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The objective of this program was to develop an accurate and fast simulation methodology for supercritical injection and mixing using molecular dynamics (MD). The use of MD allows the supercritical mixing to occur 'naturally' without the need for tracking phase boundaries and intrinsically includes all physical processes, material properties and equations of state in both subcritical and supercritical environments. MD also allows the tracking of injected liquid molecules into the chamber environment. Simulations of subcritical liquid nitrogen injection and atomization resulted in droplet sizes that matched Rayleigh theory. Subcritical breakup length as a function of pressure displayed behavior that matched experiments. Axial and radial density profiles for supercritical jet injection displayed the smooth transition of the density profiles from the high jet centerline to ambient chamber conditions and jet divergence angles that agreed in magnitude with steady state empirical models.

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Molecular Dynamics Simulations of Supercritical Sprays

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1 Jun 2001 – 30 Nov 2003

Abstract

The objective of this program was to develop an accurate and fast simulation methodology for supercritical injection and mixing using molecular dynamics (MD). The use of MD allows the supercritical mixing to occur 'naturally' without the need for tracking phase boundaries and intrinsically includes all physical processes, material properties and equations of state in both subcritical and supercritical environments. MD also allows the tracking of injected liquid molecules into the chamber gaseous environment. Simulations of subcritical liquid nitrogen injection and atomization resulted in droplet sizes that matched Rayleigh theory. Subcritical breakup length as a function of pressure displayed behavior that matched experiments. Axial and radial density profiles for supercritical jet injection displayed the smooth transition of the density profiles from the high jet centerline to ambient chamber conditions and jet divergence angles that agreed in magnitude with steady state empirical models.

Results

a) Simulation of liquid nitrogen injection

A molecular dynamics simulation of liquid nitrogen injection into gaseous nitrogen was constructed. The nitrogen molecules were simulated through the use of constraint dynamics[1, 2]. Each nitrogen atom in the molecule is simulated separately with its own Lennard-Jones 12-6 interatomic potential. A constraint force is added to the sum of the interatomic forces acting on each atom and iteratively adjusted using the RATTLE algorithm to satisfy the specified constraint, which in the case of molecular nitrogen is the fixed bond length[3].

The code is a parallel processor domain decomposition simulation developed using the MPI parallel library. The domain decomposition algorithm divides the computational region along the longitudinal axis into disk-shaped geometric domains, with each domain assigned to a separate processor. Particles are exchanged between processors when they travel between domains. A domain decomposition algorithm is the most difficult to develop but is the most computational efficient when scaled to a large number of particles and processors. A Verlet nearest neighbor list[2] was used to reduce the needed force calculations to those atoms within a cutoff radius of 2.5σ.

Approximately 5000 nitrogen molecules were used in the initial simulation region that was 4 nm in diameter and 40 nm long. The atoms were initialized at a liquid density in a cubic lattice with a Maxwellian velocity distribution representative of a given initial temperature. A stochastic boundary condition was applied on the sidewalls using diffuse reflections to obtain a no-slip boundary at a constant temperature. Periodic boundary conditions were used on the ends of the tube, if an atom exited from one end of the tube it re-entered at the other end. The time step used was 2.5 femtoseconds (fs). 10,000 time steps were used to allow the liquid argon to equilibrate, then a body force was applied to the atoms to induce a mean flow in the tube. The

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[1] Sadus, R. J., *Molecular Simulation of Fluids*, Elsevier, Amsterdam, 1999.

[2] Allan, M. P. and Tildesley, D. J., *Computer Simulation of Liquids*, Oxford University Press, New York, 1984.

[3] Andersen, H. C., "Rattle: a 'Velocity' Version of the Shake Algorithm for Molecular Dynamics Calculations," *J. Comp. Phys.*, Vol. 52, 1983, pp. 24-34.

simulation was continued for another 350,000 time steps to allow the fully developed pipe flow to reach equilibrium.

Figure 1 shows the radial velocity profile of the computed fully developed pipe flow. The analytically predicted parabolic velocity profile for the Poiseuille flow is obtained. The Reynolds number of the flow is approximately 5. The simulation requires approximately twelve hours to run on sixteen processors of our Beowulf PC cluster.

