

# Computational substantiation of technological characteristics of the closure stage of nuclear fuel cycle using code VIZART\*

Inga R. Makeyeva<sup>1,2</sup>, Vasiliy Yu. Pugachev<sup>1</sup>, Olga V. Shmidt<sup>3</sup>,  
Anastasiya A. Rykunova<sup>4</sup>, Andrey Yu. Shadrin<sup>4</sup>

1 FSUE “Russian Federal Nuclear Center – Zababakhin All-Russia Research Institute of Technical Physics”, 13 Vasiliev Str., 456770 Snezhinsk, Chelyabinsk Reg., Russia

2 South Ural State University, 76 Lenin Av., 454080, Chelyabinsk, Russia

3 JSC “PRORYV”, 2/8 Malaya Krasnoselskaya Str., 107140 Moscow, Russia

4 Private Enterprise “Science and Innovation” State Corporation Rosatom, 44 bld. 4 Bolshaya Ordynka Str., 119017 Moscow, Russia

Corresponding author: Olga V. Shmidt (shov@pnproryv.ru)

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## Abstract

There exist different variants of organizing the closure of nuclear fuel cycle (CNFC) depending on fast reactor type, fuel types, station or centralized allocation of closed nuclear fuel cycle stages. One of the ways to verify and estimate engineering solution is mathematical modeling of radiochemical technology which in the end will allow to optimize composite technological process in order to increase effectiveness and reduce cost. In order to calculate the balance of material flows of process circuits and individual production sections in the stationary and dynamic modes, with taking into account the isotopic composition evolution, a software package VIZART (Virtual Plant of Radiochemical Technologies) was developed, allowing the user to assemble the required sequence of operations for any part of the process scheme and perform the calculation of material balance for all flows of the circuit, as well as to optimize the equipment operating modes and provide the necessary data to justify the safety of certain limits and the entire process circuit. The following capabilities of code VIZART for computational substantiation of CNFC technology design and characteristics are considered: material balance calculation, cyclogram creation, determination of the most loaded parts of processing lines, estimation of fissile materials accumulating in devices and intermediate vessels, optimization of productivity of nodes and devices.

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## Keywords

technologies of the closure of nuclear fuel cycle, code VIZART, computational substantiation of technology characteristics

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## Introduction

Incorporating fast neutron reactors into the nuclear power structure needs to be accompanied by the introduction of a

closed fuel cycle, that is, a system for irradiated nuclear fuel processing and “fresh” fuel production using recycled nuclear materials (NM). Involving recycled NMs into the fuel cycle also requires ensuring that radioactive waste (RW)

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formed are handled in an environmentally friendly and safe manner. At present, neither Russia nor any other country has the complete package of closed nuclear fuel cycle (CNFC) technologies which provide for the required quantity of end and intermediate products on a commercial scale.

As part of the *Proryv* project (Adamov et al. 2015), a pilot and demonstration energy complex will be built which comprises the BREST-OD-300 lead-cooled fast neutron reactor (FNR), a spent nuclear fuel (SNF) reprocessing and RW handling module, and a fuel refabrication module (FRM). The facilities are developed within a tight schedule, and mathematical simulation of respective technologies can be used efficiently to select and justify engineering and process solutions, optimize the process conditions, and configure processing lines.

Until recently, mathematical simulation of the CNFC radiochemical processes and technologies was used by individual researchers who were involved directly in development of process operations, which has led to the absence of general approaches to simulation of processes and to the gradual loss of respective expertise and knowhow. One of the requirements in the framework of the *Proryv* project is to support the development of all facilities and technologies under design with mathematical models and codes. While there is an extensive many-year experience in simulation of the reactor plant operation, systemic activities for simulation of technologies, which encompasses the entire set of the CNFC processes, was started in 2012 exactly as part of the *Proryv*.

