Molecular Dynamics Simulations of Supercritical Jet Mixing

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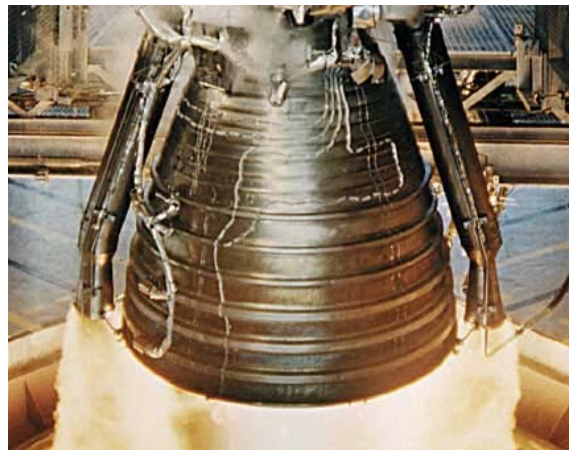
Introduction

- High pressure heterogeneous combustion systems typically operate trans- or supercritical
  - Liquid rocket engines
  - Gas turbine combustors
  - Diesel engines
- Quantitative assessments or validated theories characterizing propellant injection at near and supercritical conditions are currently limited



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Introduction

- Because these systems operate at near and supercritical conditions, it is difficult to model the injection, mixing, atomization, and vaporization using traditional CFD
  - System becomes fully 3-D
  - Material and transport properties change significantly
  - Moves from 2-phase to 1-phase
  - Complex mixture effects

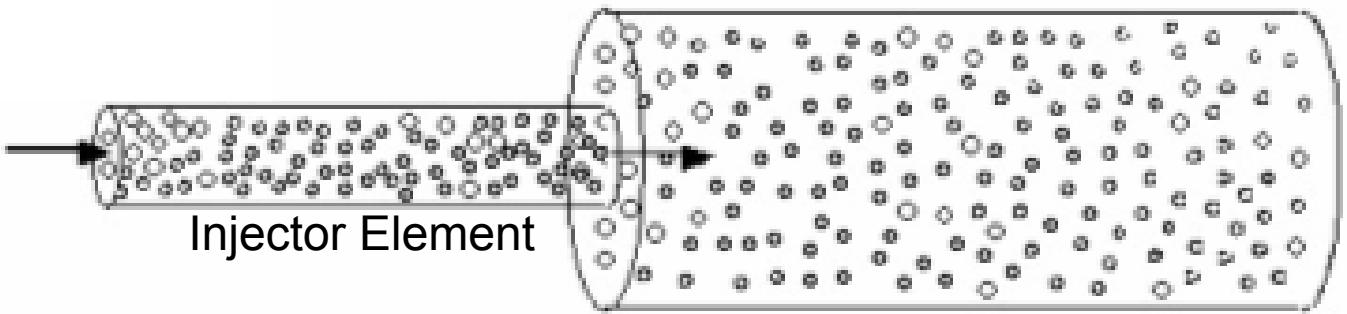
Introduction

- This research attempts to address these limitations through the use of MD as an alternate simulation tool

- Diatomic liquid nitrogen (N_2) is simulated as a non-reacting substitute to other diatomic cryogenic liquid propellants/oxidizers, i.e. H_2 or O_2

  Experimental database exists

- The simulation consists of two cylinders
  - Smaller diameter cylinder representing one injector through which simulated liquid nitrogen flows
  - Larger diameter cylinder of gaseous nitrogen into which the simulated



Introduction

- Advantages of the MD model:
  - Based purely on first principles (*F=ma*)
  - Can theoretically span all conditions; no need to track phase boundaries
  - Geometric assumptions do not need to be made
  - Equation of state, material and transport properties are not needed, and *can actually be* calculated outputs
  - Mixture effects automatically incorporated

Fundamental Concepts of MD

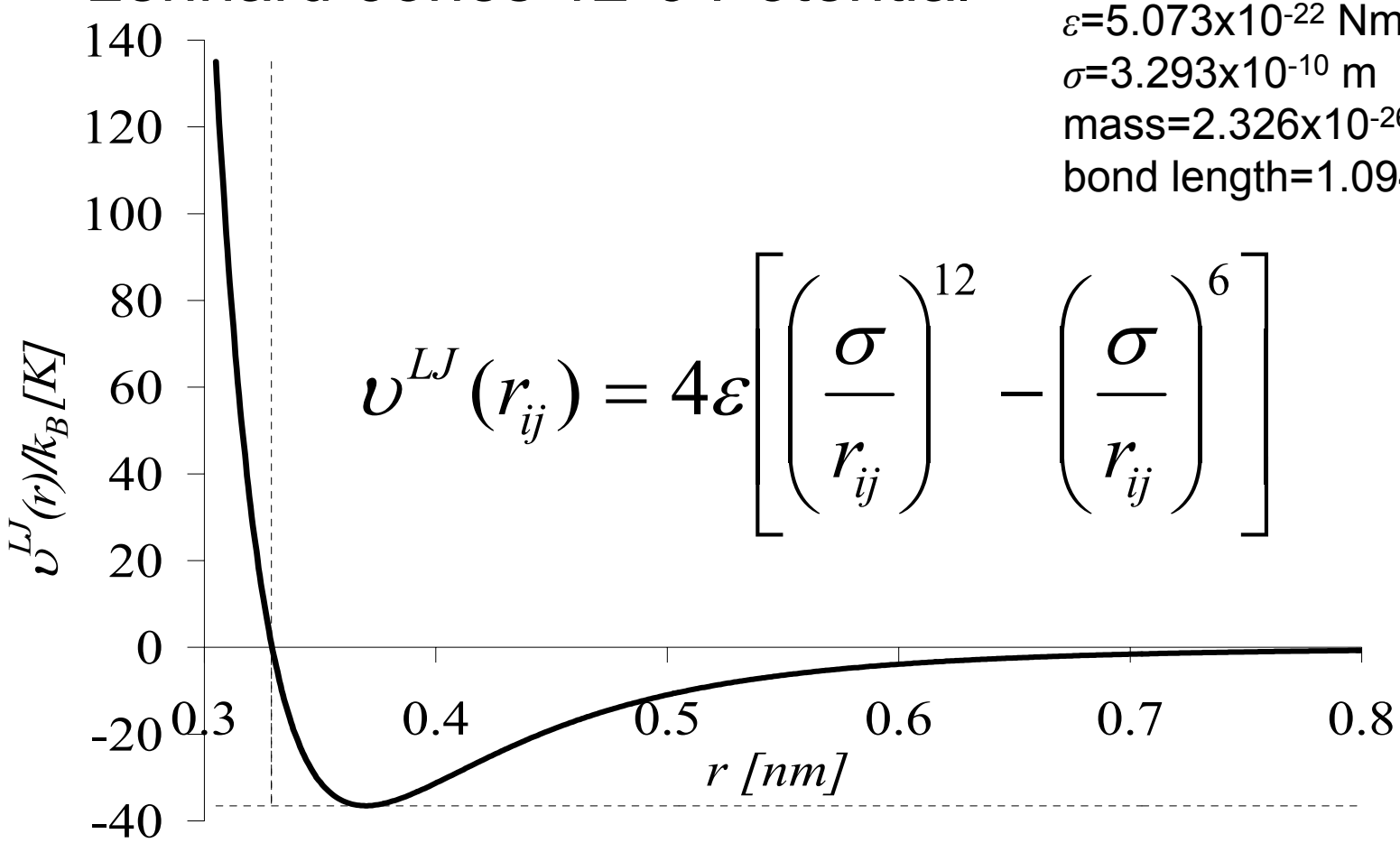
- Dynamics of interest is contained within solution to the classical N-body problem
- MD is a numerical tool used to solve Newton's Laws of Motion, applied to motions of individual atoms or molecules
  - $F = ma$ is the only equation to solve
  - Forces on atoms derived from interatomic potentials

