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Molecular Dynamics Simulations for Propulsion Applications

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Apollo Moon Missions

"one small **step for man**, one **giant leap for mankind**." – Neil Armstrong

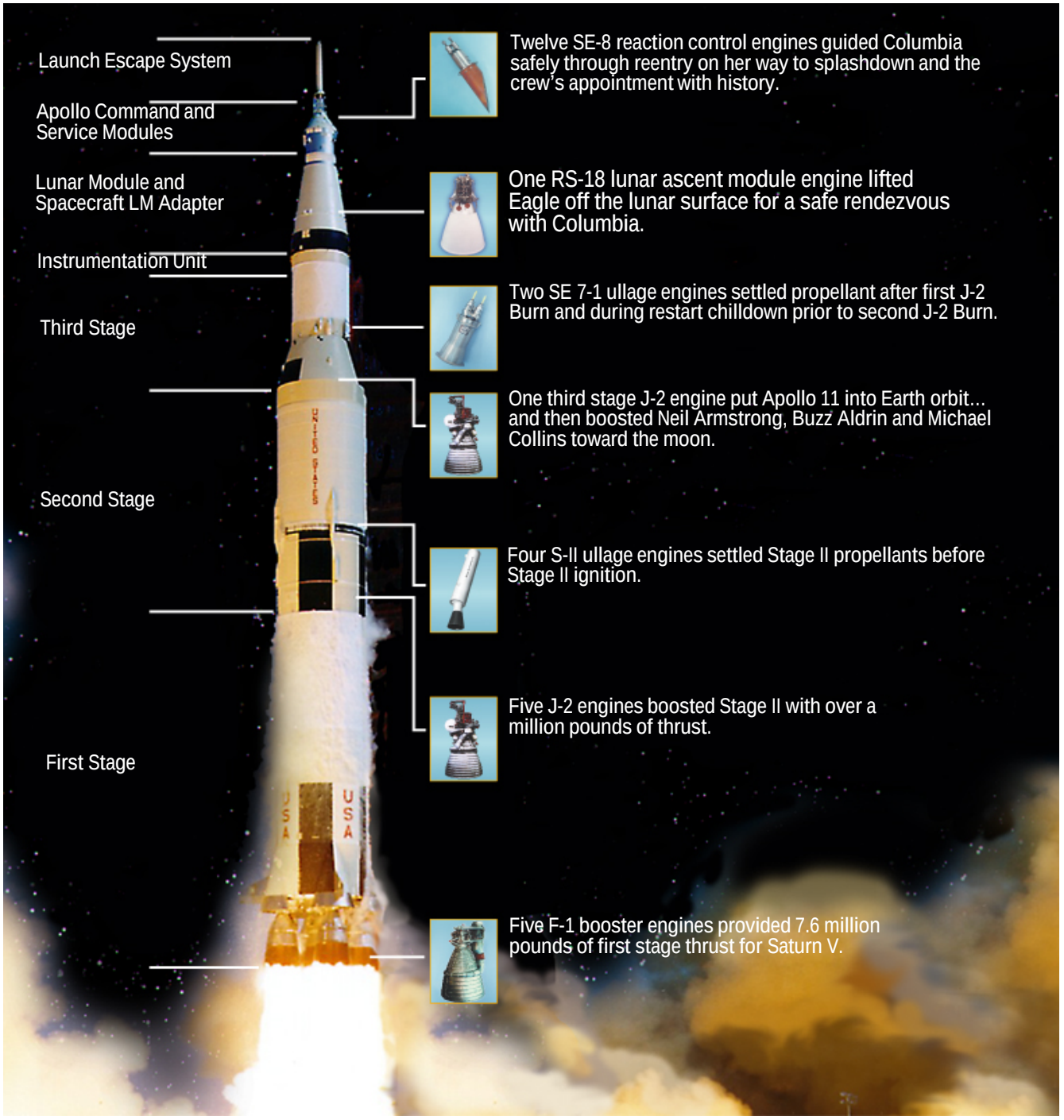
Saturn V

ΔV to Moon ~ 13 km/s

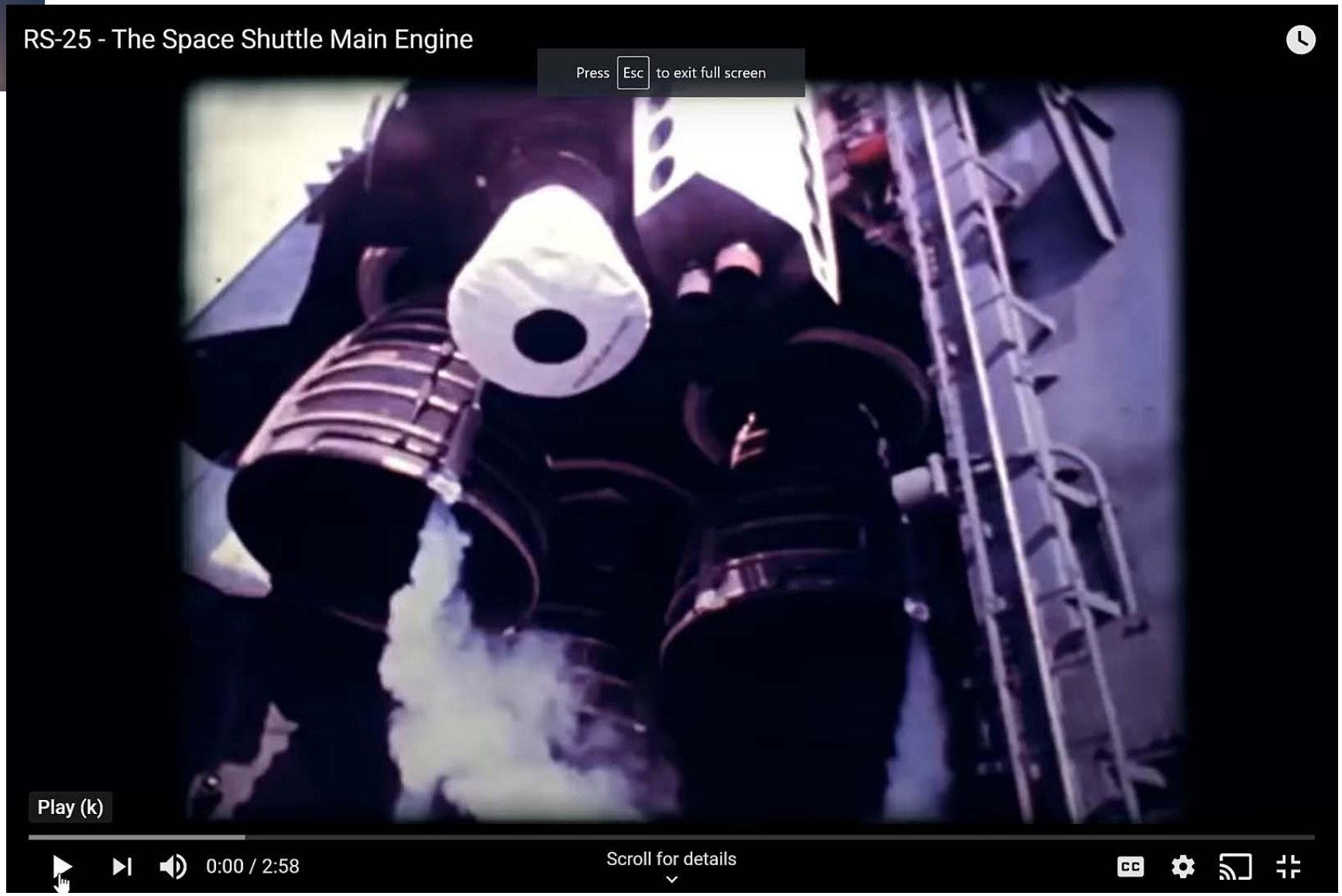
Thrust @ LO: 33,740,000 N,(7.5M lbf)
Total Mass: 3,038,500 kg (6.685M lb)
Core Diameter: 10.1 m
Total Length: 102.00 m
Launches: 13
Success Rate: 100%
First Launch Date: Nov 1967
Last Launch Date: May 1973
LEO Payload: 118,000 kg to 185 km orbit at 28.0 degrees
Payload: 47,000 kg to a translunar trajectory.
*Development Cost: $*7.5 B (1966 average dollars)
*Launch Price: $*430 M (1967 dollars)

Source: Astronautix.com

Apollo Saturn V



Space Shuttle Main Engine



•The Space Shuttle Main Engine operates at greater temperature extremes than any mechanical system in common use today. The liquid hydrogen fuel is -423 degrees Fahrenheit, the second coldest liquid on Earth. When the hydrogen is burned with liquid oxygen, the temperature in the engine's combustion chamber reaches +6000 degrees Fahrenheit - that's higher than the boiling point of Iron.