## VIZART code for simulation of the NFC backend processes

As a tool for justifying the engineering and design solutions to be used by process engineers, equipment developers and designers of out-of-pile NFC process stages, a code, VIZART (Shmidt et al. 2017), has been developed and is being evolved for simulating and optimizing both individual fuel cycle backend processes (SNF reprocessing, fuel refabrication and RW handling, including

disposal), and the nuclear fuel cycle technologies. The VIZART functions are defined by the range of issues solved by process and processing line developers when developing processes and designing the CNFC concept, and when implementing the CFNC as part of the pilot and demonstration energy complex (PDEC) and the energy production complex (EPC), this including justification of feasibility for process solutions, selection and optimization of process conditions, and assessment of solutions for the processing line configuration. Accordingly, there are three groups of functions the VIZART is responsible for:

- calculation of the material balance, including depending on time, and taking into account the evolution of the material flow nuclide compositions;
- simulation of individual processes and devices for justifying and optimizing process conditions;
- calculation of key indicators for processes and devices taking into account the performance of equipment and different process conditions.

Integrated processes, such as SNF reprocessing or fuel refabrication, used in simulations are represented as a complex flow diagram consisting of process stages, connections among them, and processed products which are transferred between process stages. Process stages consist of a set of process nodes. Processed products are transferred between process nodes via connections. Schematically, the interactions among the simulated facilities are presented in Fig. 1.

A process (process operation) is the base simulated entity. Its key functional purpose is to convert the incoming flow to an outgoing flow based on dedicated algorithms that implement the mathematical model of the process. Characteristics of the process, such as chemical reactions or dependences of the product properties on the process running conditions, are used to calculate the conversion. Each process node is a component of the flow diagram used to describe physical objects (devices, plants, etc.) in simulation problems. The key characteristic of a process node is the set of processes (consecutive or parallel) occurring on the process node. Apart from processes, a process node is characterized by a set of equipment (device, plant,...) prop-

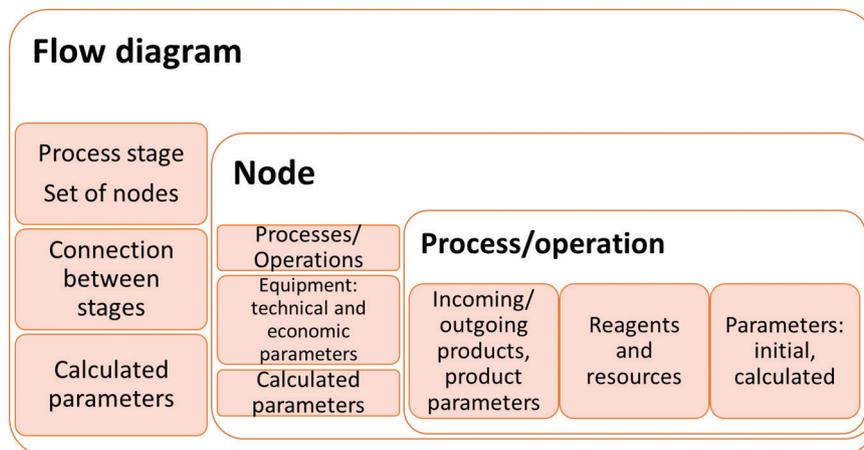


Figure 1. VIZART simulated entities.

erties, efficiency, maximum incoming flow rate (mass flow rate, volume flow rate, loading frequency and volume), as well as by the lifecycle characteristics: operating time, frequency of preventive maintenance, etc. A processed product (flow) is a combination of chemical substances (materials) entering or exiting the process node or the process.