Fundamental Concepts of MD

- Lennard-Jones 12-6 Potential

For Nitrogen Atoms:
ε=5.073x10^{-22} Nm
σ=3.293x10^{-10} m
mass=2.326x10^{-26} kg
bond length=1.094x10^{-10} m

$$\upsilon^{LJ}(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$



Fundamental Concepts of MD

- Equations of Motion

$$m_a \boldsymbol{a}_i = \boldsymbol{F}_i = \sum_{\mathrm{j=1}}^{\mathrm{N_a}} \boldsymbol{f}_{\mathrm{ij}}$$

- For Lennard-Jones Potential

$$\boldsymbol{f} = -\nabla \upsilon^{LJ}(r)$$

$$\boldsymbol{f}_{ij} = \left(\frac{48\varepsilon}{\sigma^2}\right)\left[\left(\frac{\sigma}{r_{ij}}\right)^{14} - \frac{1}{2}\left(\frac{\sigma}{r_{ij}}\right)^{8}\right]\boldsymbol{r}$$

- Solve Numerically Using Finite Difference Velocity-Verlet Algorithm

$$\boldsymbol{r}(t+\Delta t) = \boldsymbol{r}(t) + \Delta t \boldsymbol{v}(t) + \frac{\Delta t^2 \boldsymbol{a}(t)}{2}$$

$$\boldsymbol{v}(t+\Delta t/2) = \boldsymbol{v}(t) + \frac{\Delta t \boldsymbol{a}(t)}{2}$$

$$\boldsymbol{v}(t+\Delta t) = \boldsymbol{v}(t+\Delta t/2) + \frac{\Delta t \boldsymbol{a}(t+\Delta t)}{2}$$

Fundamental Concepts of MD

- Addition of Bond Constraint to Simulate Diatomic Nitrogen Molecule

$$r_{ab}^2 = \boldsymbol{r}_{ab} \cdot \boldsymbol{r}_{ab} = \text{constant}$$

$$\frac{d(r_{ab}^2)}{dt} = 2\boldsymbol{r}_{ab} \cdot \boldsymbol{v}_{ab} = 0$$

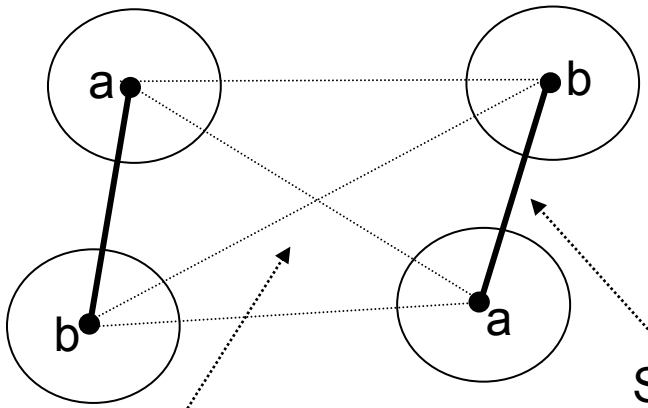
RATTLE Algorithm:

$$\boldsymbol{r}(t+\Delta t) = \boldsymbol{r}'(t+\Delta t) + \left(\frac{\Delta t^2}{2m}\right)\boldsymbol{g}(t)$$

$$\boldsymbol{v}(t+\Delta t/2) = \boldsymbol{v}'(t+\Delta t/2) + \left(\frac{\Delta t}{2m}\right)\boldsymbol{g}(t)$$

$$\boldsymbol{v}(t+\Delta t) = \boldsymbol{v}'(t+\Delta t) + \left(\frac{\Delta t}{2m}\right)\boldsymbol{g}(t+\Delta t)$$

Two N_2 Molecules:

