

# THERMODYNAMIC MODELLING IN COMPUTING BACK-END MATERIAL BALANCE

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Within the framework of “Proryv” project [1] work is underway toward mathematical modelling of spent nuclear fuel (SNF) reprocessing and fuel fabrication technologies; the software complex (SC)VIZART [2] has been developed for validation and optimization of back-end process parameters.

In modelling back-up processes some uncertainties arise related both to SNF composition of candidate reactor facilities, and to newly developed processes. Full-scale experimental development is hampered by the absence of SNF samples, and the difficulty of processing actual highly-active compositions. One of the methods to evaluate technological parameters under such circumstances is thermodynamic modelling.

For this purpose RFNC-VNIITF is currently developing SC TeDy [3], which allows computing chemical-equilibrium compositions of systems of varying complexity. The computations use the data base containing information on substance properties typical of nuclear fuel cycle (NFC) technologies. SC TeDy is able to operate standalone as an application with user interface, and it is usable in balance computations.

The results of related computations by SC VIZART and SP TeDy are used by developers of SNF reprocessing and nuclear fuel fabrication technologies to analyze and evaluate different alternative technologies.

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1. Adamov E.O., Aleksakhin R.M., Bolshov L.A., Dedul A.V., Orlov V.V., Per-shukov V.A., Rachkov V.I., Tolstoukhov D.A., Troyanov V.M. The project “PRORYV” is a technological base for large scale nuclear power engineering // *Izvestia RAN. Energetika*. 2015. No. 1. P. 5–12.
  2. Shmidt O.V., Makeeva I.R., Liventsov S.N. Modelling of back-up technological limits as a tool to create and optimize industrial processes. // *Radiokhimiya*. 2016.V. 58. No. 4. P. 316–323.
  3. Peshkichev I.V., Kuropatenko V.F., Makeeva I.R., et al. TeDy software complex to solve thermodynamic modelling problems. // *Vestnik UuUrGU. “Mathematical modelling and programming” series (Vestnik UuUrGUMMP)*. 2018.V. 11. No. 1. P. 84–94.