Due to the absence of final CNFC solutions, it is required to ensure that the computational models of the process stages could be flexibly reconfigured. An interactive designer has been developed using the VIZART code, which makes it possible to determine the model composition in a dynamic mode. Software and information models contained in the VIZART library are used to build the flow diagram model. To calculate the characteristics of flow diagrams, a set of special-purpose algorithms (managers) has been developed, which allows end-to-end calculation of the material flow throughout the flow diagram and the characteristics of process operations taking into account the mutual effects of the flow diagram components. Depending on the type of the job addressed, two key simulation modes are considered: a steady-state mode and a dynamic mode. No time characteristics of process operations, such as process time, loading frequency, and consumption rates of material flows, are taken into account in the steady-state mode. Simulation in the dynamic mode allows one to determine such processing line characteristics as continuity of equipment operation, demand for replication of assemblies and devices, and total time of reprocessing or manufacturing the preset quantity of products. Specific to the VIZART simulation is tracking of not only the material and elemental compositions of material flows but also of isotopic compositions, which makes it possible to calculate activities and power densities, and the evolution of compositions is taken into account in the dynamic mode with the use of the dedicated isotope module (Modestov 2006).

Calculations can be done both in the steady-state mode and in the dynamic mode for one and the same flow

diagram, this being supported by the VIZART object-oriented approach tools.

Fig. 2 shows the overall view of the VIZART code user interface. To build a computational model, process nodes are selected from the VIZART library (seen on the left in Fig. 2), and placed in the respective work field, and the material flow connections are established then between nodes, and characteristics of process operations, e.g., coefficients of the reaction behavior fullness, process operation duration, etc., are adjusted (seen on the right in Fig. 2). The consistency of initial information in a computational model is ensured by the VIZART databases which contain reference information on the properties of substances, and characteristics of process operations and equipment. The user-prepared calculation variant is written in the xml format and stored in the dedicated catalog along with the calculation results. The calculation results are accessible for being viewed, analyzed and compared as charts, tables and reports using the code's analytical subsystem.

## Computational simulation of the CNFC process stage characteristics

The VIZART code allows several types of simulation for the CNFS process stages, including steady-state and dynamic mode calculation of the material balance, and optimization of the characteristics of processes a processing line includes.

**Material balance calculation in the steady-state mode** is used to prepare initial data, justify the feasibility of process solutions, and estimate the RW volumes, activities and types. In this case, the reagent consumption rate per unit mass of the incoming flow is calculated, e.g., per 1 ton of SNF under reprocessing, while taking into account the return flows of process media, e.g., nitric

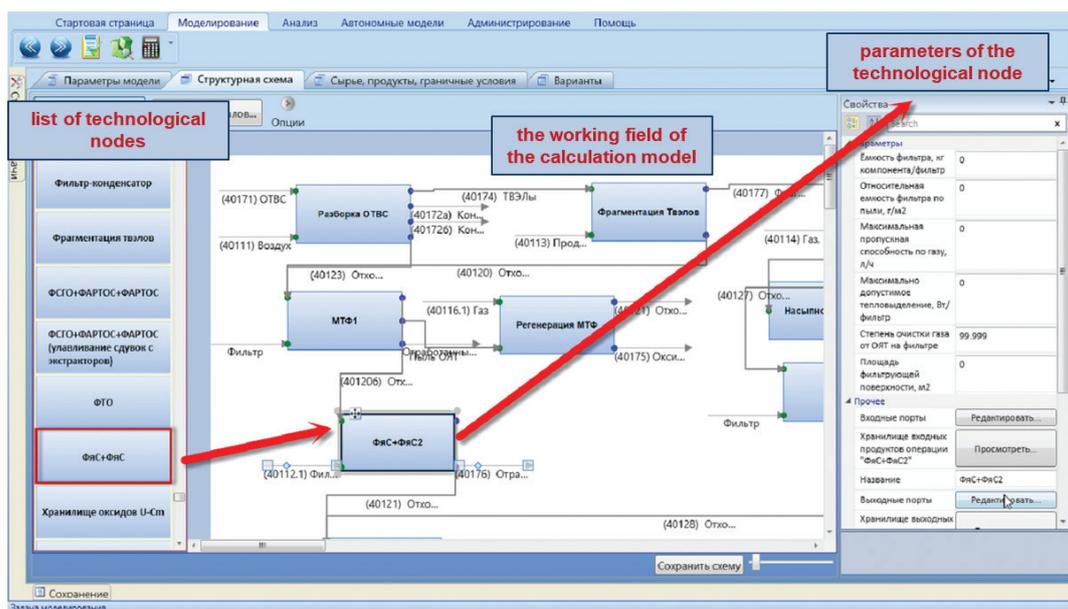


Figure 2. General view of the VIZART user interface (Russian version).