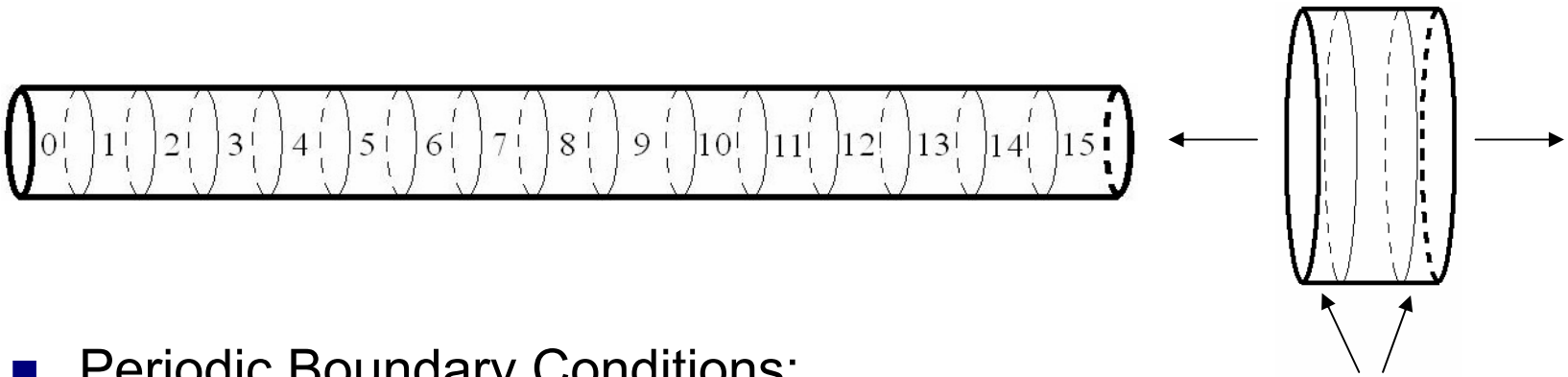


Motion of each atom in molecule simulated separately

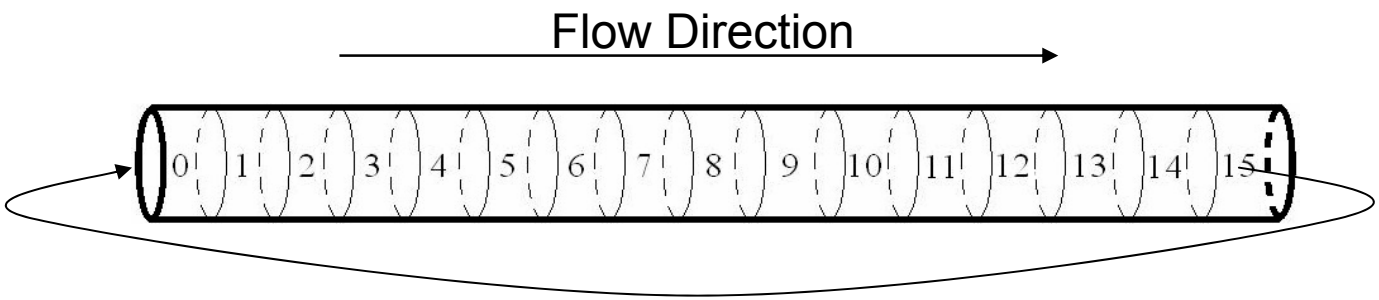
Simulated bond using RATTLE

Simulation Methodology

- Computational Domain and Processor Setup:
  - Each processor assigned to handle particles within a specific geometric region
  - As particles move, they are transferred between processors

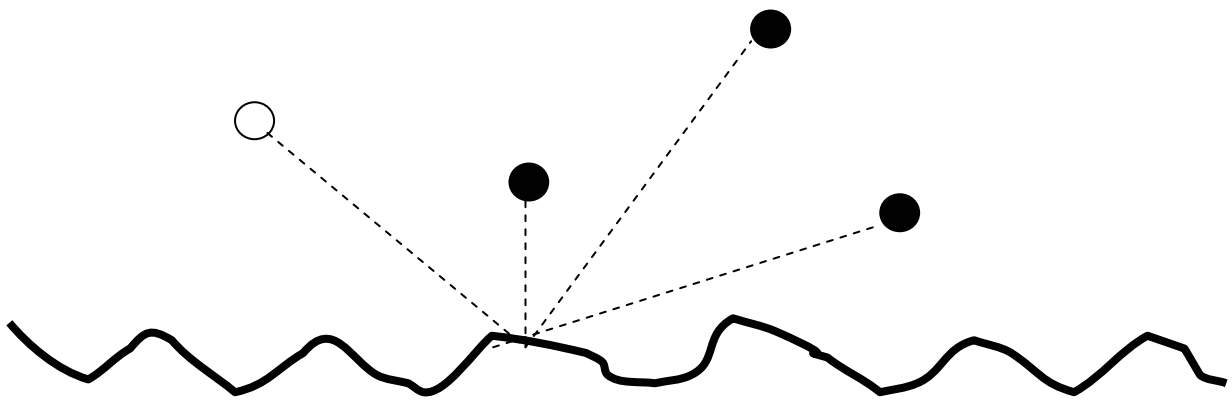


- Periodic Boundary Conditions:

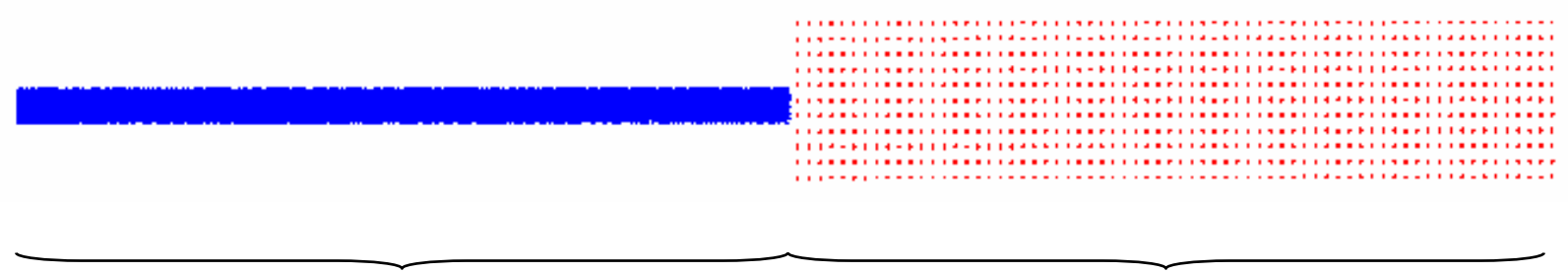


Wall Model

- Constant Temperature Wall
- Diffusely Reflecting
  - Molecules reemitted from wall in random direction with random velocity based on Maxwellian distribution scaled to the wall temperature.
  - Removes heat generated by viscous dissipation



