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
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 (N₂) is simulated as a non-reacting substitute to other diatomic cryogenic liquid propellants/oxidizers, i.e. H₂ or O₂. 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:

\[ \varepsilon = 5.073 \times 10^{-22} \text{ Nm} \]

\[ \sigma = 3.293 \times 10^{-10} \text{ m} \]

\[ \text{mass} = 2.326 \times 10^{-26} \text{ kg} \]

\[ \text{bond length} = 1.094 \times 10^{-10} \text{ m} \]

The Lennard-Jones potential is given by:

\[ u_{LJ}^{ij}(r_{ij}) = 4\varepsilon \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^{6} \]
Fundamental Concepts of MD

- **Equations of Motion**

\[ m_a a_i = F_i = \sum_{j=1}^{N_a} f_{ij} \]

- **For Lennard-Jones Potential**

\[ f = -\nabla \nu^{LJ}(r) \]

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

- **Solve Numerically Using Finite Difference Velocity-Verlet Algorithm**

\[ r(t + \Delta t) = r(t) + \Delta t \nu(t) + \frac{\Delta t^2 a(t)}{2} \]

\[ \nu(t + \Delta t / 2) = \nu(t) + \frac{\Delta t a(t)}{2} \]

\[ \nu(t + \Delta t) = \nu(t + \Delta t / 2) + \frac{\Delta t a(t + \Delta t)}{2} \]
Fundamental Concepts of MD

- Addition of Bond Constraint to Simulate Diatomic Nitrogen Molecule

\[ r_{ab}^2 = r_{ab} \cdot r_{ab} = \text{constant} \]

\[ \frac{d(r_{ab}^2)}{dt} = 2r_{ab} \cdot v_{ab} = 0 \]

RATTLE Algorithm:

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

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

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

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:
  - Cell Boundaries Each $2.5\sigma$ in Length
  - Flow Direction
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

\[
\lambda = \frac{1}{\sqrt{2\pi d^2 n}} \quad Kn = \frac{\lambda}{L}
\]

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

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

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


Demonstrating Rayleigh Breakup
Results

- **104 K, ~1.0 MPa, Re=2.07, We_l=2.18, We_g=0.14**
  - ![Images for 104 K, ~1.0 MPa, Re=2.07, We_l=2.18, We_g=0.14](image1)
  - ![Images for 104 K, ~1.0 MPa, Re=2.07, We_l=2.18, We_g=0.14](image2)
  - ![Images for 104 K, ~1.0 MPa, Re=2.07, We_l=2.18, We_g=0.14](image3)
  - ![Images for 104 K, ~1.0 MPa, Re=2.07, We_l=2.18, We_g=0.14](image4)
  - ![Images for 104 K, ~1.0 MPa, Re=2.07, We_l=2.18, We_g=0.14](image5)

- **114 K, ~2.0 MPa, Re=2.71, We_l=4.62, We_g=0.45**
  - ![Images for 114 K, ~2.0 MPa, Re=2.71, We_l=4.62, We_g=0.45](image6)
  - ![Images for 114 K, ~2.0 MPa, Re=2.71, We_l=4.62, We_g=0.45](image7)
  - ![Images for 114 K, ~2.0 MPa, Re=2.71, We_l=4.62, We_g=0.45](image8)
  - ![Images for 114 K, ~2.0 MPa, Re=2.71, We_l=4.62, We_g=0.45](image9)
  - ![Images for 114 K, ~2.0 MPa, Re=2.71, We_l=4.62, We_g=0.45](image10)
Results

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

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 \text{ m/s}

L/D=60

Total Simulation Time:
1.2625 \text{ ns}
Animation

83 K
~0.2 MPa

Re=(a)0.87, (b)1.70
We\(_i\)=(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

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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