Код продукта	Т	U	Xe	Y	Zn	Zr	Концентрация HNO <sub>3</sub> моль/л	Тепловыделение Вт	Активность Бк		
									Общая	Альфа	Бета+Гамма
Air_5							0,000	0	0	0	0
OTVS_4	14	7,5002E-001	6,6300E-003	3,5700E-004		3,7500E-003	0,000	1,56E+007	3,01E+019	2,01E+016	3,00E+019
Tvels_8	15	7,4927E-001	6,6234E-003	3,5664E-004		3,7462E-003	0,000	1,56E+007	3,00E+019	2,01E+016	3,00E+019
Tails_3							NaN	0	0	0	0
Aerosol_7	17	7,5002E-004	6,6300E-006	3,5700E-007		3,7500E-006	0,000	1,56E+004	3,01E+016	2,01E+013	3,00E+016
Air_7							0,000	0	0	0	0
Tvels_8	15	7,4927E-001	6,6234E-003	3,5664E-004		3,7462E-003	0,000	1,56E+007	3,00E+019	2,01E+016	3,00E+019

Figure 3. Material flow characteristics (Russian version).

acid or service water. Both experimental data and expert estimates from process engineers are used as design distribution coefficients to convert incoming to outgoing chemical substances if there is no information on the given process (e.g., at early stages of the technology development). Therefore, such calculations are performed, as a rule, in a particular process mode (either in a standard or conditionally ideal mode, or in a conservative mode). As information is obtained on the parameters of the process for different process nodes, calculated data for these operations are adjusted, and end-to-end calculation is performed again for the whole of the flow diagram.

Calculation results are displayed as tables (Fig. 3) which contain characteristics of flows on all flow diagram nodes: bulk and mass flow rates, chemical, elemental and isotopic compositions, as well as specific activities, power densities and other characteristics of products specific to radiochemical processes.

Automation of the material balance calculation reduces the number of routine hand computations, and cuts the number of errors and the time for preparing initial data. The dynamic environment for the computational pattern preparation and the possibility for changing the user interface parameters make it possible to consider a large number of different options for process solutions, and, accordingly, select the most appropriate alternate flow diagram.

**Material balance calculation in the dynamic mode** is used to assess and optimize:

- solutions for configurations of processing lines taking into account the existing requirements for efficiency, operating consistency of process stages, and generation dynamics for intermediate and end products;
- accumulation of fissionable and nuclear materials at different process stages, and in intermediate storages and tanks, which is initial information for assessing safety and compliance with nonproliferation criteria;
- volumes and types of generated RW.

The initial information specified for each flow diagram node in the course of dynamic calculations includes duration of the operation, loading frequency and volume, consumption rates of material flows, and capacity of devices. Based on the calculation result, the cyclogram of the equipment operation is plotted (Fig. 4), the required capacities of intermediate tanks and storages and the demand for replication of devices are defined, and the accumulation of fissionable materials in intermediate tanks and storages, and the power density and activity in the flow diagram devices are estimated.

We shall consider the possibility of selecting the parameters of process operations based on the example of a combined pyrohydrometallurgical flow diagram for reprocessing mixed nitride uranium-plutonium (MNUP) fuel for the BREST OD-300 reactor (Fig. 5), which was considered as one of the SNF processing technology options for the NFC closure (Shadrin et al. 2016).

It was shown based on the calculation results that the expected daily electrolytic cell loading of 8 kg of SNF pellets failed to allow continuous operation of the extraction and crystallization node, so the loading requires to be increased to 12 kg of SNF pellets. To ensure that the electrolytic cells operate continuously, it is required to have a decanning device for each electrolytic cell and at least 5 cadmium stripping units devices without tank filling and emptying operations taken into account. Doubling the cathode deposit granulate dissolution unit efficiency will make it possible to reduce the total SNF reprocessing time and to achieve the preset efficiency of the reprocessing module as the whole.