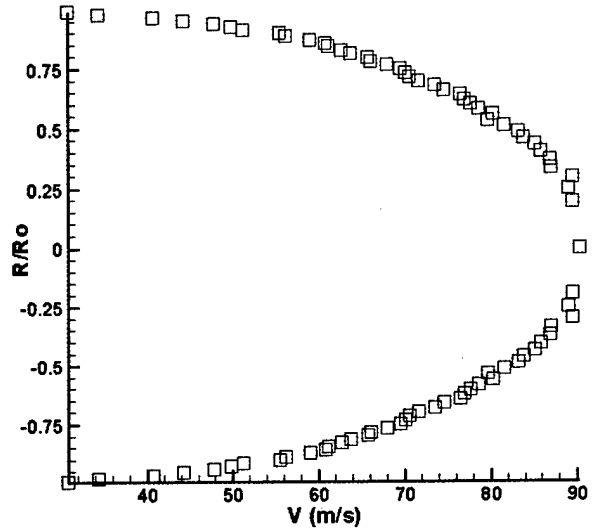

Fig. 1 Radial velocity profile for fully developed liquid nitrogen pipe flow. Re = 5.

After the liquid argon pipe flow reached equilibrium, the initial simulation region was mated to a larger diameter (20 nm) cylindrical region 40 nm long containing quiescent gaseous nitrogen at a specified pressure and temperature. The liquid nitrogen was then allowed to flow under the influence of the body force into the gaseous region. The periodic boundary conditions were removed from the upstream end of the liquid region and the downstream end of the gaseous region. The gaseous region had the same sidewall boundary condition as the liquid region, i.e., no-slip and a specified temperature. An additional eight processors were used for the gaseous region utilizing the same domain decomposition scheme as for the liquid region. Figure 2 shows a schematic of the initialization of the jet injection simulation.

b) Implementation of molecular tagging

In order to follow the mixing of the injected liquid nitrogen into the gaseous nitrogen, a means to track the initially liquid and initially gas molecules was implemented in the simulation. Figure 3 shows an initialized simulation where the molecules initially in the liquid are colored

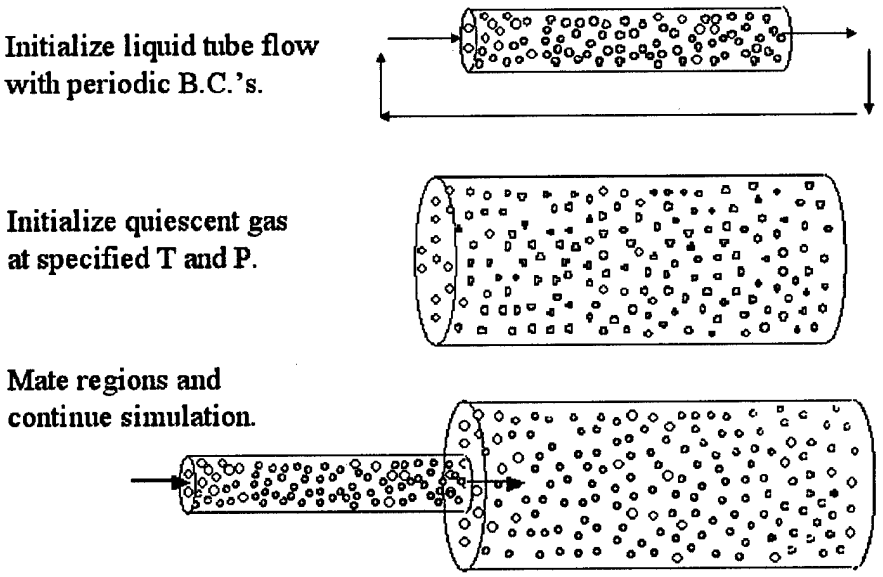

Fig. 2 Schematic of initialization of molecular dynamics jet injection simulation.

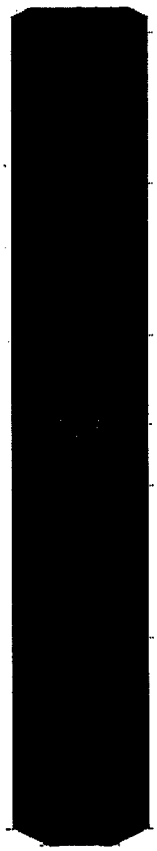

Fig. 3 Molecular tagging: red molecules are initially in the liquid while green molecules are initially in the gas. Both molecules are nitrogen.

red while the molecules initially in the gas are colored green. The molecules retain their initial color as the simulation proceeds, allowing the mixing of the liquid into the gas to be followed.

