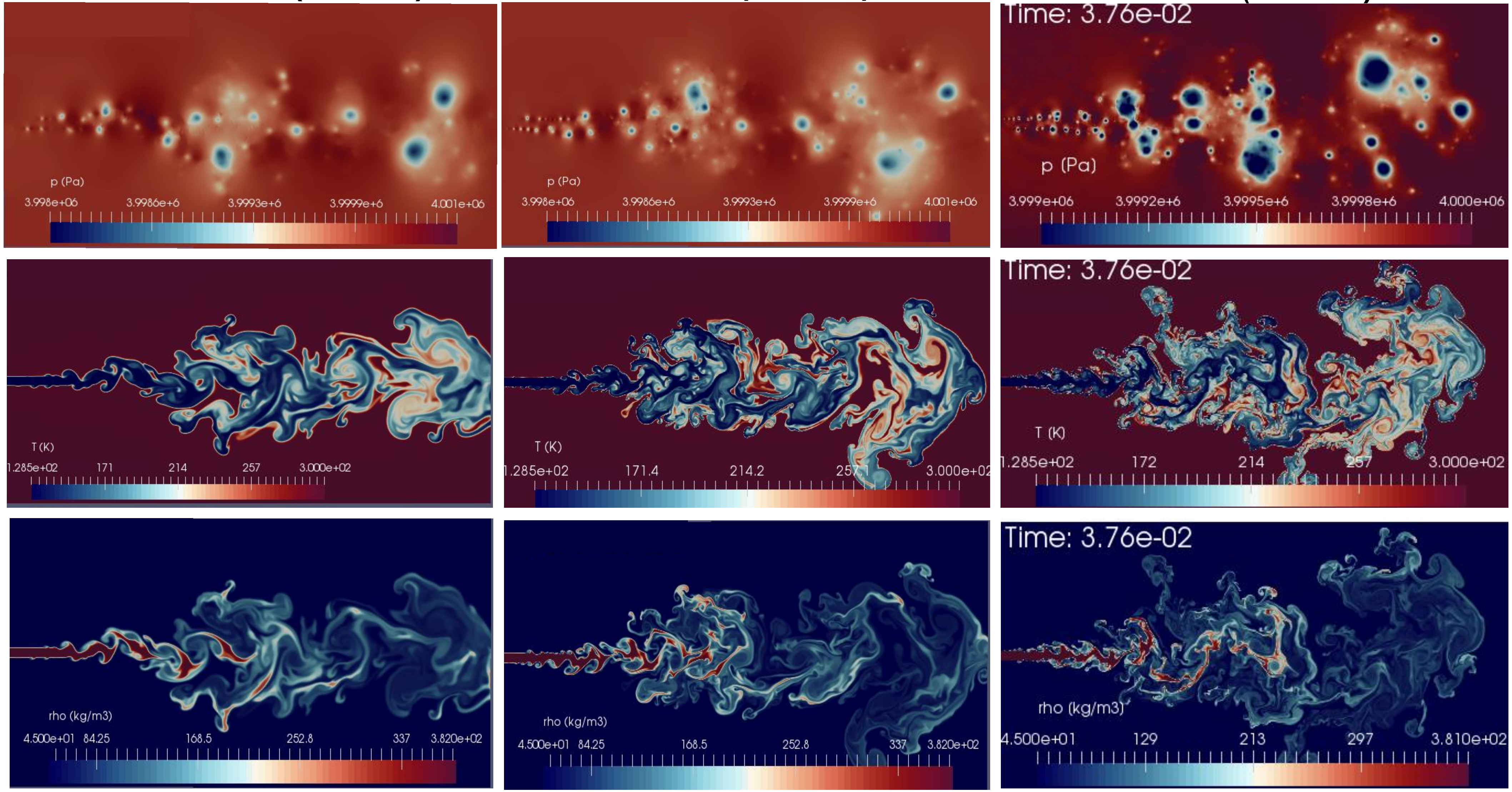
- **Grid Sensitivity study**

0.32×10^6 cells ($\Delta x/d = 16$) | 1.28×10^6 cells ($\Delta x/d = 32$) | 2.88×10^6 cells ($\Delta x/d = 48$)

