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Molecular dynamic simulation of water vapor interaction with various types of pores using hybrid computing structures

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Theoretical and experimental investigations of water vapor interaction with porous materials are very needful for various fields of science and tech-nology. Not only studies of the interaction of water vapor and porous material as a continuous medium, but also the study of the interaction of water vapor with individual pore is very important in these researches. Mathematical mod-eling occupies an important place in these investigations.Conventional ap-proaches to solve problems of mathematical research of the processes of inter-action of water vapor with individual pore are the following. The first ap-proach is based on the use of diffusion equation for description of interaction of water vapor with a pore. It is so called macro approach.The second ap-proach is based on various particle methods like, for example, molecular dy-namics (MD). These methods essentially consider the microstructure of the in-vestigated system consisting of water vapor and a pore. This second approach can be called a micro approach.

At the macro level, the influence of the arrangement structure of individ-ual pores on the processes of water vapor interaction with porous material as a continuous medium is studied. At the micro level, it is very interesting to in-vestigate the dependence of the characteristics of the water vapor interaction with porous media on the geometry and dimensions of the individual pore. Both approaches require the most efficient calculation methods as far as pos-sible with the current level of development of computational technologies. Us-age of efficient calculation methods is necessary because the degree of approx-imation for simulating system is largely determined by the dimensionality of the system of equation being solved at every time step. Number of time steps is also quite large.

In this work, a study of efficiency of various implementations algorithms for MD simulation of water vapor interaction with individual pore is carried out. A great disadvantage of MD is its requirement of a relatively large compu-tational effort and long time in simulations. These problems can be drastically reduced by parallel calculations. In this work we investigate dependence of time required for simulations on different parameters, like number of particles in the system, shape of pores, and so on. The results of parallel calculations are compared with the results obtained by serial calculations.

Keywords: porous media, molecular dynamics, macroscopic diffusion model, parallel calculations

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