c) Subcritical liquid nitrogen injection

In order the validate the accuracy of the molecular dynamics simulation to model supercritical injection and mixing, simulations were initially conducted to model subcritical liquid nitrogen injection for comparison to classical analytical theories. Figure 4 shows the simulation of subcritical liquid nitrogen at 84 K and 0.5 MPa injected into gaseous nitrogen at the same conditions. The blue molecules are initially liquid and the red molecules are initially gas. The injection velocity was 44 m/s, corresponding to a Reynolds number Re=1.14. The pinch-off and formation of two liquid nitrogen droplets can be seen. The diameter of the drops matches the Rayleigh theory predicted size for low Reynolds number flow of 1.89 times the diameter of the liquid jet[4]. Clearly the instability of the liquid jet due to the surface tension is reproduced.

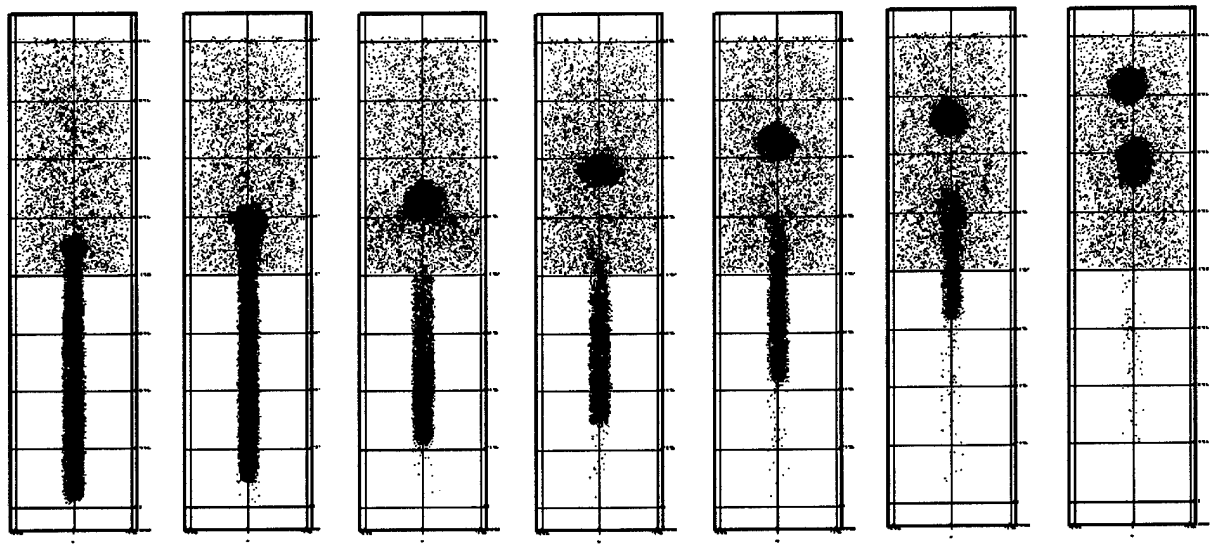

Fig. 4 Molecular dynamics simulation of subcritical liquid nitrogen injection at 0.5 MPa and 84 K demonstrating Rayleigh break-up.

Simulations have also been conducted at 1, 2 and 3 MPa liquid and gas pressures (critical pressure for nitrogen is 3.38 MPa). The Rayleigh atomization is still reproduced at these higher pressures, although the droplets are more difficult to visualize due to the increased gas density. The liquid core breakup length as a function of pressure is shown in Figure 5. The expected decrease in breakup length with an increase in ambient pressure is observed[5]. 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.

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[4] Rayleigh, Lord, "On the Instability of Jets," *Proc. Lond. Math. Soc.*, Vol. 10, 1878, pp. 4-13.

[5] Lefebvre, A. H., *Atomization and Sprays*, Hemisphere Publishing, New York, 1988, pp. 57-59.