**Optimization of the flow diagram parameters.** It will be reasonable that a system analysis methodology by Moiseev 1981, as part of which methods are evolved for designing complex engineering, manufacturing, environmental and other systems, be used to develop such complex engineering systems, one of which is the set of the CNFC technologies. System analysis combines principles of the operations research theory by Taha 1985 and the

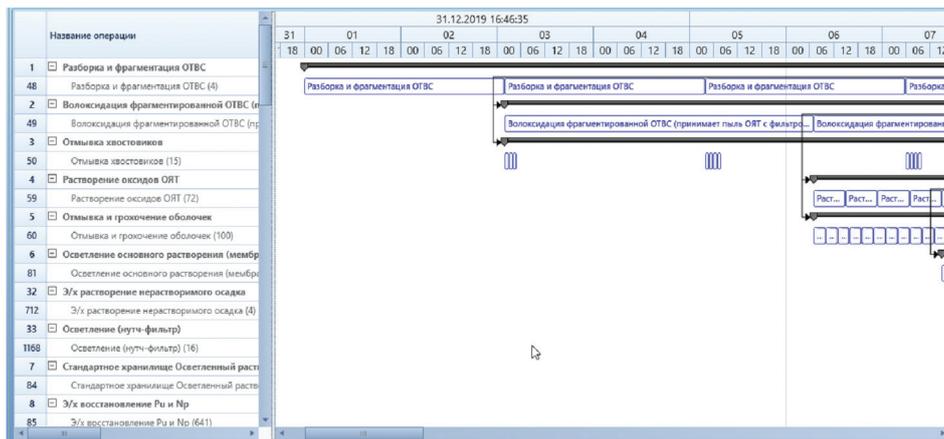


Figure 4. Example of the equipment operation cyclogram calculated in the VIZART code (Russian version).