Simulation Methodology



Initialized Liquid Nitrogen Flow

Initialized Gas Chamber

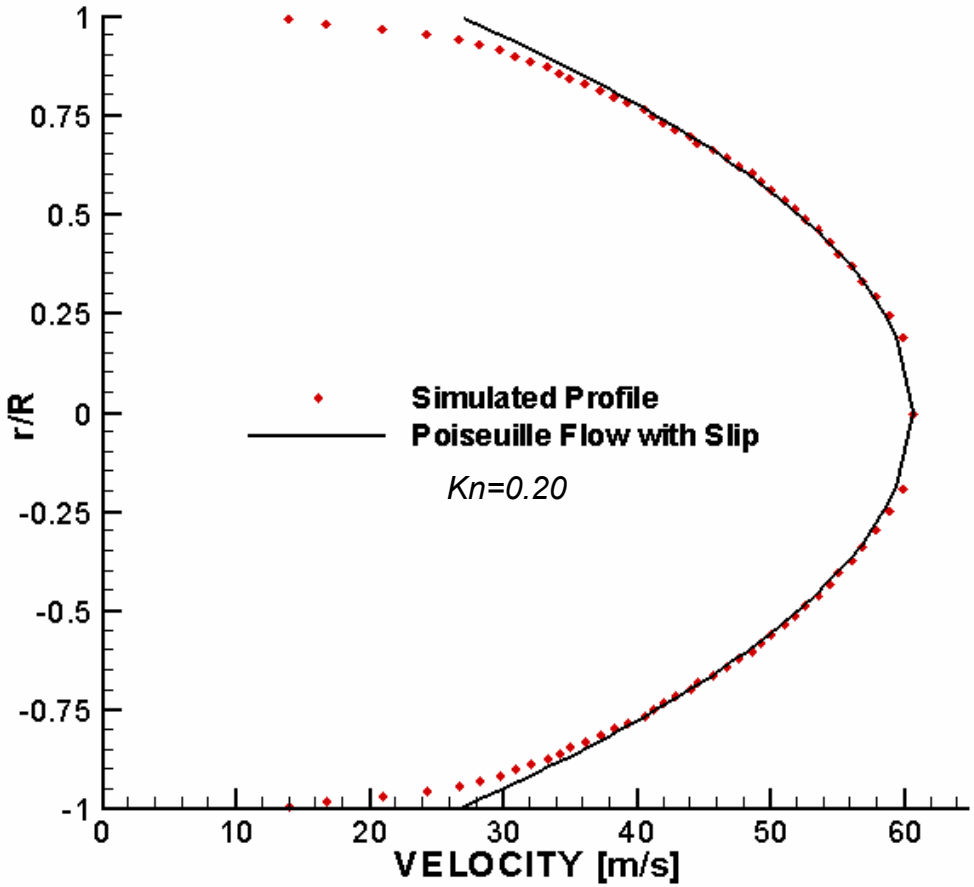
Results

- Velocity Profile

$$\lambda = \frac{1}{\sqrt{2}\pi d^2 n} \qquad Kn = \frac{\lambda}{L}$$

$$u(r) = u_{\max} - \frac{u_{\max}}{1 + 4Kn}\left(\frac{r}{R}\right)^2$$

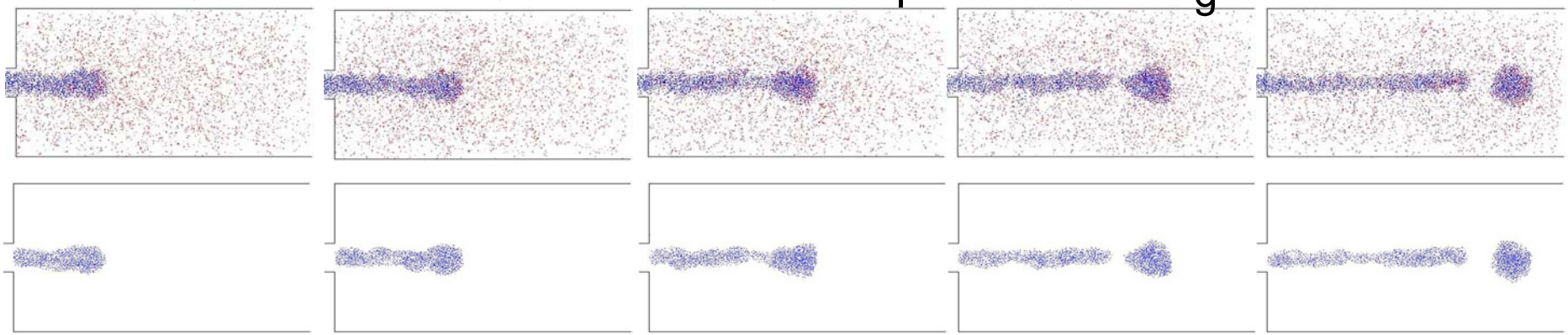
$$u(R) = -\lambda\left(\frac{du}{dr}\right)_{r=R}$$



Radial Velocity Profile

Results

- 94 K, ~0.5 MPa, Re=1.63, We_l=1.50, We_g=0.04

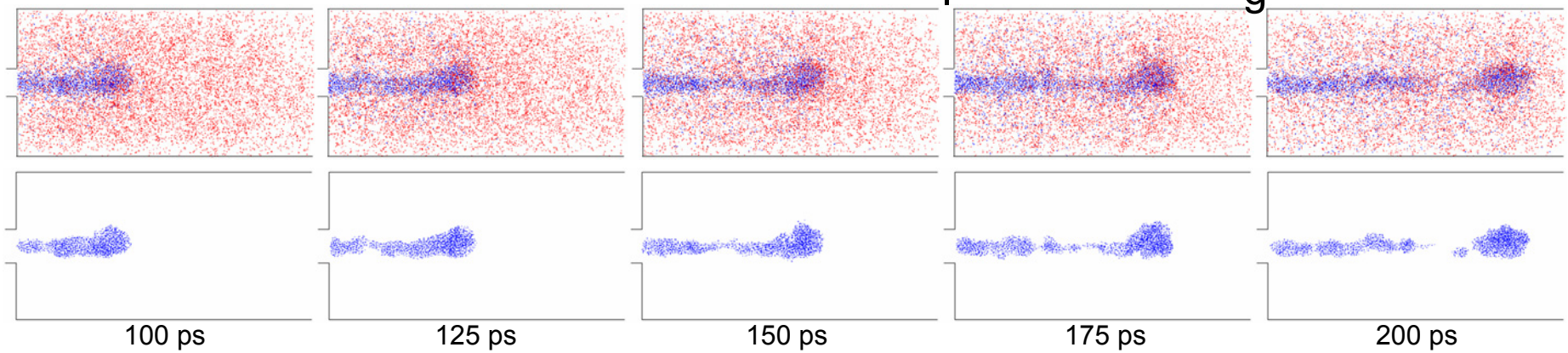


Source: Mayer, W. O., and Telaar, J., "Investigation of Breakup of Turbulent Cryogenic Variable-Density Jets." *Atomization and Sprays*, **12**, 651-666, 2002.