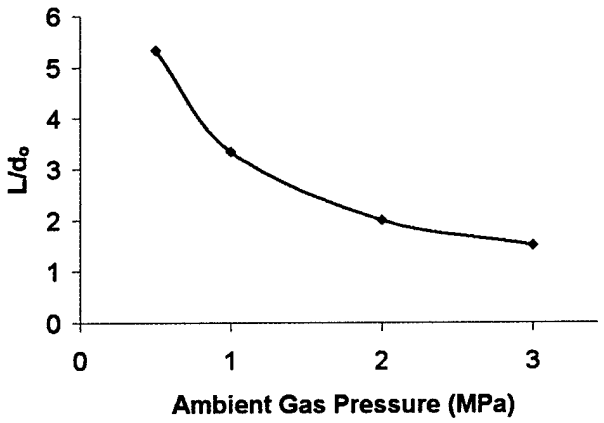

Fig. 5 Influence of ambient gas pressure on subcritical jet breakup length from molecular dynamics simulations.

d) Supercritical liquid nitrogen injection

Simulations have been initiated of liquid nitrogen injection into a supercritical nitrogen environment. The low Reynolds number of the molecular dynamics simulations results in a laminar flow injection of the liquid nitrogen. Although these can be compared to measurements of jet spreading angle and radial and axial density profiles taken from Raman measurements at DLR[6] and AFRL[7] of turbulent liquid nitrogen injection, current work at DLR is focussed on repeating these measurements for laminar flow injection for comparison to the simulations. Previous work at DLR as shown that the nondimensionalized density profiles are not a function of the jet diameter[8], thus allowing the comparison of the experimental results to the molecular dynamics simulations. Figure 6 shows a shadowgraph image of a turbulent supercritical nitrogen jet at 4 MPa and 130 K taken at DLR[5]. In order to quantitatively compare results from the molecular dynamics simulations to the experimental measurements, means for calculating the radial and axial density profiles produced by the MD simulations are being developed. Figure 7 shows radial density profiles taken from Raman measurements for a variety of pressures and temperatures from the experiments at DLR[5]. Figure 8 shows the radial density profile progression at various axial locations downstream of the injector obtained from a molecular dynamics simulation of nitrogen injection at 40 m/s, 4 MPa and 123 K. The smooth curves are indicative of the supercritical nature of the flow. Since there is no jet surface, the expected density profile is a smooth transition from the high jet centerline density dropping off to the ambient chamber conditions.

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[6] Mayer, W., Telaar, J., Branam, R., Schneider, G. and Hussong, J., "Raman Measurements of Cryogenic Injection at Supercritical Pressure," scheduled for publication in *Int. J. of Heat and Mass Transfer*, 2003.

[7] Cheroudi, B., Cohn, R. and Talley, D., "Cryogenic Shear Layers: Experiments and Phenomenological Modeling of the Initial Growth Rate under Subcritical and Supercritical Conditions," *Int. J. of Heat and Fluid Flow*, Vol. 23, 2002, pp. 554-563.

[8] Branam, R. and Mayer, W., "Characterization of Cryogenic Injection at Supercritical Pressure," *Journal of Propulsion and Power*, Vol. 19, No. 3, May-June 2003, pp. 342-355.

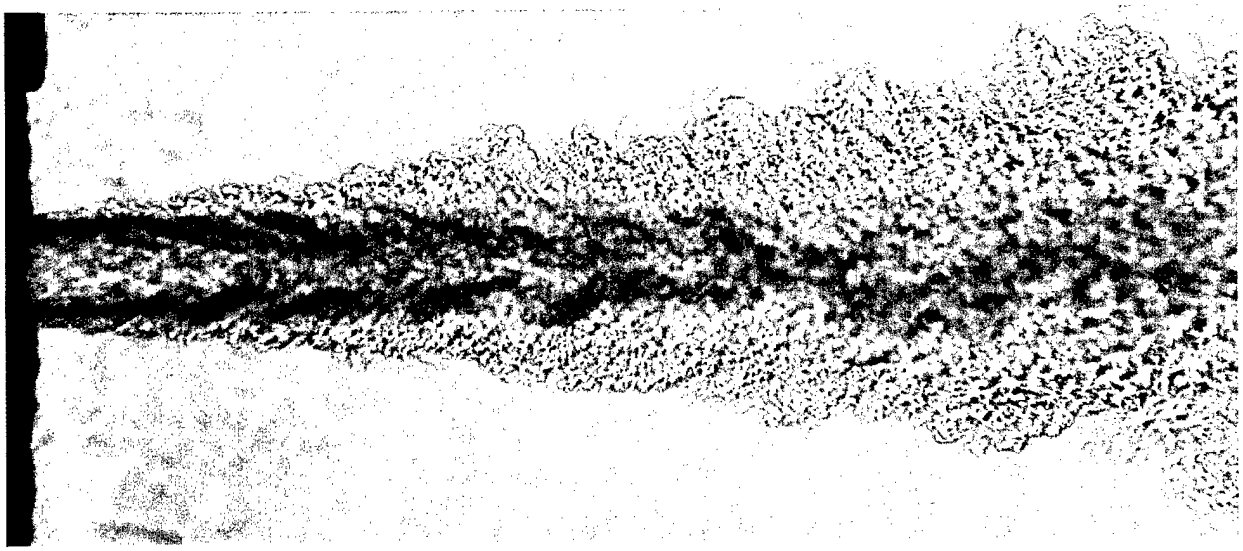

Fig. 6 Shadowgraph image of supercritical liquid nitrogen jet at 4 MPa and 130 K[5].

