THE INFLUENCE OF FLUID LAYER STRUCTURE ON FLUID MOBILITY IN MICROPORES: MOLECULAR DYNAMICS SIMULATION

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The lattice-gas model (LGM) was successfully applied to the description of mass transfer processes in highly heterogeneous media in last years [1]. Considerable attention has been focused on application of this model to the calculation of the basic kinetic coefficients (self-diffusion coefficients, heat conductivity, value and shear viscosity) in narrow pores. Comparison of the values of kinetic coefficients obtained by the LGM, by molecular dynamics simulation (MD) and by the kinetic theory of a liquid demonstrated satisfactory agreement. However, fields of this method application as well as accuracy of results obtained are not essentially up to now. In particular, it is no clear, from what time intervals the lattice-gas model is applicable, and how strong is the influence of density and temperature on the model parameters.

A molecular dynamics simulation of Lennard-Jones (LJ) fluid in narrow slit pores and a calculation of same system in the framework of LGM were carried out for the study these problems. The fluid was confined between parallel structured walls [2]. All fluid and wall particles are interacting to each other with cut off LJ (12-6) potential with σ-ε parameters. The masses and dimensions σ of all atoms (wall and fluid) were equal, but fluid-wall and fluid-fluid particle interaction was changed from repulsive to high attractive potential ($\varepsilon_{wf}/\varepsilon_{ff}$=9.24). Two pore widths were studied, 5.5 σ and 13 σ, which allows the fluid to form 6 and 12 layers respectively. The fluid temperature was varied over a wide range from freezing to super critical temperatures.

The obtained results demonstrate that the lattice-gas model can be a convenient interpolation tool for quantitative description of dynamics of particles redistribution between layers and the longitudinal self-diffusion coefficients. Comparison of MD simulation results and LGM calculations allows us to determine the parameters of the lattice gas model and to use it for LGM calculations at large time scales.

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References

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