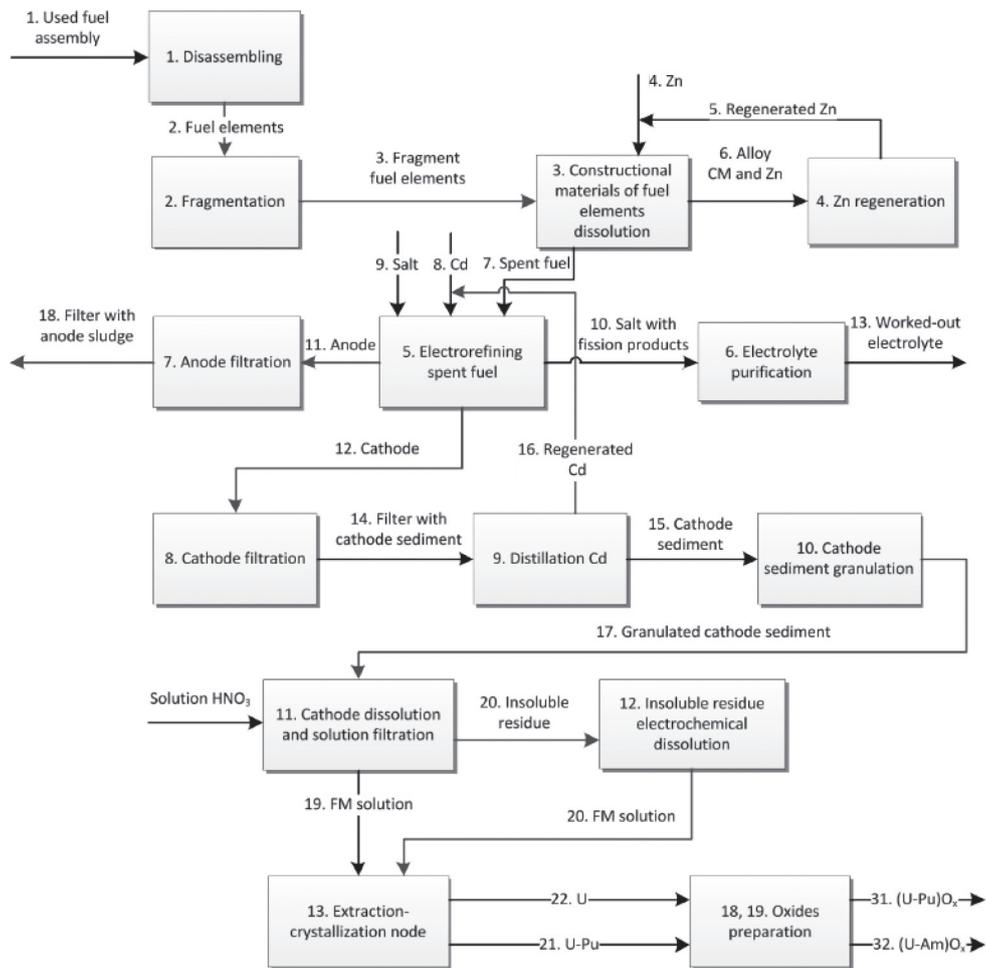


Figure 5. Overall view of a combined SNF MNUP reprocessing flow diagram.

control theory methods by Alekseev et al. 1979. Among other things, specific to system analysis is methods for building system hierarchies which cannot be done in the field of only formal mathematical procedures, particularly when choosing the detailing level and the adequate mathematical model. Different methods, e.g., the event tree method by Glushkov 1969 or the solving matrix method by Pospelov et al. 1980, are used for decomposing a complex problem. Essential to all these methods is that the optimum is searched for individual parts of the project such that the “global” project objectives are achieved.

Building the package of the CNFC technologies suits naturally such logic.

The CNFC technologies can be optimized via:

- optimizing the processing line configuration using a set of process nodes and operations;
- optimizing the processing line configuration in terms of efficiency and the material flow processing time;
- optimizing process modes and operations to comply with the *Proryv* project general requirements, e.g.,

such as the efficiency of the reprocessing module (RM) and the fuel fabrication module (FRM), requirements for the RM and FRM products, and the level of the fissionable materials recycle.

As a rule, the replacement of nodes and operations leads to a major change to the entire process chain or, at least, to the nodes associated with them. Automation of such changes is hard to implement. In this case, one can speak about optimization only in terms of comparing a number of the layout options based on the preset integral characteristics of the flow diagram as the whole, and the notion of global optimum becomes indefinite. Therefore, optimization, as understood in the classical mathematical theory, can be spoken about only in the event that the set of process nodes is defined and fixed. Therefore, no flow diagram is expected to be varied in the course of optimization.

A classical optimization problem is formulated as follows:

$$f(x) \rightarrow \min, x \in G, \quad (1)$$

where  $x$  is a component of a certain normalized space,  $E$ , defined by the model nature; and  $Q \subset E$  is the set that can have a however complex nature defined by the model structure and the peculiarities of the problem solved.

The structure of set  $G$  is defined by the set of conditions and constraints which define the permissible domain of the problem parameter variation. The optimization problem having been formulated, one of the known solution methods, e.g., the feasible directions method by Zoutendijk 1960, the sliding access method by Himmelblau 1975, and other nonlinear programming methods, given the constraints, can be used to solve it. One of the most reliable methods for searching for the global extremum of functions in geometrically complex multidimensional domains is the modified simplex method by Nelder, Mead 1965.

The solution of the optimization problem is traditionally broken down into three stages:

- construction of the processing line (process) model;
- statement of the optimization problem, that is, definition of the target function, variable parameters, and the set of constraints;
- solution of the optimization problem using the selected method.

The process model is built using the VIZART user interface. To solve the extremum problem, a dedicated subsystem has been developed, which includes window interface forms for setting the optimization parameters, and modules which allow one to search for the target function extremum and to compute the target function values based on the results of calculating the flow diagram characteristics. Variable optimization parameters are process modes and the efficiency and loading characteristics of equipment.

