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Improvement and bench-testing of computer simulation of transient behavior in the PUREX process units of various function and structure

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A mathematical model has been proposed for calculating distribution coefficients of NPP spent fuel components in extraction systems with 30% TBP in a hydrocarbon diluent using the improved Rozen's model based on the semi-empirical extraction equations. A computer code has been developed for simulation of the steady-state component concentration profiles throughout the extraction multistage unit, as well as the code for calculating the transient regime in the head and backwashing units of various PUREX process options for high burn-up spent fuel from nuclear power plants (NPP) with WWER (PWR) water-cooled reactors. The analysis of published and newly obtained data on the influence of component concentration and temperature made possible to describe the equilibrium extraction of HNO_3 and hexa- and tetravalent acti-nides as well as Zr and $HTcO_4$ from nitric acid solutions into 30% TBP in the Purex process conditions in different extraction units except the ki-netics of ox-red reactions because of uncertainty of induction period. The results of long-term bench experiments concerning transient regime of the head mixer–settler unit of the RT-1 complex were in good agreement with simulation results for entering the beyond-design-basis regime using the model of ideal mixing in a settling chamber, while the return from this regime is better described by plung-flow model. The effect of significant extraction of Pu at limiting loading of the solvent with uranium was confirmed allowing adequate description of the Pu accumulation in the uranium-free zone of the extraction–scrubbing unit. The adequacy of the ideal mixing model for a unit of centrifugal con-tactors was demonstrated as applied to reprocessing of SNF from fast reactors. A separate experiment has shown that the Pu accumulation in the uranium-free zone does not occur in this case because of higher acidity of the aqueous phase and higher process temperature (so called IMPUREX process), while the Pu distribution between the contac-tor steps correlates with the U distribution. The bench tests on transient regime in uranium backwashing unit have indicated on the applicability of the above model. The drawbacks of Rozen's model such as ignoring of hydrolyses and extraction of partially hydrolyzed or complexed species leading to the high number of empirical corrections, as well as impossibility to de-scribe salting-out effect and extraction by high concentration TBP urged us to look for a new approach to simulation of interphase equilibrium. The new "multireaction" model describes the extraction of actinides in various valent states, some fission products and admixed acids from nitric acid media in the presence of salting out agents by diluted TBP. It is based on a set of simultaneous chemical reactions of unlimited number of components, including salvation, hydrolysis, complexing and other reactions, characterized by apparent concentration constants.

Biography

Egor A. Puzikov graduated from Physico-Chemical Department of SPb Institute of Technology (Technical University), St-Petersburg, Russia, in 1989 and received there his PhD in 1995. He has been working at Khlopin Radium Institute for 23 years and currently holds the position of a senior researcher at Department of Applied Radiochemistry. He works in the team of scientists headed by prof. B.Ya.Zilberman. His main interests are computer simulation of extraction, precipitation and evaporation equilibrium applied to Nuclear Fuel reprocessing. He has developed several software packages for simulation of stationary and dynamic component distribution through the stages of extraction units. He has publishes more than 20 papers and is working currently on his full doctor of science thesis.

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