Extended Abstract

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Fluid & Aerodynamics 2018_ The scaling problem of oxide materials hydrothermal synthesis for various autoclave reactors with considering natural convection_ I V Sharikov_ Saint Petersburg Mining University, Russia

I V Sharikov

Saint Petersburg Mining University, Russia

Hydrothermal synthesis is widely used for the assembly of varied nanodispersed oxide materials. Reactions under hydrothermal conditions are complicated and usually they are accompanied with heat generation or heat absorption. Heat flux calorimetry may be a powerful instrument for kinetic study and developing mathematical models of hydrothermal reactions. A mathematical model makes it possible to determine optimal experimental conditions for the production of a definite material on the base of a limited number of kinetic calorimetric runs. But so as to use the kinetic data to reactors of larger volume one should take under consideration heat transfer, mass transfer phenomena and non-uniform temperature distribution during a definite apparatus at the chosen initial conditions and in course of hydrothermal synthesis. Reaction vessel of C80 Calvet calorimeter (SETARAM Instrumentation) may be a micro-autoclave of 8.5 cm3 volume without mechanical stirring. Heat transfer and mass transfer inside it are run due to natural convection while heating to a chosen temperature of an isothermal run. And temperature gradient in this case is rather moderate (yet not negligible) as the reactor is relatively small. If we pass to the reactor of a larger volume (e.g., 1 liter) ??? we find that the important temperature mode in it's faraway from that during a kinetic vessel at an equivalent initial conditions. In order to take into account the temperature and conversion distribution due to natural convection in course of a definite hydrothermal synthesis we have developed a mathematical model that takes into account convection inside a hydrothermal reactor together with the chemical reaction. Convective flows were described at the base of Business approach and the differential equations system was solved with applying Convex program package that takes into account size and geometry of the reactor, reaction mixture properties, heat transfer peculiarities inside and out of doors and warmth generation thanks to reaction . It was found that temperature and conversion distributions in the calorimetric vessel and in the 1 liter reactor were rather different at similar initial conditions from the very beginning. Time of reaching the stationary temperature profile in the bigger vessel at implementing, e.g., isothermal mode is comparable with total duration of the run, and stationary temperature gradient is bigger as well. This indicates of the necessity to estimate rigorously the natural convection and heat transfer phenomena at scaling the hydrothermal synthesis for the reactor of bigger volume without mixing. Kinetic models developed on the base of calorimetric data cannot be directly applied to simulating the hydrothermal synthesis process in such a reactor. Recent Publications 1. Byrappa K and Yoshimura M (2001) Handbook of hydrothermal technology. A technology for crystal growth and materials processing. New York: William Andrew Publishing, ISBN 081551445X. 2. Ivanov V K, Kopitsa G P, Sharikov F Yu, et al. (2010) Ultrasound-induced changes in mesostructure of amorphous iron (III) hydroxide xerogels: A small-angle neutron scattering study. Physical Review B 81:174201. 3. Gershunin G Z and Zhukhjvitskii E M (1989) Stability of convection flows. PMM 31(2):272-281. It include the ability to create crystalline phases which are not stable at the melting point. Also, materials which have a high vapor pressure near their melting points are often grown by the hydrothermal method. The method is additionally particularly suitable for the expansion of huge good-quality crystals while maintaining control over their composition. Disadvantages of the method include the need of expensive autoclaves, and the impossibility of observing the crystal as it grows if a steel tube is used.

Email:yvshar@mail.ru