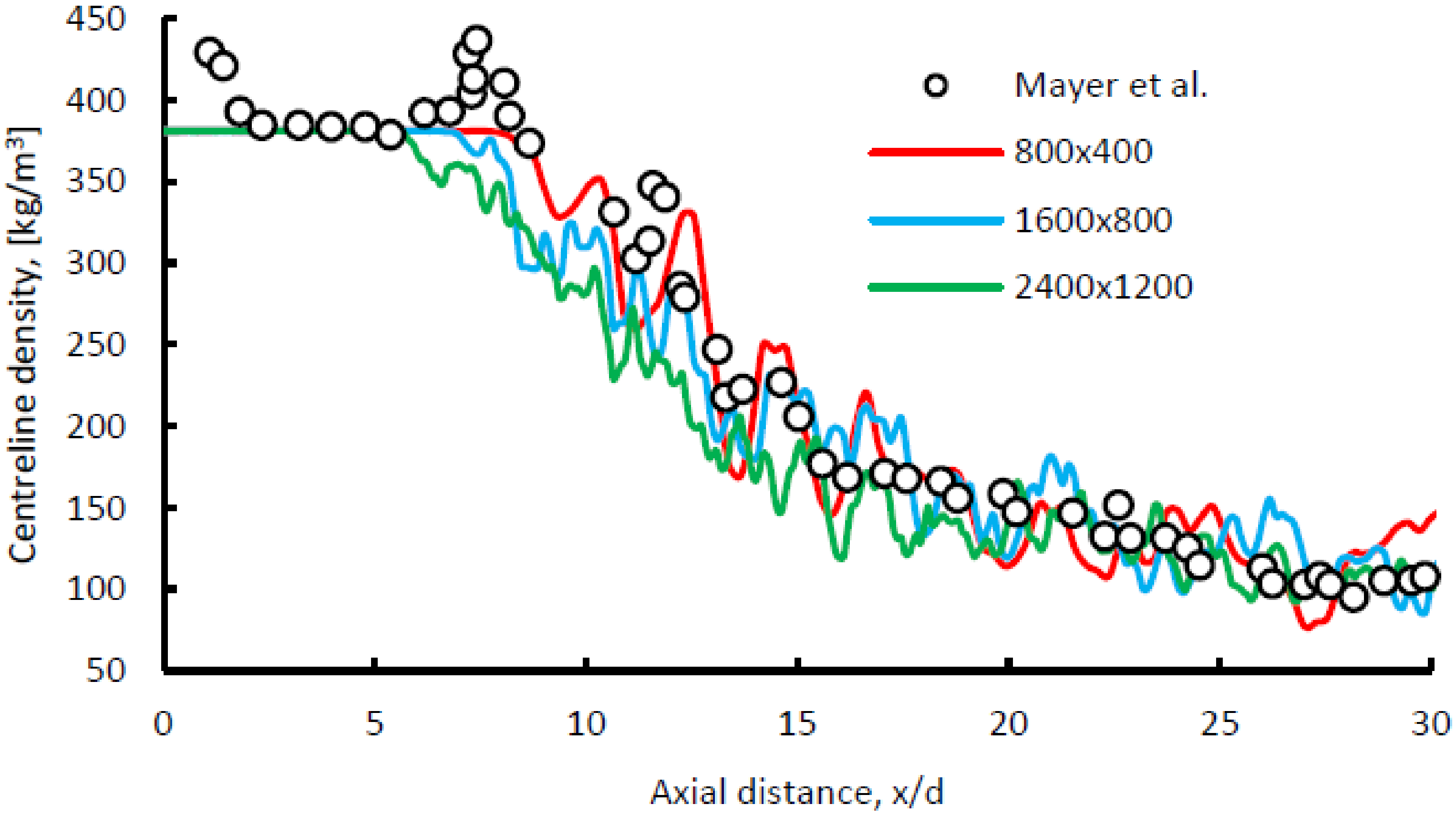
Pressure (MPa)