•The energy released by three of Rocketdyne's Space Shuttle Main engines is equivalent to the output of 23 Hoover Dams.

•If water, instead of fuel, were pumped by the three Space Shuttle Main Engines, the average home swimming pool could be filled in 25 seconds.

•The SSME high-pressure fuel turbopump main shaft rotates at 37,000 rpm compared to about 3,000 rpm for an automobile operating at 60 mph.

•The discharge pressure (head) of the high-pressure fuel pump is equivalent to a 36-mile-high column of liquid hydrogen

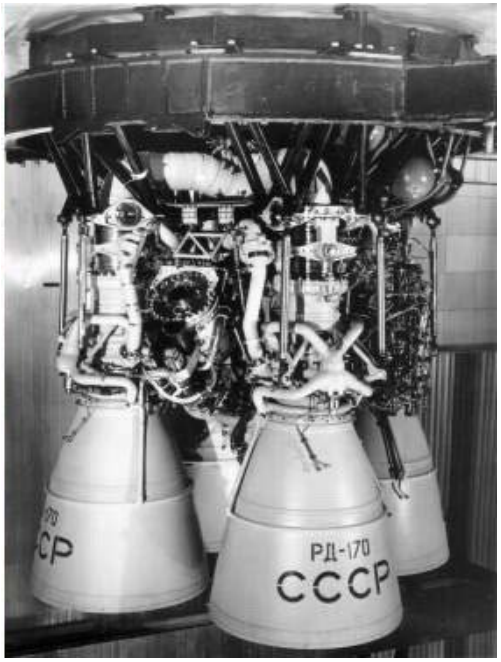
Chemical Propulsion Research

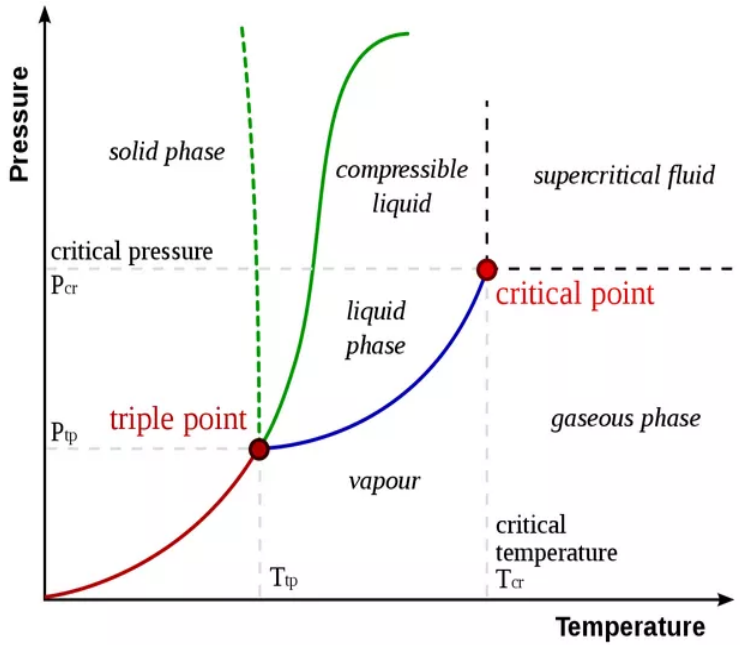
BE-4 rocket engine
(**Blue Origin**)

Reusability: making human life multi-planetary (**SpaceX**)

