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Research Article

Isotope kinetics modeling in a circulating fuel system: a case study of the MBIR reactor loop*

Dariya S. Kuzenkova[1], Victor Yu. Blandinskiy[1]

1 *National Research Center «Kurchatov Institute», 1 Academician Kurchatov Sq., 123182 Moscow, Russia*

Corresponding author: Dariya S. Kuzenkova (Kuzenkova_DS@nrcki.ru)

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Abstract

The paper presents the results of modeling of changes in the isotopic composition of the liquid-salt fuel circulating in the experimental channel of the MBIR reactor facility. The authors tested the ISTAR software environment adapted for solving burnup equations in problems with variable power levels. The loop channel parameters, including two heat exchanger options, were estimated to obtain the appropriate salt transit time through the loop channel zones. Two problems of a circulating fuel system (loop) modeling are considered, namely: (1) modeling the equilibrium salt isotope composition in such a system; and (2) developing a technique for modeling nonstationary isotope kinetics in the MBIR reactor loop. Non-stationary isotope kinetics can be modeled as sequential burnup of nuclides in the neutron field and decay during movement in the external circuit. The authors also developed an algorithm for modeling changes in the isotopic composition of fuel salt during its circulation, taking into account the sequential transfer of a given salt volume from the burnup zone to the zone outside the reactor core. Based on this algorithm, a software package was created using the Python 3.9 programming language and ISTAR modules. In addition, a description of the calculation methodology was given and some calculation results obtained using the software were presented. In the process of working with the program, it was found that, for the given times of the fuel being in each of the zones (2 and 200 seconds, respectively), modeling the change in the isotopic composition during the fuel campaign (500 days) will require the calculation of more than 500 thousand steps. In order to save time, it is necessary to find out whether it will be possible to reduce the number of calls to the neutronic calculation code due to a slight change in the isotopic composition of the fuel in the loop per one burnup step. Work is currently underway to optimize this process.

Keywords

MBIR, molten-salt reactors, molten-salt loop, ISTAR software, modeling, neutronic characteristics

Introduction

Molten salt fuel compositions can be used both in advanced nuclear reactors (Blinkin and Novikov 1978; Novikov et al. 1993; Ignatiev et al. 2019) and in blankets of hybrid fusion reactors. Using thorium fuel compositions in the blanket of a fusion source of neutrons will make it possible to generate ^{233}U, this expected to allow addressing issues of providing the nuclear fuel market with resources for a long period of time. The Advanced Research Reactor, MBIR (Dragunov et al. 2012), is planned to replace the BOR-60 reactor and is equipped with standalone loop devices for testing of materials and fuel, including molten salts. This study is a continuation of Blandinskiy and Kuzenkova 2020.

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The paper deals with simulation of a loop channel and evolution of the isotope composition in the molten salt fuel in the experimental channel of the MBIR rector facility.

Loop channel parameters

A loop channel can be conditionally divided into two areas: that in the reactor core and the outside circuit. The area in the neutron field is described in detail in Blandinskiy and Kuzenkova 2020. It has a complex structure: a tube from EP-450Sh steel, which, with an allowance for the argon-filled gas gap, accommodates a Hastelloy H tube that contacts the circulating fuel salt. The outside circuit is formed by pipelines and an intermediate heat exchanger. The intermediate heat exchanger transfers heat from the primary circuit fuel salt to the secondary circuit coolant. Further neutronic calculations require estimating the volume of fuel salt in each of the circuit parts.

Selection of the heat exchanger

To start the heat exchanger calculations, one needs to determine the key parameters of fuel salt: density, specific heat capacity, dynamic viscosity and thermal conductivity. The justification for the LiF–ThF_4 system and its density calculation are described in Blandinskiy and Kuzenkova 2020. The thermophysical properties of the LiF–ThF_4 system for the required composition were estimated based on published experimental data.

The compound's heat capacity was estimated using the Neumann-Kopp rule based on known data for some of the components (LiF and ThF_4 (Capelli et al. 2013)) and is equal to 908.1 J/(K·kg).

The dynamic viscosity at the working temperature is 0.0209 Pa·s (Benesh and Konings 2009). No experiments were undertaken with such salt composition to determine the heat conduction coefficient, so, as shown in Benesh and Konings 2009, it is proposed to assume that $\lambda = 1.5$ W/(m·K).