T (K)

Density (kg/m^3)



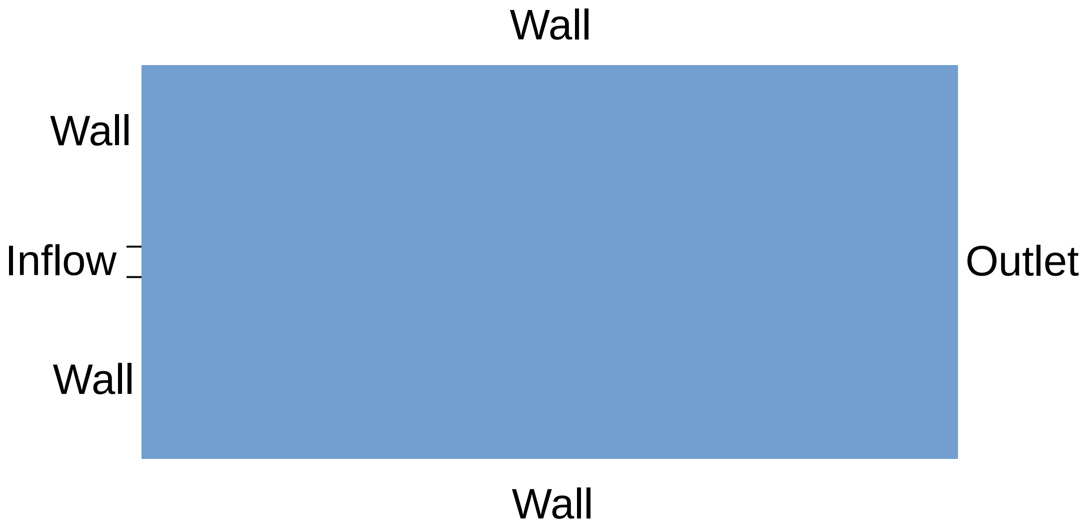
Time averaged centreline density for the 3 grids



- Good agreement of jet core density with experimental data
- Ealier jet dispersion with finer grids