Maurice J. Zucrow Laboratories

Science of Rocket Propulsion





Combustion chamber pressure: 245 bar

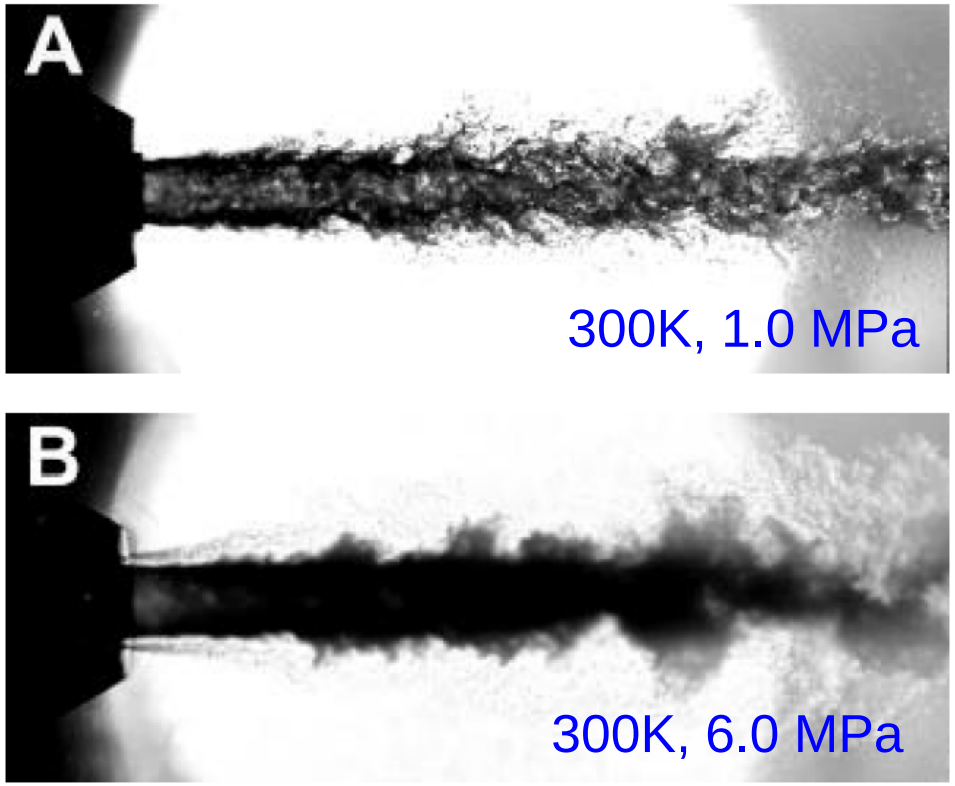
High-pressure phenomena are far from well understood:

- Very limited experimental data for understanding physics/chemistry;
- Many assumptions and empirical correlations used in various models have not been validated.

Transcritical and Supercritical Behaviors

Liquid N_2 (97K) injected into gaseous He

Mayer et al. (1998)



Question: At what conditions transition from the classical two-phase atomization to the one-phase diffusion-controlled mixing will take place? What are the dominant mechanisms controlling such transition?

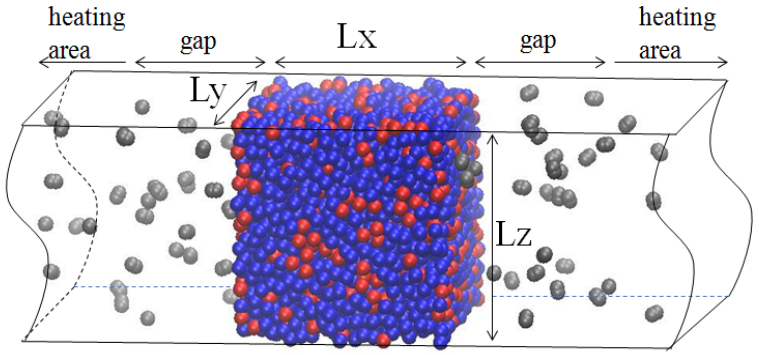
Molecular Dynamics Simulations

- **Predicting the time evolution of a system of interacting particles (initial condition + interaction potential).**
- At high pressures, molecules are very close to each other that ideal gas law breaks down and **intermolecular forces become non-negligible (ideal gas law is no long valid)**.
- The introduction of **thermodynamic nonidealities and transport anomalies** near the critical point is one of the main challenges to model these phenomena.
- The biggest advantage of the molecular dynamic approach is that no assumptions are made about the process to be investigated; the only input is a potential model that describes intermolecular interaction.
- **Equation of State, mixing rules, thermodynamics and transport properties of mixtures are not required**.