The following integral characteristics calculated in the course of the simulation are used as optimization criteria:

- deviation of concentrations of chemical elements in end and intermediate products from preset values;
- efficiency of the processing line;
- deviation of the physicochemical characteristics of intermediate and end products from target values to be transferred to further operations and stages (density, particle size, flow temperature, flow composition).

Refabrication cost of 1 kg of nuclear fuel (with capital costs taken or not taken into account) can be used as the versatile criterion for the entire package of the CNFC technologies. Apart from material flows, this requires the whole range of cost and financial and economic characteristics to be taken into account for simulation, which is a promising area of development activities. At present, the VIZART code includes a dedicated subsystem that allows optimization of process parameters using mathematical methods, including optimization of the RW handling cost with regard for different classes of generated waste (Makeyeva et al. 2021; Kashcheev et al. 2022). And the set of variable parameters is selected by the user immediately when preparing calculation tasks.

One of the most frequently solved problems in optimizing processing lines of radiochemical production facilities is harmonization of efficiencies for different operations production departments or the entire flow diagram include. Thus, optimization was demonstrated in Makeyeva et al. 2017 for different stages of the dissolution nodes that comprises operations for dissolution of SNF oxides, membrane filtration of solution, and electrochemical after-dissolution of undissolved deposit, as the result of which it became possible to reduce the equipment idle time 20%.

In connection with the complexity of the simulated system, it is not possible to formulate assumptions with respect to the target function topology and the global extremum location, including the target function continuity and smoothness. No gradient methods, which require computation of derivatives, can be used therefore for the extremum problem solution. Among non-gradient methods, the modified deformed polygon method has proved to perform well (in Nelder, Mead 1965). The major issue in employing this method is its convergence to the local minimum that depends on the selected initial approximation. A combined algorithm has been therefore developed when a set of initial approximations is selected at the initial stage using a genetic algorithm (in Different Evolution: genetic algorithm for functional optimization), for each of which the optimal value of the target function is determined. The global minimum is determined based on the obtained target function values.

Considered as the test problem for demonstrating the operation of the proposed algorithm was the problem of optimizing based on the VIZART code the characteristics of the fuel fabrication flow diagram fragment comprising the following operations: disintegration of uranium and plutonium nitrides, granulation of powders, mixing of powders with zinc stearate, compaction of fresh pellets (Fig. 6).

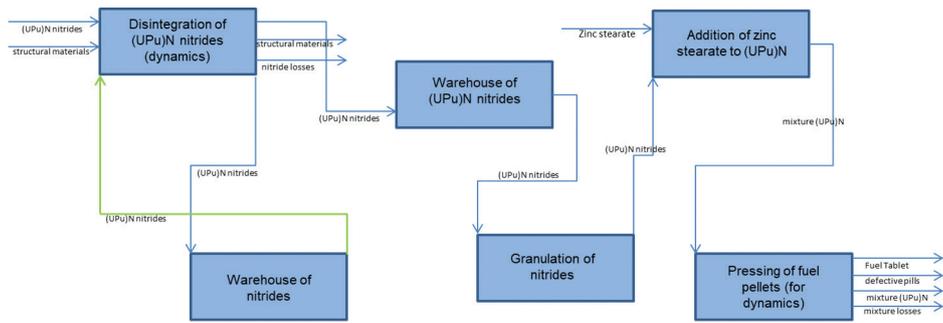


Figure 6. A fragment of the fuel fabrication flow diagram.

