Multiscale modeling of particles supercritical drying process

Menshutina N.V., Kolnoochenko A.V., Lebedev A.E.

The process of supercritical drying is the only way to obtain promising highly porous nanostructured materials - aerogels. This process is highly complex, it requires accurate maintenance and the correct choice of the most effective parameters: temperature, pressure and supercritical fluid flowrate. Industrial technology of aerogel particles production realization requires considerable capital expenditure, since it is associated with the need to use high-pressure equipment. The use of high-precision mathematical models in such cases will make it much easier to understand the course of the process, increase its efficiency and simplify the scale up.

In the framework of this study, an approach for multiscale modeling of the supercritical particle drying process is proposed. This approach includes modeling the process at three levels: nano-, micro- and macro. At the first level, the internal porous structure of the dried material is generated using various methods. At the second level, with the use of obtained structures, the phenomenon of diffusion of the solvent through the pores of the material, its adsorption and desorption on the inner surface were investigated. The obtained data were used to calculate the energy of interaction of the solvent with the internal surface of the dried material and the effective diffusion coefficient of the solvent through it, depending on the concentration. At the considered levels, cellural automata models were used. To predict the supercritical drying process at the macrolevel, CFD method was used, it is based on the provisions of continuum mechanics. This method makes it possible to calculate hydrodynamics, heat and mass transfer at each local point of the studied system for arbitrary boundary and initial conditions. Thus, it can be used to predict the course of the process in apparatuses of laboratory and industrial scale. The implementation of the proposed multiscale approach will make it possible to obtain results that are close to reality and needs minimal possible computational costs. This approach was used to increase the efficiency of the process of supercritical drying of particles in apparatuses of various volumes. The processing of the obtained results made it possible to identify the most significant parameters and phenomena that have to taken into account when scaling the supercritical drying process.