Molecular Simulations for Gas/Liquid Interface

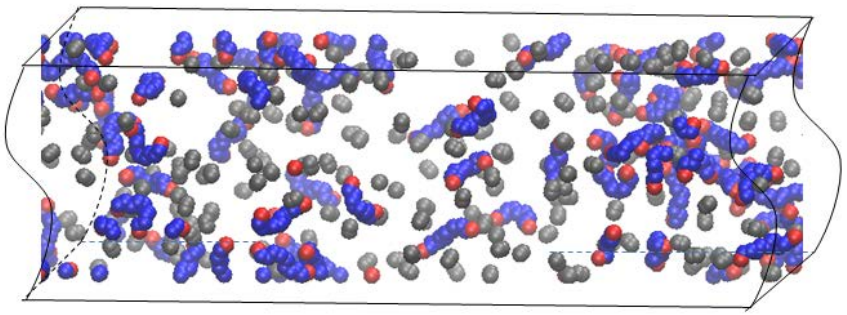
NVT ensembles

Number of alkane molecules	600 - 2400
Number of N_2 molecules	10000 - 30000
Liquid slab thickness (nm)	10-20
Cross section area (nm^2)	5*5
Reduced temperature (T/T_c)	0.8 – 2.4
Reduce pressure (P/P_c)	0.55 – 14.3
Boundary conditions	Periodic
Equilibrium time	5 ns
Statistical time	1 ns
Time step	2 fs
Bin length	2 Å



Initial configurations

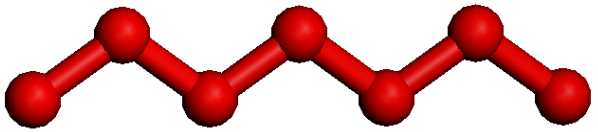
Atoms: red (CH_3), blue (CH_2), grey (N).



End of evaporation

Computational Method

- Open source code – Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) developed by Sandia National Lab.
- For n-alkanes: SKS (united atom) *Smit* et al. (1995) - treat each CHx as one atom.
- For N_2: Rivera et al. (2002)



CH_3-$(CH_2)_5$-CH_3

- Equations of atom motion were integrated by Verlet algorithm.

