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MOLECULAR DYNAMIC SIMULATION OF WATER VAPOR INTERACTION WITH BLIND PORE OF DEAD-END AND SACCATE TYPE

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One of the varieties of pores, often found in natural or artificial building materials, are the so-called blind pores of dead-end or saccate type. Three-dimensional model of such kind of pore has been developed in this work. This model has been used for simulation of water vapor interaction with individual pore by molecular dynamic method [1]. Special investigations have been done to find dependencies between thermostats implementations and conservation of thermodynamic and statistical values of water vapor - pore system. The all types of evolutions of water –pore system have been investigated: drying and wetting of the pore. Full research of diffusion coefficient, diffusion velocity and other diffusion parameters has been made. Simulation results analysis demonstrates an importance of the investigation of the water vapor interaction with individual pore from point of view the control of water penetration into building material and protection of building material from wetting.

References

[1] Gould H., Tobochnik J., Christian W., An Introduction to Computer Simulation Methods, Third edition, 2005.

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