MOLECULAR DYNAMIC SIMULATION OF WET WATER VAPOR TRANSPORTATION PROCESSES IN A POROUS MEDIUM

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Studies of the transportation of wet water vapor are relevant for various areas of human activity, including the construction and production of building materials [1], mining, agriculture, environmental safety of technological processes, scientific research. In particular, one of the methods for extracting highly viscous bitumen grades of oil from the subterranean depths is based on the dilution of the contents of the porous medium by means of pumping coolants. The simplest and environmentally friendly coolant is wet steam containing small drops of water [2]. In addition, with the help of heated water vapor, the filtering elements of collectors are cleaned from sediments of the solid phase (for example, paraffins, gas hydrates and ice floes) on the walls of the porous medium.

For realistic modeling of the processes of filtration and heat and mass transfer during the injection of wet steam into a porous medium, it is necessary to investigate the characteristics of the interaction of saturated water vapor with individual through-type pores. In this paper, a study was carried out through mathematical modeling of the dependence of the diffusion rate of wet water vapor on the pressure difference outside the pore that occurs when water vapor is injected into a porous medium. The dependences of the diffusion rate on the pore cross section, the magnitude of vapor adsorption on the pore walls, as well as the effect of water vapor temperature on all these processes were also investigated. Of practical interest is the study of the influence of the rate of cooling of water vapor on the diffusion rate and the adsorption of water vapor on the wall of the pores. The calculations were carried out using a hybrid type model that combines molecular dynamics and macro-diffusion approaches to describe the interaction of water vapor with individual pores [3,4].

References

- 1. *Krus M.*, Moisture transport and storage coefficients of porous mineral building materials: Theoretical principals and new test method. Fraunhofer IRB Verlag, Stuttgart, 1996. 175 p.
- 2. *Shagapov V.Sh.*, *Rakhmatillin I.R.*, *Nasyrova L.A.*, On the theory of injection of wet steam into a porous medium. *High Temperature*, **42**:6, 951–960 (2004).
- 3. *Nikonov E.G., Pavluš M., Popovičová M.*, 2D microscopic and macroscopic simulation of water and porous material interaction, arXiv:1709.05878 [physics.flu-dyn]
- 4. *Nikonov E.G., Pavluš M., Popovičová M.,* Molecular dynamic simulation of water vapor interaction with blind pore of dead-end and saccate type. arXiv:1708.06216 [physics.flu-dyn]