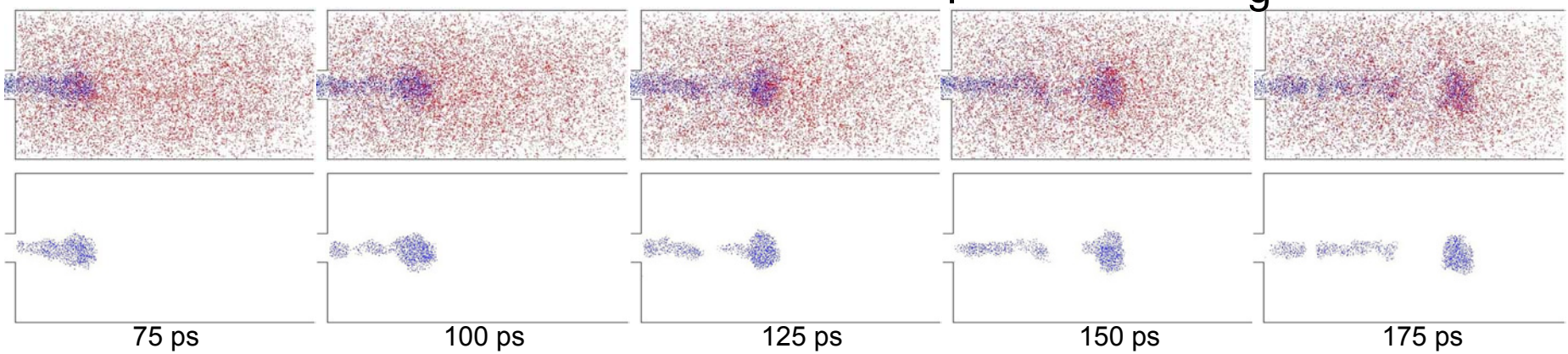
Demonstrating Rayleigh Breakup

Results

- 104 K, ~1.0 MPa, Re=2.07, We_l=2.18, We_g=0.14

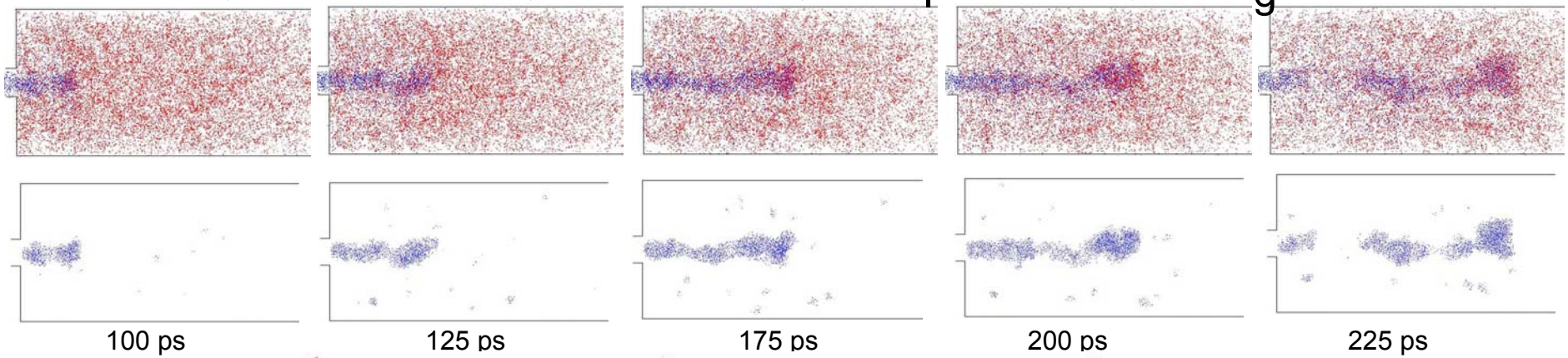


- 114 K, ~2.0 MPa, Re=2.71, We_l=4.62, We_g=0.45



Results

- 124 K, ~3.0 MPa, Re=4.04, We_l=41.53, We_g=7.06



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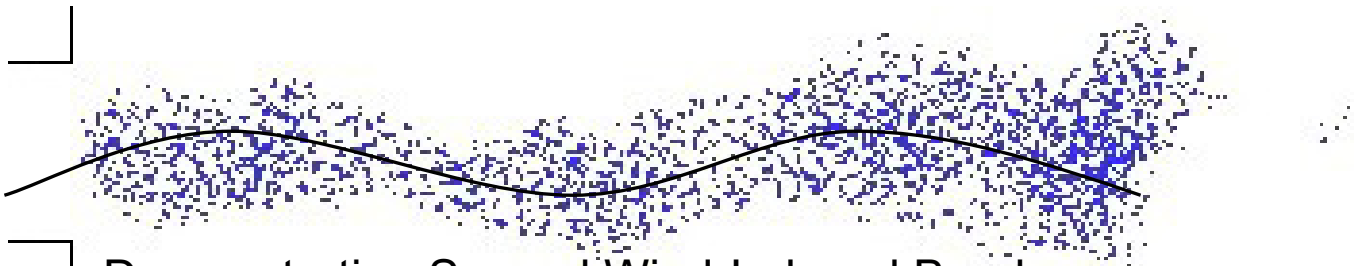
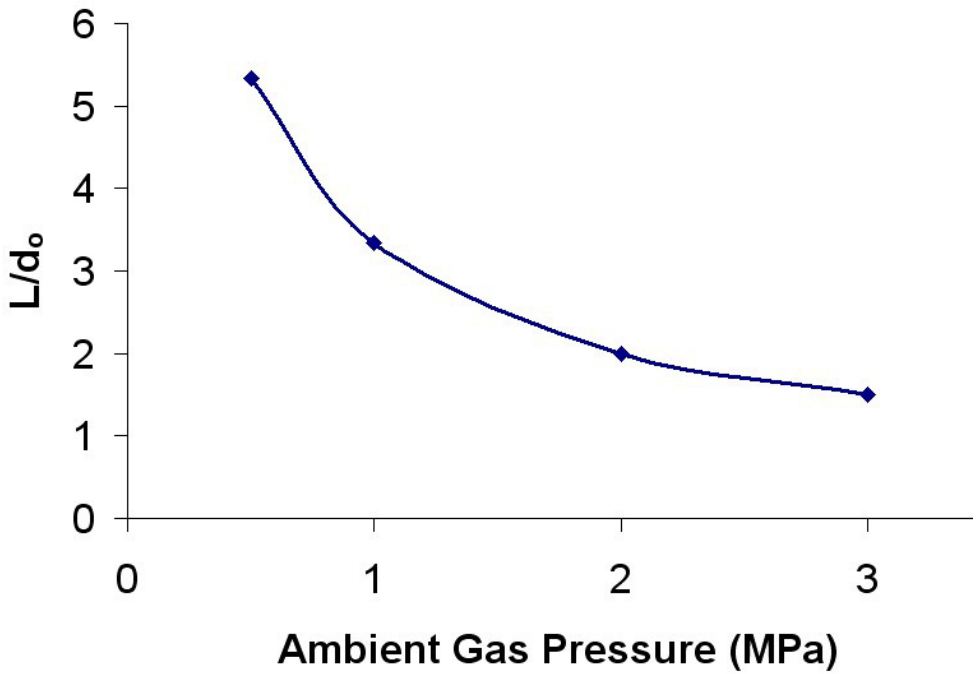