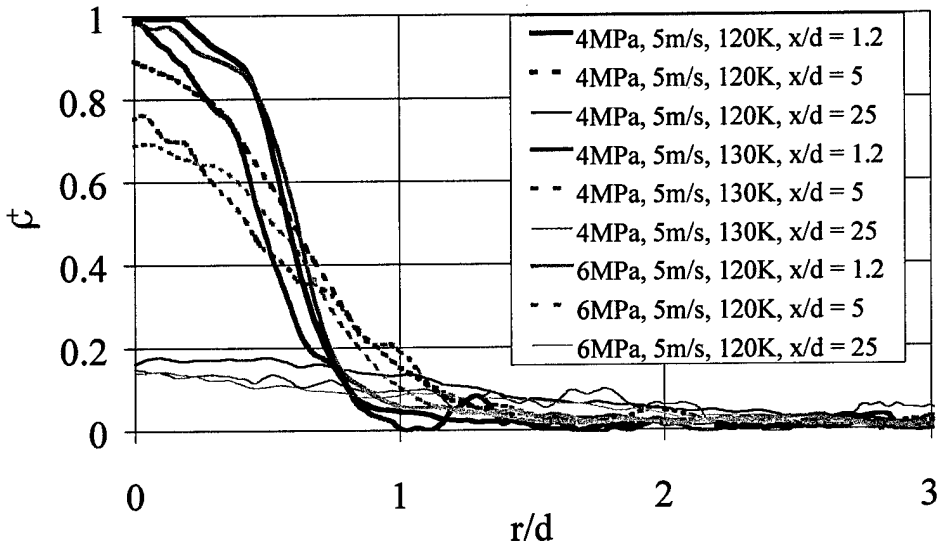

Fig. 7 Raman measured nondimensionalized radial density profiles for liquid nitrogen injection[5].

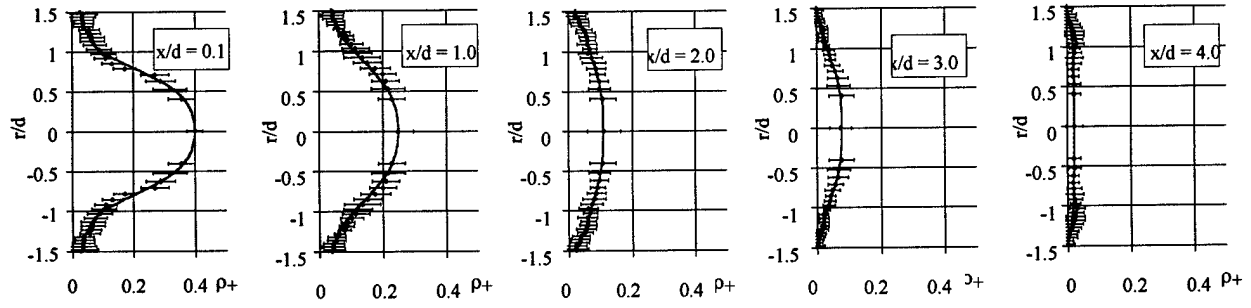

Fig. 8 Radial density profile progression from molecular dynamics simulation; 4 MPa, 123 K, 40 m/s.

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Graduate Students:	Major Richard Branam, USAF Kurt Ludwig

Publications:

Molecular Dynamics Calculations of Near-Critical LOX Droplet Surface Tension. Submitted to Atomization and Sprays, June 2003. Revision submitted March 2004.

Molecular Dynamics Calculations of Near-Critical LOX Droplet Surface Tension. Proceedings of ICLASS 2003, Sorrento, Italy, July 13-18, 2003.

Experiments and Molecular Dynamics Simulations of Supercritical Nitrogen Injection. Proceedings of ICLASS 2003, Sorrento, Italy, July 13-18, 2003.