$$\frac{3}{2}k_bTN = \sum_{i=1}^{N}\frac{1}{2}m_iv_i^2$$

$$P = \frac{NK_bT}{V} + (\sum_{i=1}^{N} r_iF_i)/dV$$

kinetic energy term

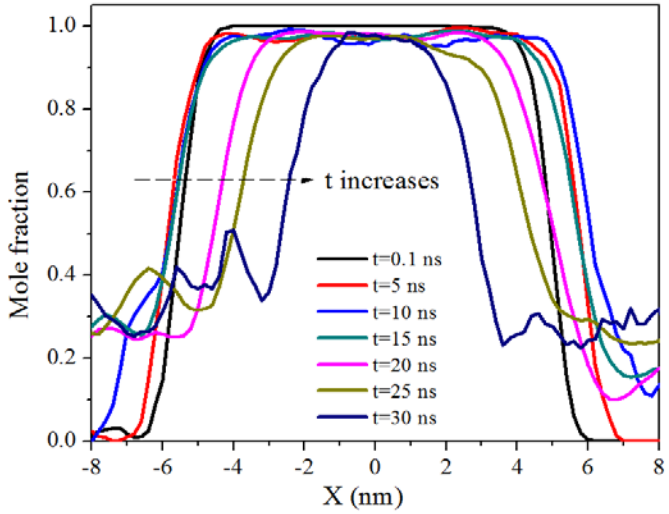
virial term

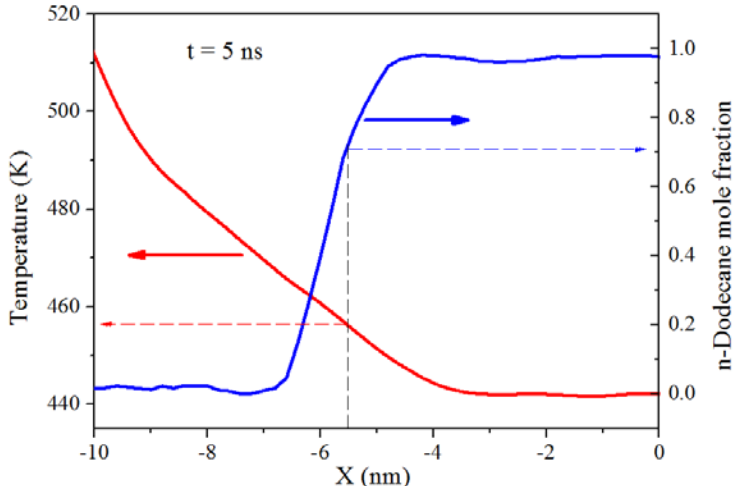
- The integrated difference between the normal and tangential pressure-tensors is the surface tension of the liquid. It was calculated according to the Kirkwood and Buff method :

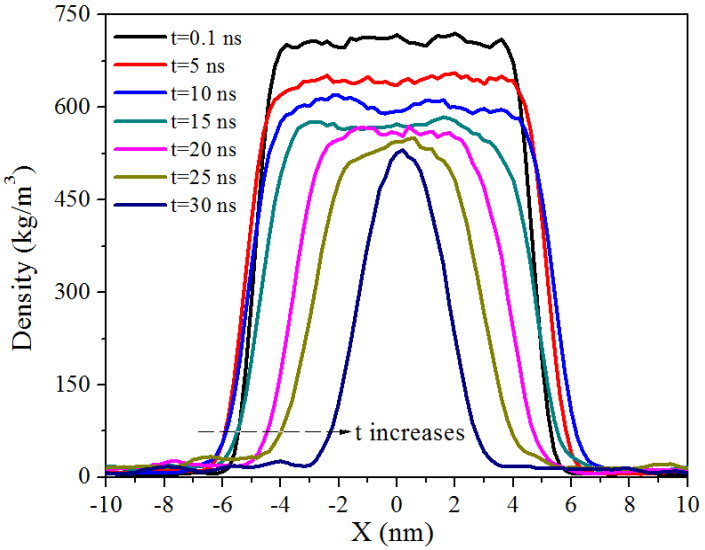
$$\gamma = 0.5\int_{-\infty}^{\infty}(p_n(x) - p_t(x))dx$$

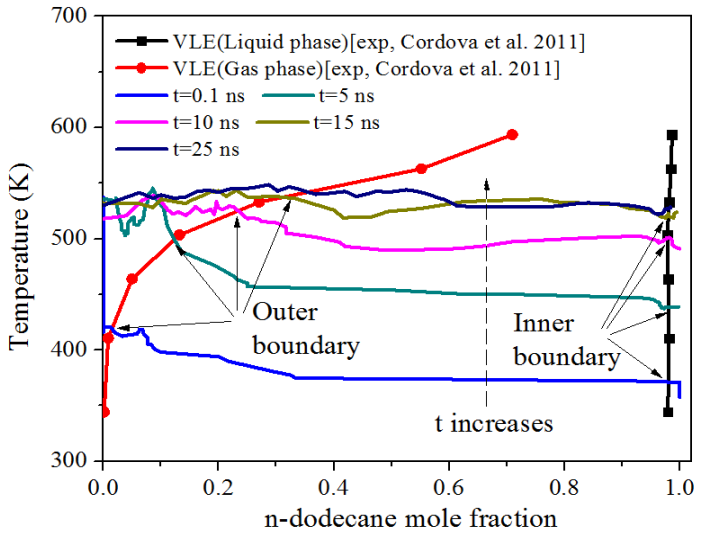
Subcritical Evaporation

n-Dodecane: T_c= 658 K, P_c = 1.817 Mpa, T_{init} = 363 K. **Ambient:** 526 K and 1 Mpa.