2D n-dodecane/nitrogen jet flows

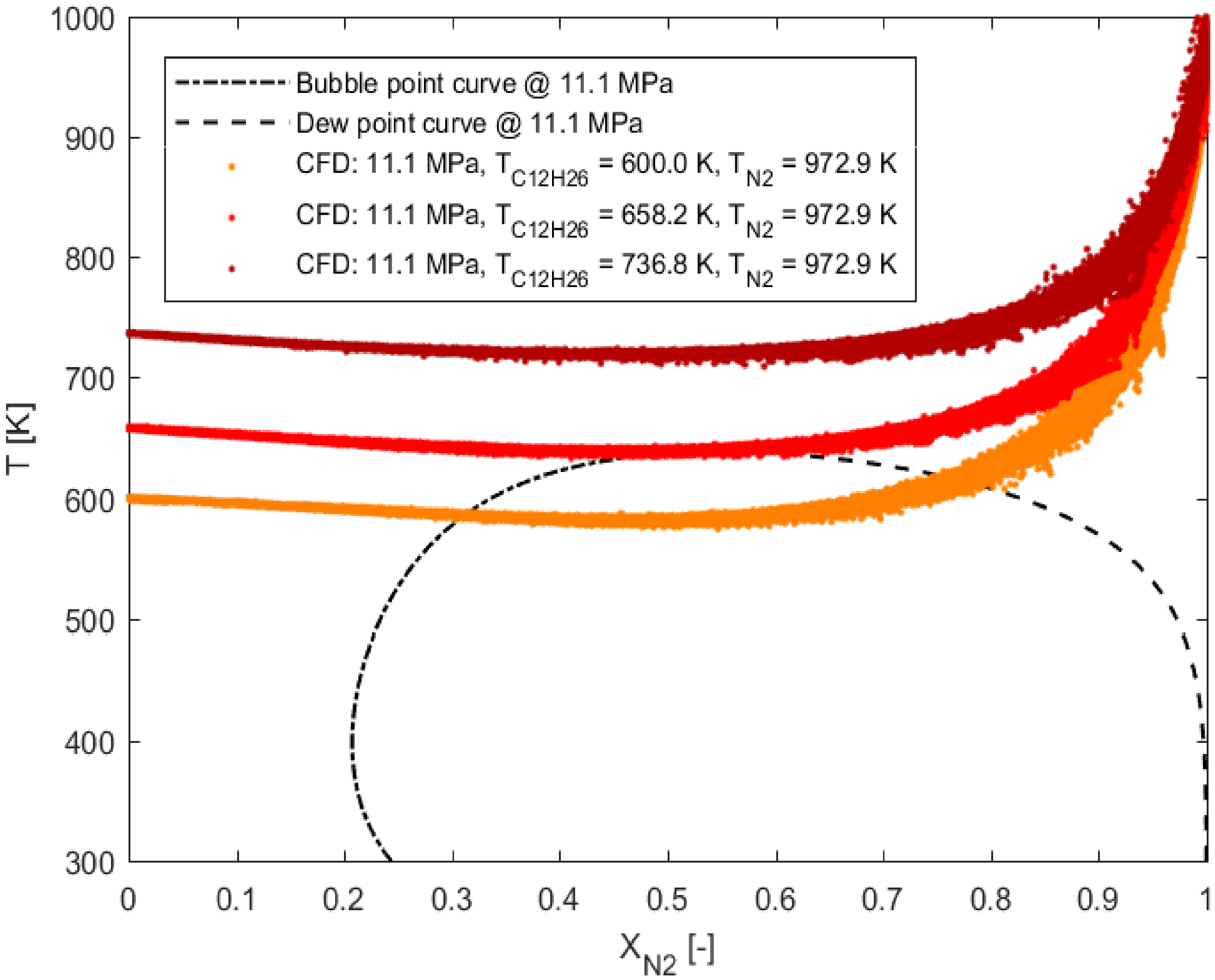
Injected fluid	n-dodecane
Ambient gas	nitrogen
Computational 2D domain, $L \times H$	5 mm × 2.5 mm
Diameter of nozzle jet, d	0.1 mm
Jet inlet velocity, u_{inj}	200 m/s (uniform)
Chamber temperature, T_{amb}	972.9 K
Chamber pressure, p_{amb}	6.0 MPa and <u>11.1 MPa</u>
Jet inlet temperature, T_{inj}	600 K, <u>658.2 K</u> and 736.8 K



Critical properties of $C_{12}H_{26}$:

- P_{cr} = 1.8 MPa
- T_{cr} = 658.2 K

Effect of inlet jet temperature



- Lower temperature case crosses the two-phase region for a substantial part of the CFD states
- Intermediate case touches the VLE curves but remaining basically above

