Modeling and scale up of aerogel production processes

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There are some complicated processes during the production of aerogel and composites based on them, which may require special high-pressure equipment: solvent exchange, supercritical drying, and supercritical adsorption. These processes involve heat and mass transfer in continuous and multiphase medium, and it is important to take into account rapid changes in density with change of process parameters. In order to develop adequate mathematical model of such systems it is required to use accurate and specific equations for hydrodynamics, heat and mass transfer and physical properties calculation. This model should allow to investigate and improve the efficiency of the processes, to carry out its optimization. Also, such model should be suitable for using for the modeling of aerogels production in form of particles and monoliths. Nowadays, when industrial production of aerogels gathers pace, modeling is essential for processes scale-up in order to receive large industrial apparatus and there are only few tries of scaling presented in the literature [1].

In the present work the model to describe the hydrodynamics, mass and heat transfer under high pressure has been proposed. It is based on the provisions of continuum mechanics, using CFD [2]. The calculations were performed using Peng-Robinson equation of state, He and Yu, Tin and Calus equations for diffusion coefficients, first order kinetics to calculate the adsorption phenomena. For different processes the adequacy of the model was validated. The developed model was used for the design of various large-scale reactor geometry and its optimization.

References

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