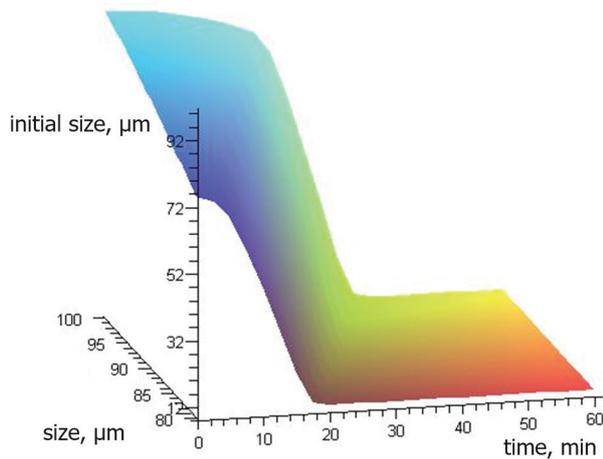


Figure 7. Powder granule size as a function of time and initial size.

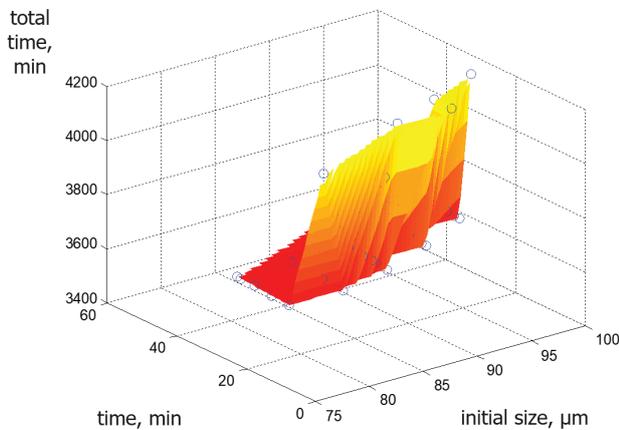


Figure 8. Total process duration as a function of initial size and disintegration time.

The problem consisted in minimizing the time for the fresh pellet production from the preset number of mixed nitrides.

The parameter “compaction time” was varied at stage 1. The overall process duration depends linearly on the durations of process operations, and, therefore, a trivial task was considered. As an answer, the optimization process produced the optimal value at the lower range boundary, having confirmed so that all components of the optimization subsystem operate correctly.

The parameter “nitride disintegration time” was varied at stage 2. For the preset parameters of the powder gran-

ule disintegration time and size limits, equal to 60 min and 10 μm respectively, the dependence of the granule size on the initial size and time changes according to the law shown in Fig. 7. The nitride disintegration time affects the size of the powder granules, which are disintegrated repeatedly if failing to comply with specification requirements, that is, affects nonlinearly the total time of the fresh fuel pellet production. An overall view of the target function is presented in Fig. 8.

As a result of the optimization, the nitride disintegration time (33.2 min) was found which ensured the smallest possible process duration of 69 h 23 min.

## Conclusions

The VIZART code makes it possible to solve a broad range of problems involved in development, justification and optimization of the CNFC processes. At present, the code is used to prepare initial data for developing and designing radiochemical process stages of the nuclear fuel cycle, and to select and justify the processing line configurations. The flow diagram designer and the VIZART process operation model library allow changing flexibly the computational pattern composition and the parameters of processes, increasing so the number of the options considered and cutting the time required to analyze and justify the adopted solutions. Dedicated modules used in the code for the isotopic composition, activity and power density calculation allows one to calculate the parameters specific for radiochemical production facilities, e.g., maximum one-time content of nuclear materials in tanks and vessels, taking into account the evolution in the content of isotopes in the nuclear fuel components, and, therefore, the change in chemical properties, and radioactivity and power density characteristics. Such calculations are used to estimate the effect of the product heat release on the working temperature of the process and equipment, for defining the end forms and volume of radioactive products, as well as for justifying the nuclear safety of technologies used.

Application of mathematical optimization methods makes it possible to update the characteristics of processes based on integral criteria. Target functions need to be described for these to be used more efficiently.

At present, the VIZART code addresses primarily prediction problems due to which it does not require

certification. To confirm the adequacy of the VIZART-based calculation results, tests are conducted to find out if the calculations used in the code algorithm coincide with the calculations obtained by an alternative method

or with the results of operating real production facilities. The code will require to be certified in the event of the calculation results used in justifying safety of processing facilities.

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