Effect of inlet jet temperature

T_{inj}= 600 K

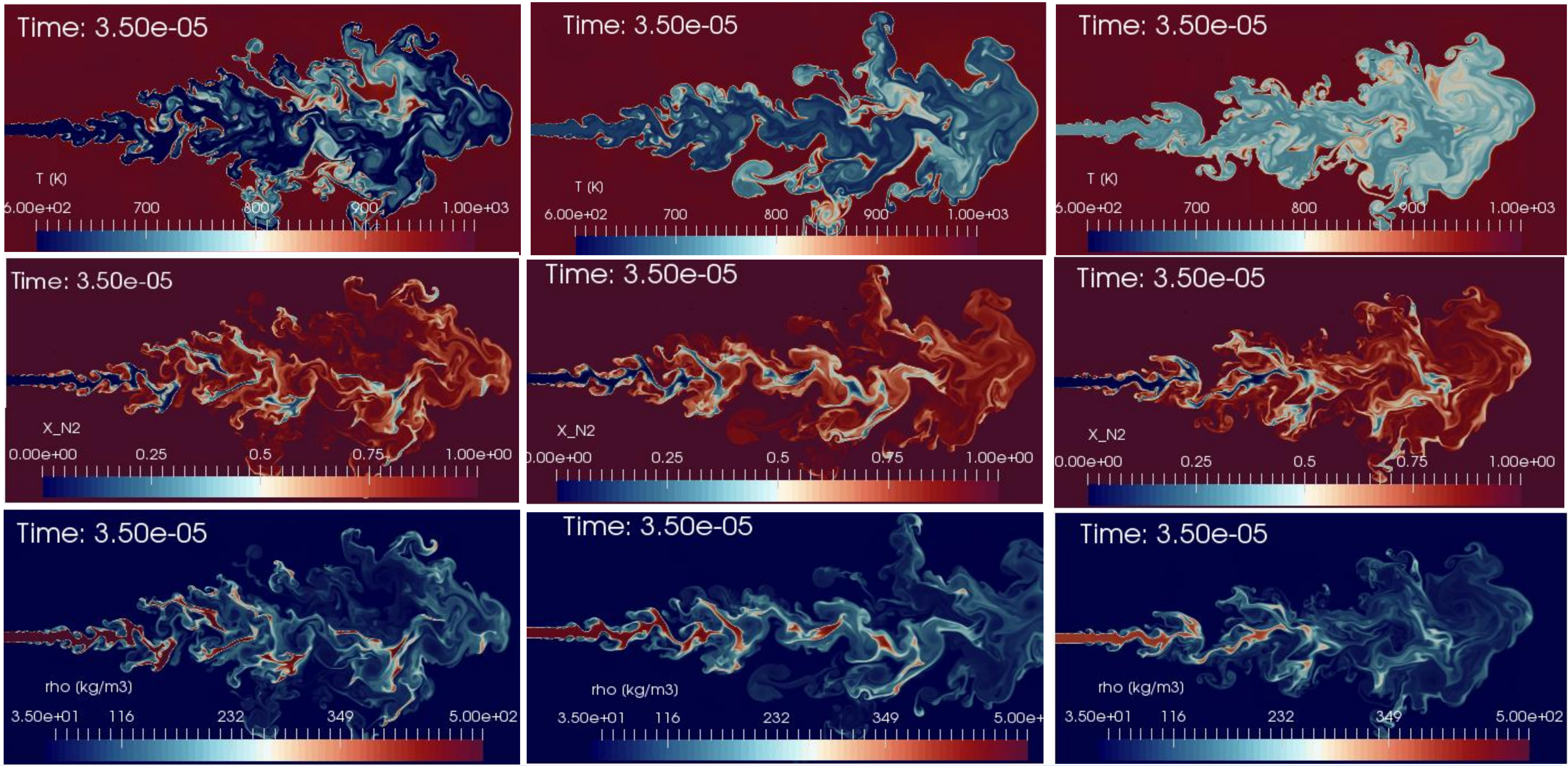
T_{inj}= 658.2 K

T_{inj}= 736.8 K

T (K)

Mole Fraction

Density (kg/m^3)