Demonstrating Second Wind-Induced Breakup

Results



- A decrease in breakup length with an increase in ambient pressure is observed
- The difference in breakup length between the higher ambient pressure cases is also less, indicative of higher pressures having less of an effect on breakup length

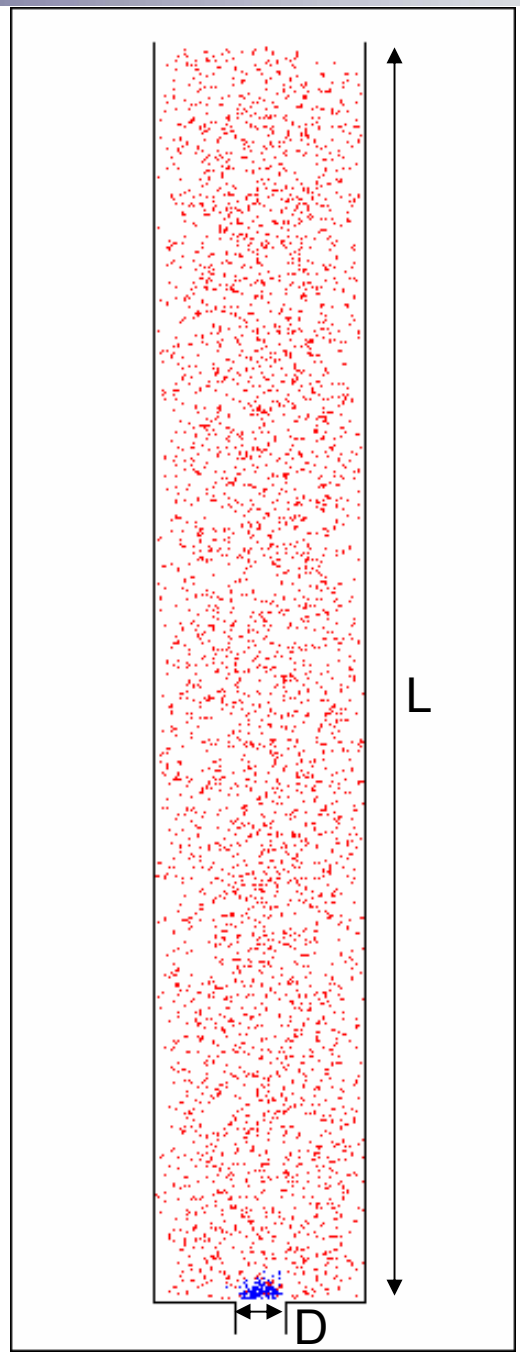
Animation

83 K
~0.2 MPa

Re=1.09
We_l=0.84
We_g=0.009

u_{avg}=45.3 m/s

L/D=60



Case1prev_nf.avi

Total Simulation Time:
1.2625 ns

Animation

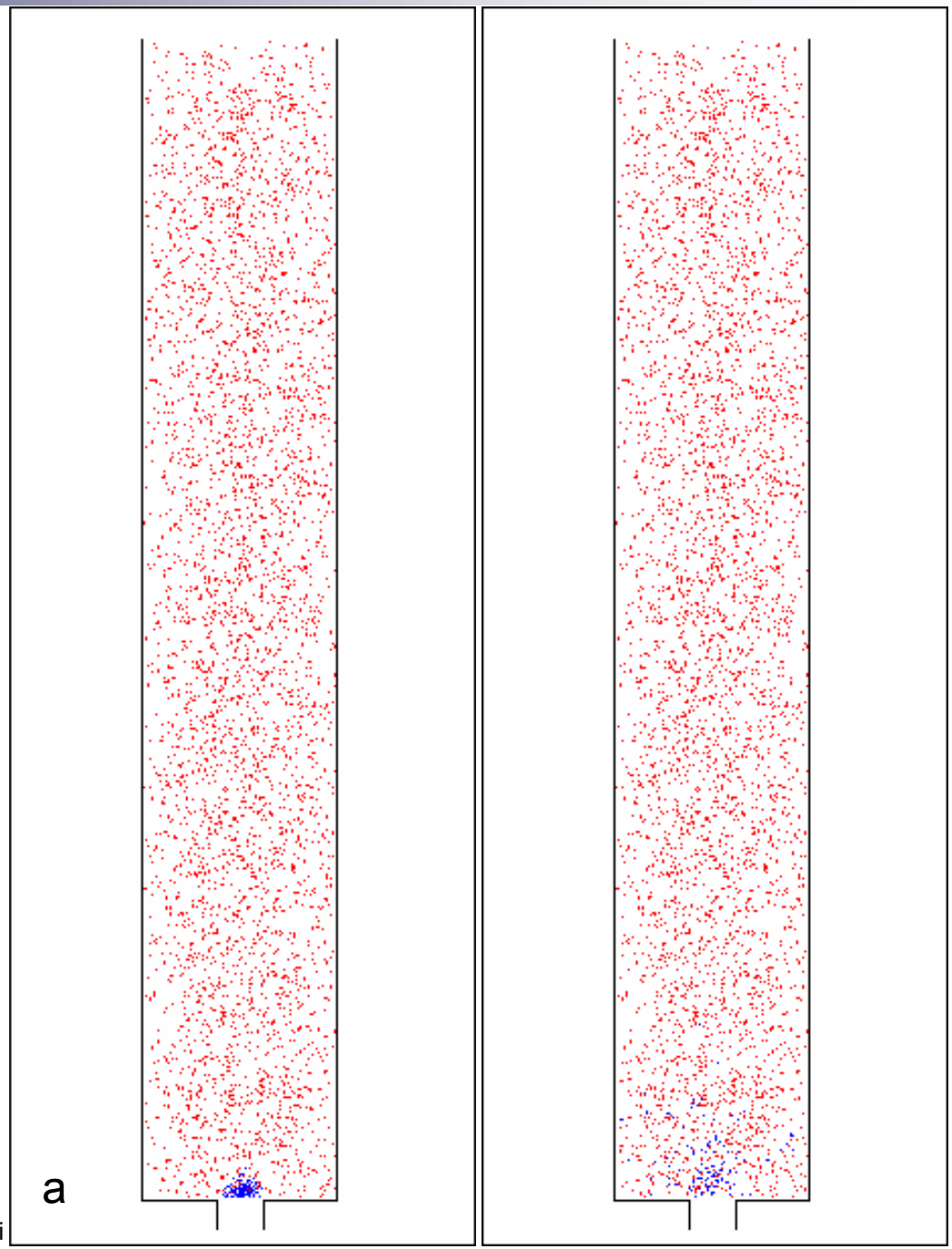
83 K
~0.2 MPa

Re=(a)0.87, (b)1.70
We_l=(a)0.50, (b)1.90
We_g=(a)0.005, (b)0.021

u_{avg}=(a)33.8 m/s
(b)66.1 m/s

L/D=60

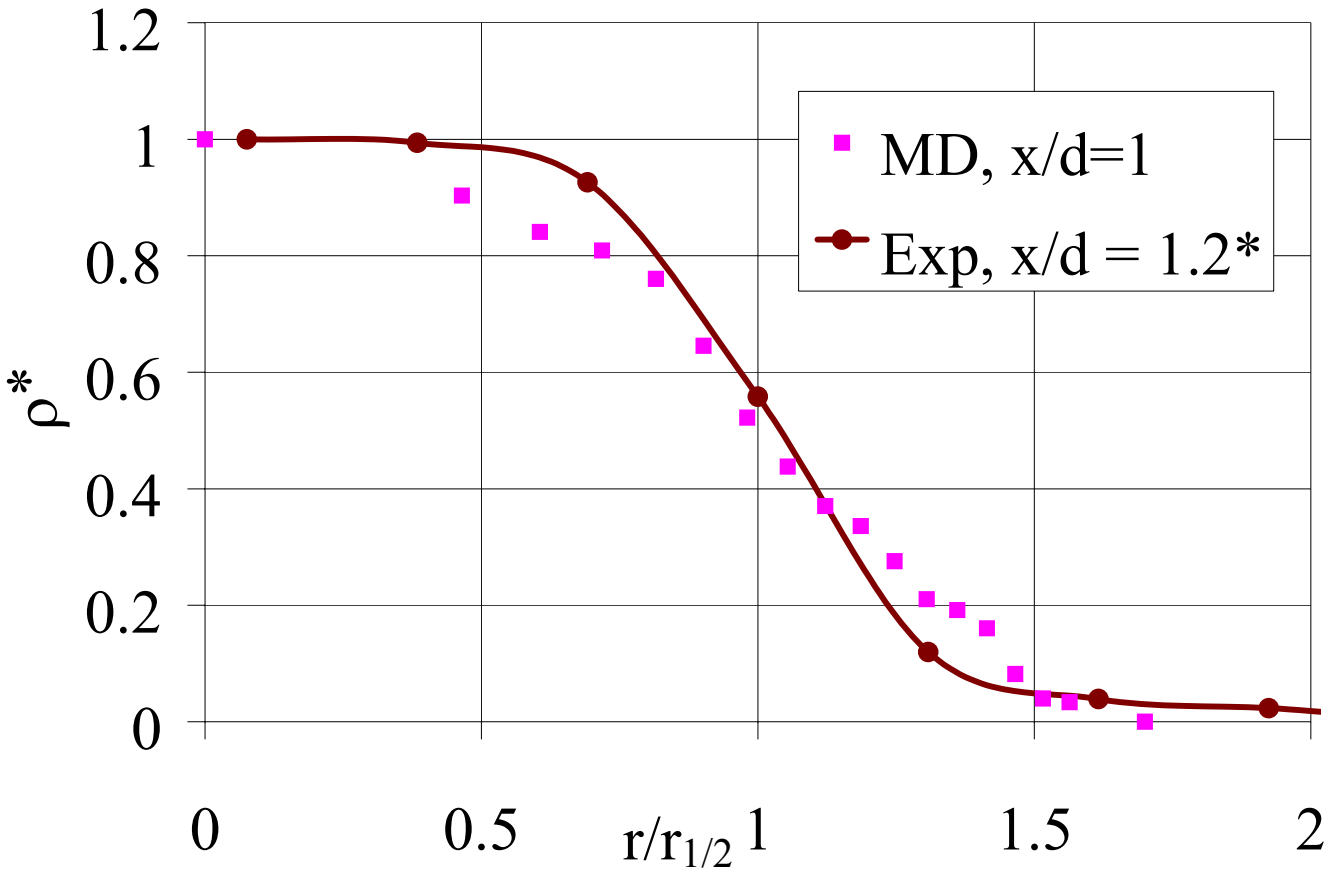
Total Simulation Time:
1.2625 ns



(a) Case1new.avi, (b) fgrav2xspray.avi