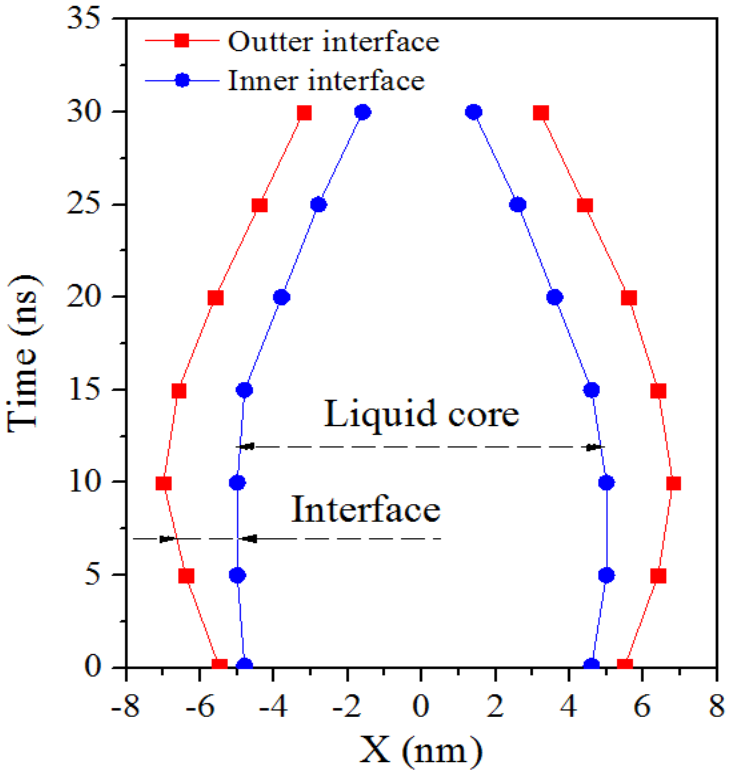




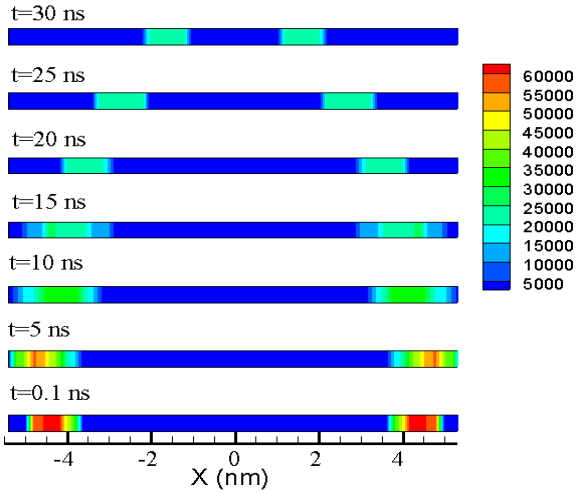




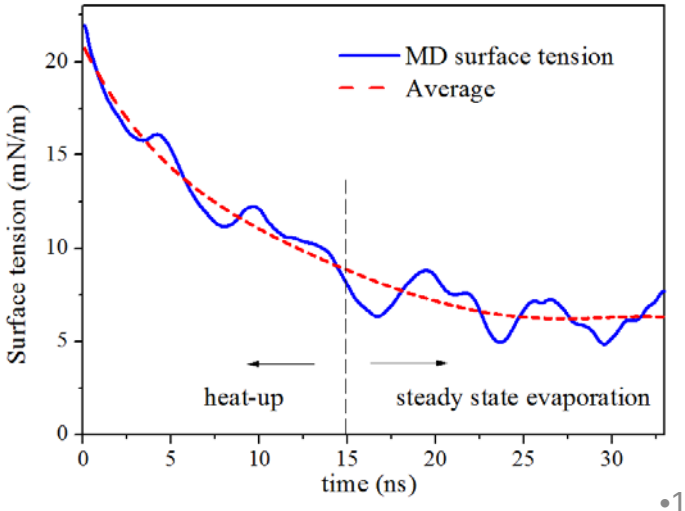
Evolution of the Interface and Surface Tension



Evolution of the gas/liquid interface; about 2 nm after the heat up stage.



Variation of the surface tension



Supercritical Evaporation

n-Dodecane: T_c=658 K, P_c=1.817 MPa, T_{init}=363K. **Ambient:** 1052 K and 20 MPa