Effect of inlet jet temperature

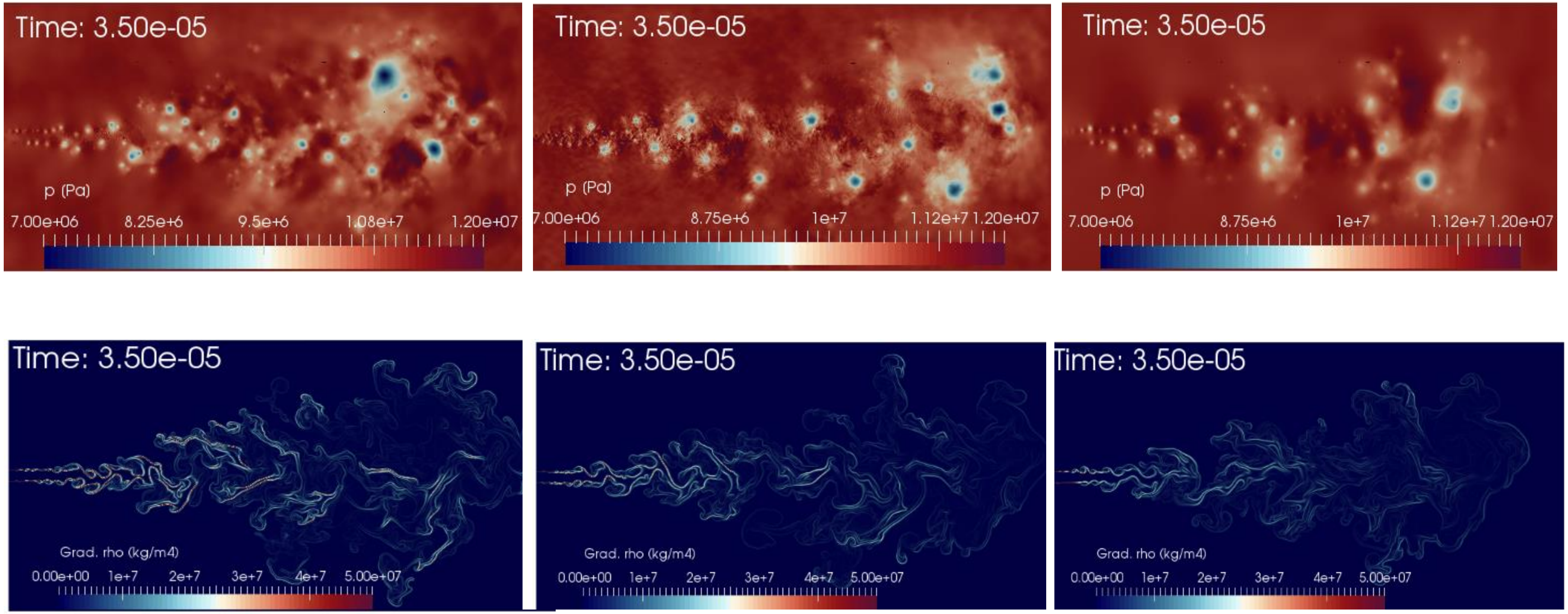
T_{inj}= 600 K

T_{inj}= 658.2 K

T_{inj}= 736.8 K

P (Pa)

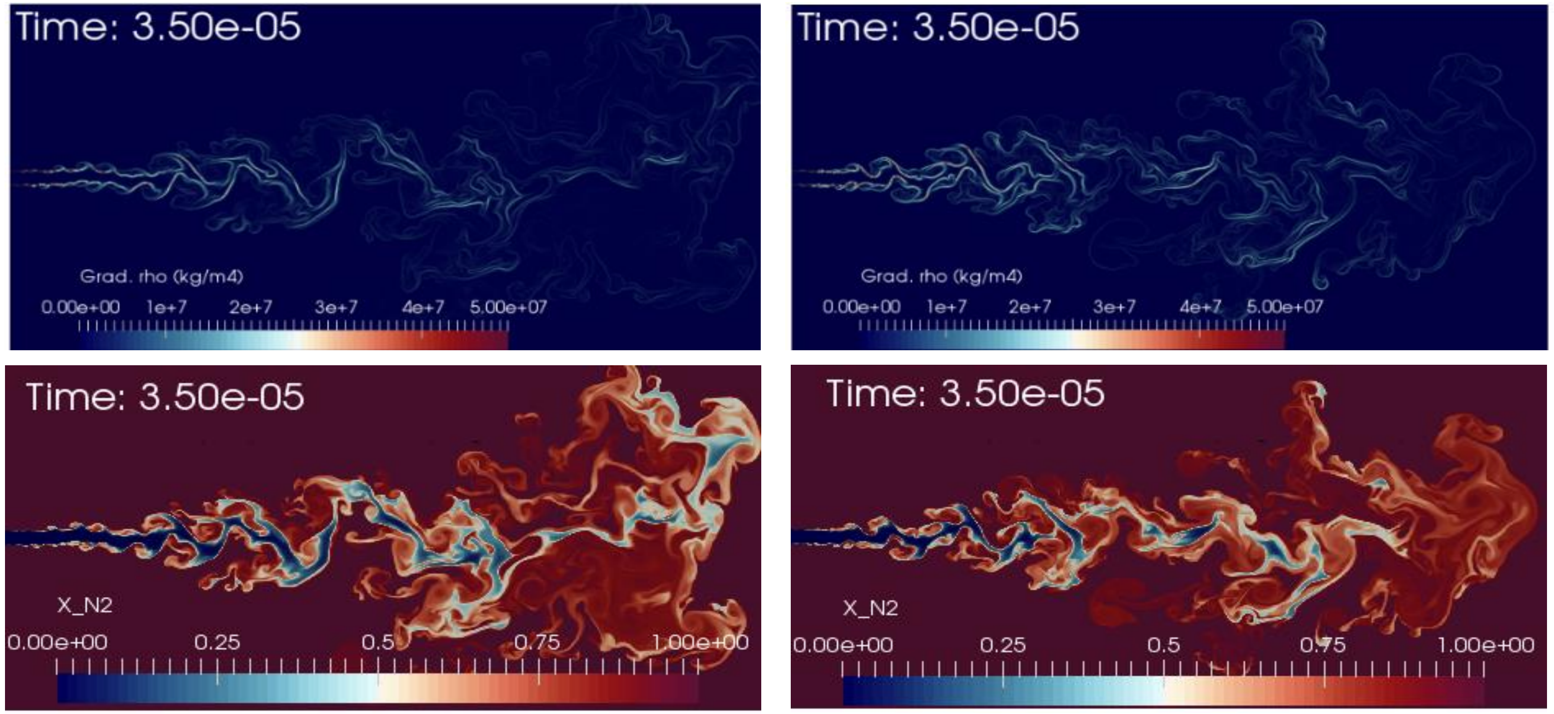
Density gradient (kg/m^4)



