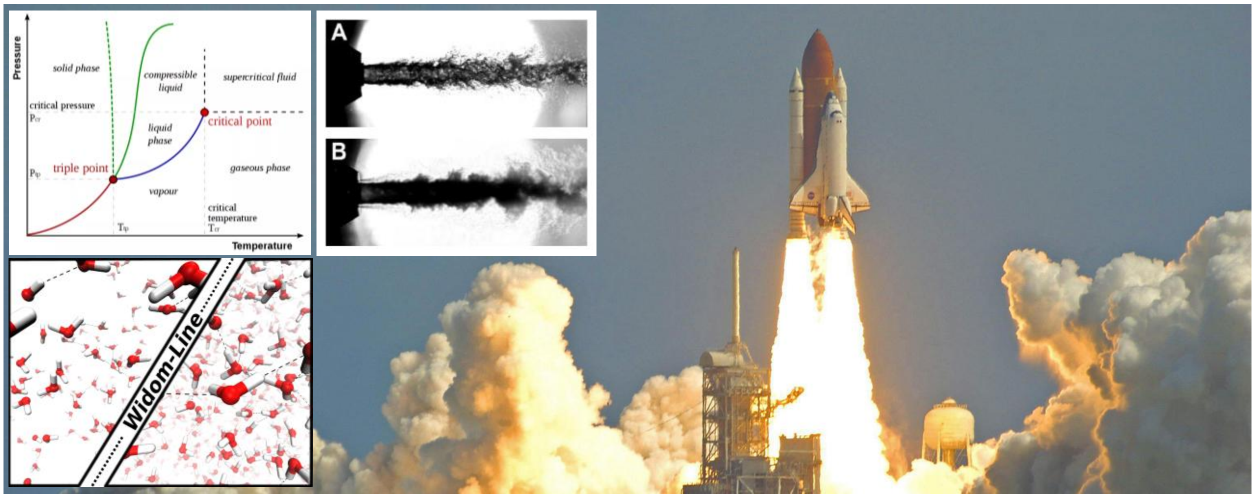

AAE 590: Physics of Non-ideal Fluids

with

Applications in High-pressure Reacting Flows

Fall 2020

Practical propulsion systems operate at high pressures, e.g., the chamber pressure of the RD 170 family developed by the Soviet Union in 1970s, one of the most powerful liquid-fueled rockets, is around 245 bar. As a result of the high pressure, the injected fuel may be at transcritical or supercritical state during the mixing, evaporation and combustion processes. Modeling these processes has serious challenges due to the non-equilibrium and unsteady nature of the phenomena, lack of a physical interface, and departure from the ideal gas behavior. This course will focus on the thermodynamics of non-ideal gases with applications in high-pressure propulsion systems such as rockets, gas turbines and internal combustion engines. Topics include basic concepts of gas kinetic theory and statistical thermodynamics, intermolecular potential and molecular dynamics, real-gas equation of state (EOS) for pure fluids and mixtures and mixing rules, phase diagrams and equilibria, vapor-liquid equilibrium calculations, and critical enhancement phenomena. The course will also discuss recent progress in understanding and modeling high-pressure chemical reacting flows, including supercritical droplets, jets and flames, and combustion chemistry at high pressures.

Instructor: Professor Li Qiao
Email: lqiao@purdue.edu
Phone: 494-2040
https://web.ics.purdue.edu/~lqiao/index.htm

Prerequisite: ME 200 Thermodynamics

Course Outline

Weeks 1-4: Basic concepts of thermodynamics

Gas kinetic theory:

- Macroscopic quantities: density, pressure, translational energy, ideal gas law, velocity speed, internal energy
- Molecular collisions: mean free path, collision rate, Knudsen number
- Molecular transport process: diffusion, viscosity, thermal conductivity
- Velocity distribution function (VDF) Boltzmann equation; Maxwellian VDF

Statistical Mechanics:

- Statistical counting method
- Distribution of energy states
- Relation to thermodynamics
- Partition function

Week 5-7: Molecular dynamics

- Interatomic potential models: Born-Oppenheimer approximation and pair potentials
- Molecular dynamics simulations: basics, initial conditions, defining and maintaining temperature and pressure, boundary conditions, equilibrium and dynamic properties
- LAMMPS demonstration

Week 8-12: Phase equilibria and EOS

- Phase behavior for pure fluids and mixtures, compressibility, fugacity
- Vapor-liquid equilibrium calculations
- Empirical EOS: Van der Waals EOS, Redlick-Kwong EOS, Soave-redlich-Kwong EOS, Peng-Robinson EOS
- The Virial EOS and the Second Virial Coefficient
- Perturbed-Chain SAFT: An EOS based on Perturbation Thoery for Chian molecules
- EOS for mixtures and mixing rules
- Applications of EOS

Week 13-15: Recent progress in modeling high-pressure reacting flows

- Droplet evaporation in high-temperature and pressure environment
- Sub-to-supercritical transition and different spray regimes
- Transcritical and supercritical jets
- Combustion chemistry at high pressures