Two coolant options have been considered for the heat removal circuit: liquid sodium used as coolant for the MBIR reactor, and molten salt in the FLiBe form (LiF–BeF_2). The calculation results for the key values of the two intermediate heat exchanger versions were estimated based on a procedure in Usynin et al. 1981 and are presented in a summary Table 1.

Table 1. Key characteristics of heat exchangers

Measured value	Secondary coolant	
	Na	LiF–BeF_2
Mass flow rate of primary fuel salt, kg/s	22	22
Mass flow rate of secondary coolant, kg/s	16	9.5
Heat-exchange surface area, m^2	80.8	458.7
Outer shell diameter, m	0.42	1.02
Pressure loss, kPa	126	126
Fuel salt volume in IHX, m^3	0.14	0.76

The dimensions of the intermediate heat exchanger (IHX) were estimated and the volume of the fuel salt it contains was calculated. The fuel salt volume is 0.14 m^3 when liquid sodium is used as coolant and 0.76 m^3 when molten salt is used.

Consolidated data on the volumes of all elements in the loop channel circuit are presented in Table 2.

Table 2. Volumes of fuel salt in different sections of the loop channel for two coolant options, m^3

Loop channel section	Secondary coolant	
	Na	LiF–BeF_2
Channel's in-core part	0.143	0.143
Pipelines	0.014	0.014
Heat-exchanger	0.136	0.759
Entire loop channel	0.293	0.915

Computational model and software tools

Simulation of the circulating fuel isotopic kinetics requires software tools to calculate the power density and fuel burnup in variable-power zones.

The power density in the loop is determined using the Monte Carlo MCNP code (Monte Carlo Team 2008). Inside of the MBIR reactor loop, power density of distributed by zones that contain fuel materials (core, blankets, in-core storage, molten salt loop). The power density distribution for each of the zones is calculated in Blandinskiy and Kuzenkova 2020: core – 88.17%, blankets – 8.61%, in-core storage – 3.16%, loop channel – 0.06%. The low value of power in the loop channel is explained by the fact that the salt in the starting state contains only raw ^{232}Th isotopes. Power will grow as ^{233}U is accumulated. This is followed by normalization against the MBIR total thermal power (150 MW).

The ISTAR software tool (Dudnikov 2020) makes it possible to calculate both the equilibrium state and the isotope composition change. It is designed to investigate complex structures of nuclear power systems, including different processes of nuclide transformation at different nuclear power complex facilities. The model of a nuclear power system is defined as a specific structure consisting of a set of processes, physical zones, storages, NFC facilities, and nuclide flows between these. Calculations can be undertaken both for burnup and cooling steady-state modes and transients (Alekseevsky 2008; Blandinskiy and Dudnikov 2018). Each process (physical zone) uses a pointwise single-group isotope kinetics model; it is assumed that all nuclides have zone-average and energy-integral parameters of interaction with neutrons and are in a zone-average and energy-integral neutron flux. A need arose for testing the adaptation of the ISTAR software environment for problem-solving in calculation of the nuclide kinetics in variable-power zones.

Heavy fissile nuclei are contained in the reactor core, in the blankets and in the loop channel (4 zones in total). A decision was made to simulate these zones, calculate the burnup in each of the zones, beginning from the starting salt composition with a step of 20 days (10 steps), knowing the total power density in the core, in the blankets, and in the loop channel. As the result of the burnup calculation, apart from the isotope composition, the ISTAR retains the power density distribution by steps in each of the four zones. With known values of the power distribution in the loop channel for each time step, the burnup problem has been solved for only one burnup zone (loop channel).

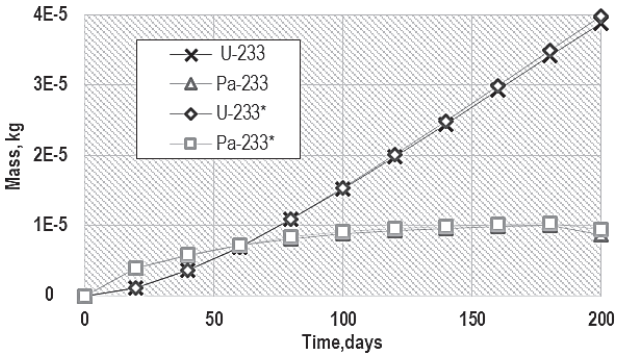

Figure 1. Comparative ^{233}Pa and ^{233}U mass diagrams for two types of calculations depending on time. The asterisk (*) marks calculations with power density defined inside of a particular zone.