Effects of ambient pressure

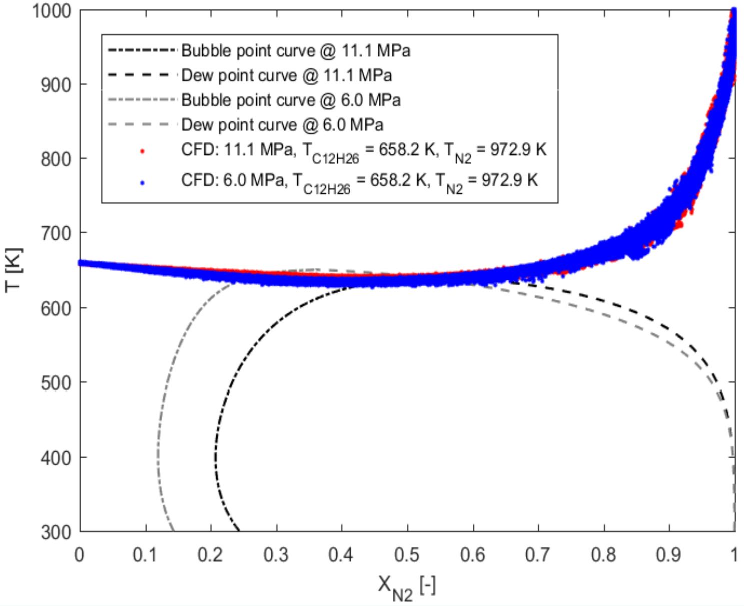
Density gradient (kg/m^4)

Mole Fraction



6 MPa

11 MPa



The lower pressure case shows marked subcritical features, such as strong ligament persistence

Conclusions

- Pressure based numerical formulation was able to capture density and temperature without severe spikes of pressure and velocity

- Capability to handle multi-species mixing processes accounting for real-fluid properties

→ Current framework has adequate accuracy and potential for further developments

Work in progress

- Implementing more advanced mixing rules

$$a\alpha = \sum_i \sum_j a_{ij}\alpha_{ij}x_i x_j \qquad b = \sum_i x_i b_i \qquad a_{ij}\alpha_{ij} = \sqrt{a_i a_j \alpha_i \alpha_j}\left(1 - k_{ij}\right)$$

- Implementing multi-species mass diffusivity models based on binary coefficients
- Including phase stability tests and phase splitting
- Further improving the solver efficiency

thank you

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