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Molecular dynamic simulation of convective heat transfer from supercritical Argon flow in a nanochannel

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The convective heat transfer from single-phase supercritical argon flow in a nanochannel is studied by means of molecular dynamics simulations. Forced convection in micro- and nano-channels is one of the most efficient cooling methods for small-scale devices with high power density, which can dissipate heat fluxes in excess of 1000 W/cm^2. In this context, the prospective development of quantum computer technologies, which operate at temperatures close to the absolute zero, requires efficient low-temperature thermal management systems. With a boiling point of 87.3 K at atmospheric pressure, Argon (refrigerant R-740) is one of the most promising candidates as heat transfer fluid in low-temperature heat exchangers.

In the present work, a numerical setup for the simulation of Poiseuille flow is proposed, incorporating an alternative temperature control strategy, which divides the channel into five zones to mitigate the artefact backward diffusion due to periodical boundary conditions. The channel consists of two solid copper (12 Å thickness) parallel walls containing the fluid at a distance of 120 Å from each other, while their length in the flow direction is 400 Å. Periodic boundary conditions are applied in the directions parallel to the walls.

A lattice structure of face-centered cubic unit cells is used to model the solid walls, and the argon atoms are randomly distributed between the two walls according to their density. The interatomic interactions between the argon atoms as well as those between the copper and the argon atoms are described by the Lennard-Jones 12-6 model potential. The Langevin thermostat is used to keep the wall temperature constant, while an external driving force is used to induce the flow. A timestep of 1 fs is used in all simulations.

Four cases with inlet temperature of 300 K, mean flow velocities ranging between 2 m/s and 32 m/s, and wall temperatures of 200 K and 250 K, respectively, are simulated to obtain the temperature distribution in the channel and to calculate the local heat transfer coefficient as well as the corresponding Nusselt number.

Fig.1 displays temperature profiles at different distances from the inlet for a mean flow velocity of 1.92 m/s and a wall temperature of 200 K, as well as the local Nusselt number along the channel for the four cases investigated. With the exception of the developing region near the inlet temperature profiles are parabolic, however one can observe a steeper temperature gradient in the near-wall region, which can be interpreted as an effective thermal slip. The Nusselt number converges rapidly to a constant steady-state value, which is independent of the flow velocity and weakly dependent on the wall temperature. Its magnitude is about 25% higher than the theoretical value expected for a Poiseuille flow (the discontinuous horizontal line in the figure), which is consistent with numerical simulations of forced convection in supercritical CO_2 flows [1].

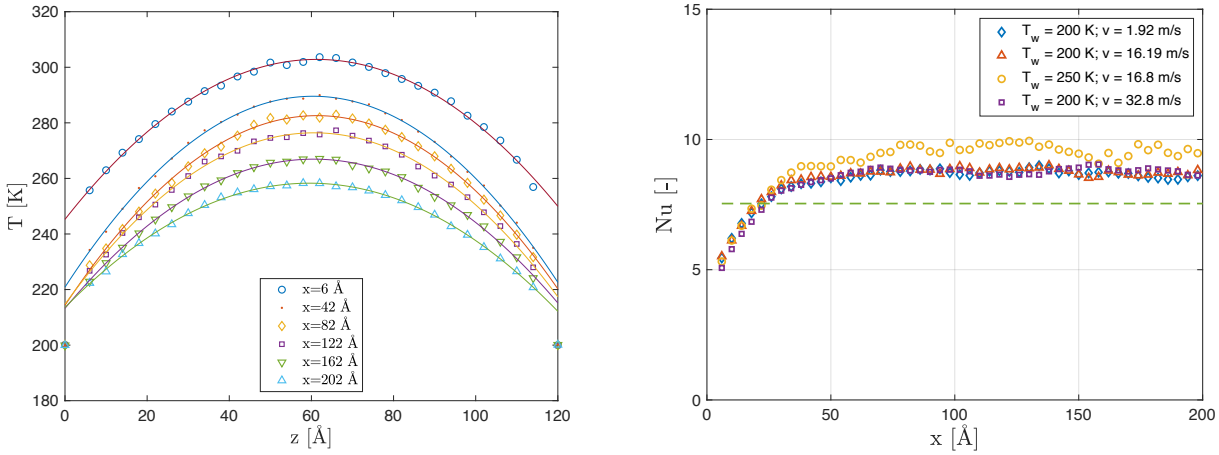

Fig. 1. Temperature profiles of supercritical argon for v = 1.92 m/s and T_w = 200 K (left), and Nusselt number of supercritical argon flow along the channel for different simulation parameters (right).

References

[1] X. R. Zhang, H. Yamaguchi, "Forced convection heat transfer of supercritical CO_2 in a horizontal circular tube", Journal of Supercritical Fluids 41 (2007) 412-420.