Supercritical - Comparison to Raman measurement

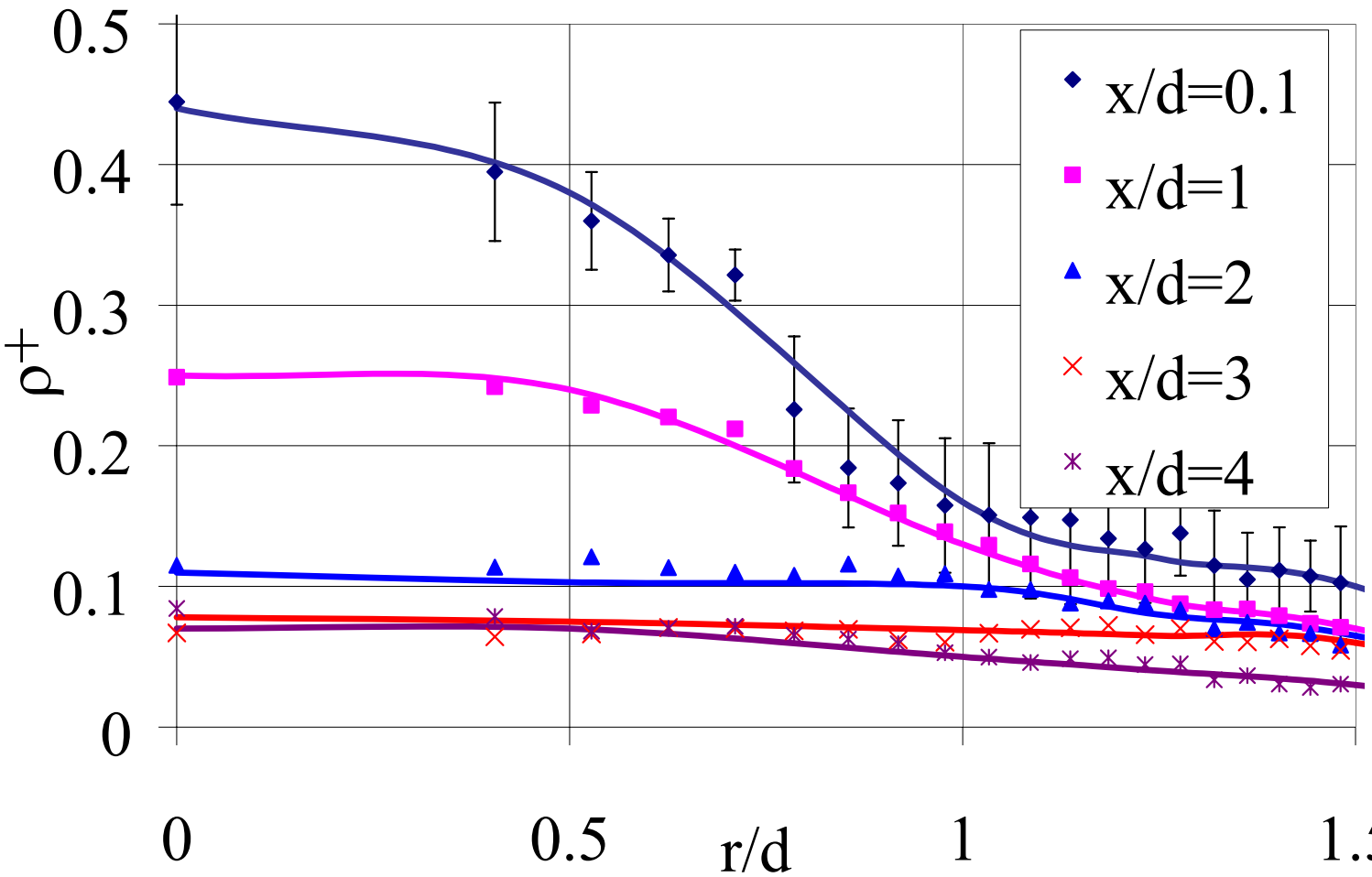
- 4 MPa, 123 K



*Branam, R. and Mayer, W., "Characterization of Cryogenic Injection at Supercritical Pressure," *J. Prop. and Pow.*, Vol. 19, No. 3, May-June 2003, pp. 342-355.

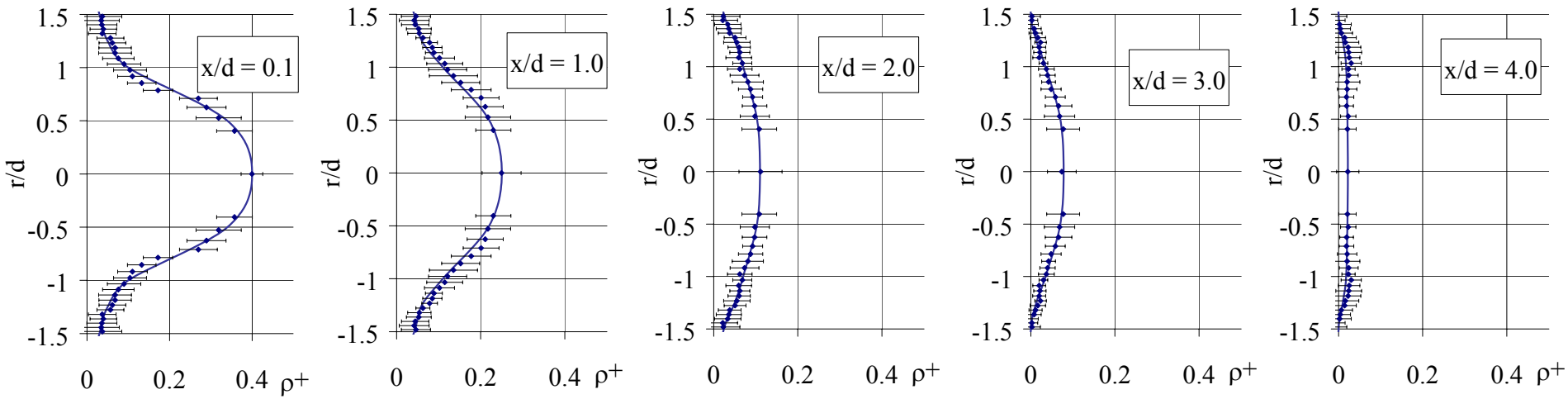
Supercritical - Computed radial density profiles

- Target conditions, 6 MPa, 123 K, 40 m/s



Supercritical - Evolution of computed density profiles

- Developing Flow
  - At a given time
  - Average of five independent simulations
- Supercritical conditions, 4 MPa, 123 K



Summary

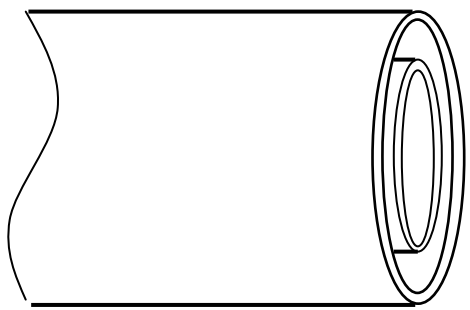
- Subcritical Injection Simulations:
  - Rayleigh breakup is reproduced, resulting in formation of droplets due to capillary instabilities in the jet driven by surface tension
  - The onset of aerodynamic effects, including the second wind-induced breakup regime, can also be seen in the cases of higher gas pressures

Summary (II)

- Supercritical Injection Simulations:
  - MD simulations match Raman measurements near injector exit (potential core)
  - Simulated flow still transient further downstream

Future work

- Resolve wall B.C. rotational accommodation
- Increase size of simulations
  - Generating injected particles
  - Increase tube diameter
  - Increase Re, decrease Kn
- Future work to focus more on ethanol and other hydrocarbons
- Extend geometry to include coaxial tube



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