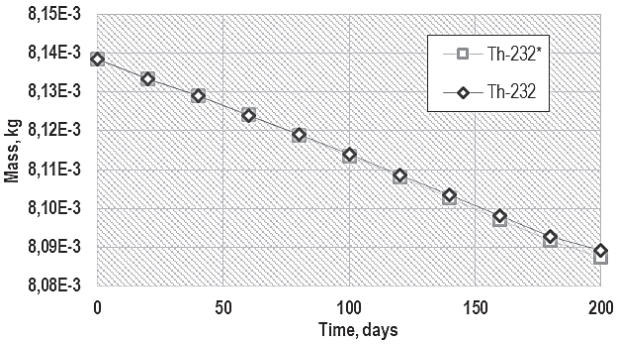

Figure 2. Comparative ^{232}Th mass diagrams for two types of calculations depending on time. The asterisk (*) marks calculations with the power density defined inside of a particular zone.

Comparative calculations were undertaken to solve the isotope kinetics problems using different methods: by defining the reactor's total power and the power density in the loop channel only knowing the power density fractions for each portion. A new isotope composition was obtained at each calculation step. The figures present comparative isotope mass diagrams for ^{233}Pa, ^{233}U (Fig. 1) and ^{232}Th (Fig. 2), for each of the calculations described above depending on time (in days). The calculations of the isotope compositions, with total power and power density defined inside of the loop channel only for a step, coincide, which allows one to count the burnup in variable-power zones.

Approaches to simulation of circulation

There are two simulation approaches for a system (loop) with circulating fuel:

- to change the content of isotopes in the fuel composition in the neutron field with the neutron flux density averaged over the entire loop circuit;
- to change the isotope composition with the consistent burnup of nuclides in the neutron field (the loop in the reactor core) and cooling in the course of movement in the outside circuit.

This paper deals with the evolution of the latter approach. An algorithm has been developed and a software tool has been implemented in the Python 3.9 language using ISTAR code modules to simulate the isotope kinetics of the fuel composition of interest that circulates among the zones with and with no neutron field in any preset time interval.

Simulation of the fuel salt circulation in the loop channel

A preliminary thermal-hydraulic calculation was undertaken which has made it possible to estimate the time of the fuel salt residence in the neutron field, that is, immediately in the MBIR reactor loop channel (2 seconds), and in the outside circuit portion beyond the core (200 seconds).

A code has been developed for calculation of the isotope kinetics in systems with circulating fuel based on the ISTAR software tools (Kuzenkova and Blandinskiy 2022), intended to calculate the isotope composition in molten fuel salt in the course of its circulation in the research reactor loop channel using the ISTAR. The code simulates the consistent transport of the elementary liquid fuel volume from the burnup zone to a zone beyond the reactor core.

The code startup requires entering a number of key parameters, including the initial fuel salt composition, power density in the in-core channel portion, the number of burnup steps, and the time of the salt residence in each loop part. A step corresponds to one program run stage that simulates one of two processes: burnup (reactions in the neutron field) or natural decay.

We shall look in detail at how the code operates. Step 1, similarly to all further odd steps, deals with burnup simulation: the ISTAR code's module of the same name is started, the operation of which results in a changed isotope composition of fuel, and calculation is started further to determine more precisely the power density for the new fuel composition, after which the obtained data are rerecorded as starting for the further process. Step 2, likewise all other even steps, simulates natural decays of nuclides in fuel, the composition of which is obtained in the previous step. The code sequentially starts the executed modules for the

preset number of times. As the result of the operation, each step creates a text file with a table that contains data on the isotope composition of fuel, as well as a text file with the recounted power density values. The data for each step are aggregated in a summary table (in the CSV format).

The developed software tool was verified. Hand procedures were used to calculate 20 program run steps. The results of the power density and isotope composition calculations using hand procedures and the developed research tool have coincided in full (Fig. 3). The ISTAR software tool was verified earlier for the burnup calculation (Blandinskiy and Dudnikov 2018).

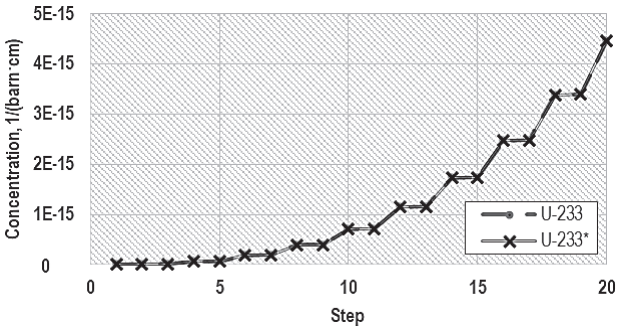

Figure 3. Comparative diagrams of the ^{233}U concentration change in time based on hand procedures and using the developed research tool. The asterisk (*) marks hand calculations.

