

SIMULATION OF MULTIPHASE SYSTEMS IN EXTRACTION PROCESSES OF SNF REPROCESSING

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The development of process equipment in various industries involves generating of digital twins. Digital twins make it possible to choose the most preferred solutions for equipment development, as well as to significantly reduce the cost of prototyping and bench testing. To generate a digital twin, it is necessary to choose a set of models that reliably describe the processes in the device being developed.

The existing flowsheets for spent nuclear fuel reprocessing are based on extraction processes. Extraction is a procedure of separating liquid or solid substances in a mixture using selective solvents (extractants). A centrifugal extractor is divided into two zones: a mixing chamber, in which two phases come into contact for the transition of a key component, and a separation chamber in which the phases are separated by centrifugal force. The 3D hydrodynamic simulation of the processes occurring in the extractor (mass transfer between phases, phase separation, distribution of undissolved sediment, and formation of a gas phase) is of interest for a preliminary assessment and selection of the most preferred technological solutions.

There are various approaches to describe a flow of a multicomponent or multiphase mixture. The industrial applications often utilize the Volume of Fluid (VOF) methods [1]. In the VOF method, only one set of equations of motion, energy, and turbulence is solved, while a special equation (similar to the continuity equation) is introduced to track the position of the phase boundary. The values of the parameters characterizing the phase properties (density, viscosity, thermal conductivity, etc.) when passing through the phase interface, “switch” so that each point of space would correspond to the phase existing at that point [1]. The finite volume method is the most suitable method for approximating the terms of the general system of equations of motion in hydrodynamic calculations [2].

This approach is implemented in the interFoam [3] and multiPhaseEulerFoam [4] solvers of the free OpenFOAM software package [5]. These are the two solvers selected for the simulation. To solve the system of equations of motion, the splitting method implemented in the PIMPLE algorithm is used. The method is based on splitting the effects of various terms on the change in momentum in the computational grid [6].

To describe the process of mass transfer of a chemical component, the standard solver has been modified using the method described in [7]. The method is based on the introduction of the VOF method (an additional equation that describes the mass transfer of the component) into the system of equations.

The paper presents the models of hydrodynamic and mass transfer processes that make it possible to simulate phase mixing, mass transfer across the interface, and phase separation induced by the centrifugal force. The proposed models can be used to build a system of computer models to generate a digital twin of a centrifugal extractor.

References

1. **Bykov, L. V.** Fundamentals of computational heat transfer and hydrodynamics [Text] : textbook / L. V. Bykov, A. N. Molchanov, D. S. Yanyshchev. – 2nd edition, revised and enlarged. (in Russian).
2. **Ferziger, Joel H.** Computational Methods for Fluid Dynamics [Text] / Joel H. Ferziger, Milovan Perić. – Fourth Edition. – Springer Nature Switzerland, 2020. [Electronic resource]. – <https://doi.org/10.1007/978-3-319-99693-6>.
3. [Electronic resource] <http://www.openfoamwiki.net/index.php/interfoam>.
4. Surya Kaundinya Oruganti, Implementation of cavitation models into the multiPhaseEulerFoam solver. – URL: <https://www.researchgate.net/publication/327692025>.
5. [Electronic resource] <http://www.OpenFOAM.org>.
6. **Kraposhin, M. V.** Numerical simulation of compressible flows using a hybrid method of approximation of convective flows. – 2016. [Electronic resource] https://www.keldysh.ru/council/3/D00202403/kraposhin_diss.pdf (in Russian).

7. **Haroun, Y.** Volume of fluid method for interfacial reactive mass transfer: application to stable liquid film [Text] / Y. Haroun, D. Legendre, L. Raynal // Chem. Eng. Sci. – 2010b. – Vol. 65. – P. 2896–2909.
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