Conclusions

A computational model has been developed and the experimental loop channel key parameters have been estimated. The circulation of fuel salt in a loop channel was simulated (consistent transport of the preset amount of salt from the burnup zone to a zone beyond the reactor core).

It was found in the course of the code operation that the calculation time for each process matters with the preset times of fuel residence in each of the zones (2 and 200 seconds). Knowing that the MBIR reactor fuel life is 500 days, the number of such steps will be more than 500 thousand. One calculation may take several months, so the code was upgraded. Proceeding from the fact that the fuel composition changes insignificantly for 200 seconds (let alone for 2 seconds), power density can be recounted once in a number of steps. Work is under way to optimize this process.

References

- Alekseevsky LD (2008) Search for a possible structure of a stationary system for future nuclear power engineering with a closed nuclear fuel cycle based on the study of nuclide balances. VANT. Ser. Fizika Yadernykh Reaktorov 2: 21–26. [in Russian]
- Benesh O, Konings RJM (2009) Thermodynamic properties and phase diagrams of fluoride salts for nuclear applications. Journal of Fluorine Chemistry 130(1): 22–29. https://doi.org/10.1016/j.jfluchem.2008.07.014
- Blandinskiy VYu, Dudnikov AA (2018) Calculations of spent fuel isotopic composition for fuel rod from VVER-440 fuel assembly benchmark using several evaluated nuclear data libraries. Kerntechnik 83(4): 325–330. https://doi.org/10.3139/124.110917
- Blandinskiy VYu, Kuzenkova DS (2020) Computational validation of experiments with molten-salt thorium-uranium fuel compositions in MBIR test loop. Atomic Energy 128(5): 271–276. https://doi.org/10.1007/s10512-020-00687-3
- Blinkin VL, Novikov VM (1978) Molten Salt Nuclear Reactors. Atomizdat Publ., Moscow, 112 pp. [in Russian]
- Capelli E, Benesh O, Beilmann M, Konings RJM (2013) Thermodynamic investigation of the LiF-ThF4 system. The Journal of Chemical Thermodynamics 58: 110–116. https://doi.org/10.1016/j.jct.2012.10.013
- Dragunov YuG, Tretiyakov IT, Lopatkin AV, Romanova NV, Lukasevich IB (2012) MBIR multipurpose fast reactor – innovative tool for the development of nuclear power technologies. Atomic Energy 113(1): 24–28. https://doi.org/10.1007/s10512-012-9590-x
- Dudnikov AA (2020) Program for Modeling Isotope Kinetics in Multicomponent Structure of Nuclear Industry «ISTAR». Certificate RF: computer software No. RU 2020619218. [Available at:] https://www.elibrary.ru/item.asp?id=43889370 [accessed Sep. 19, 2022] [in Russian]
- Ignatiev VV, Kormilitsyn MV, Kormilitsyna LA, Semchenkov YuM, Fedorov YuS, Feinberg OS, Kryukov OV, Khaperskaya AV (2019) Molten-salt reactor for nuclear fuel cycle closure on all actinides. Atomic Energy 125(5): 279–283. https://doi.org/10.1007/s10512-019-00481-w
- Kuzenkova DS, Blandinskiy VYu (2022) Program for Calculating Isotope Kinetics in Circulating Fuel Systems Based on the ISTAR PS. Certificate RF: computer software No. RU 2022614236. [Available at:] https://www.elibrary.ru/item.asp?id=48139601 [accessed Sep. 19, 2022] [in Russian]
- Monte Carlo Team (2008) MCNP – A General Monte Carlo N-Particle Transport Code. Version 5/X-5 Monte Carlo Team (2008) LA-UR-03-1987, LLC. [Available at:] https://mcnp.lanl.gov/pdf_files/la-ur-03-1987.pdf [accessed Sep. 19, 2022]
- Novikov VM, Slesarev IS, Alekseev PN, Ignatiev VV, Subbotin SA (1993) Nuclear Reactors of Increased Safety (Analysis of Conceptual Designs). Energoatomizdat Publ., Moscow, 348 pp. [in Russian]
- Usynin GB, Karabasov AS, Chirkov VA (1981) Optimization Models of Fast Reactors. Atomizdat Publ., Moscow, 232 pp. [in Russian]