CNFC process codes

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Abstract. The following models and codes for technological stages of CNFC are being developed in the frames of “Proryv” project:

- Mathematical models of technological processes describing physical and chemical, gas/hydrodynamic, kinetic and phase processes occurring in apparatus. The models are focused on reasoning the range of technical parameters under normal, transitional and abnormal modes and on reasoning and optimization of mass-dimensional characteristics of the equipment and calculation of separate units lifetime;
- KOD TP code is intended for real-time simulation of the operation of technological schemes in order to define the functionality, controllability and to optimize the technology including control systems and simulation of accidents;
- Kinematic model of processing lines is intended for virtual definition of commutated workability both separate processes, nodes and facilities and processing lines in all. Starting, transitional, stationary modes are considered as 4D-models taking into account kinematic and technological features and restrictions.

Developing models and codes are currently used when technologies for closing stages of CNFC are designed (preparing initial data for equipment design and construction). Calculation models allow to detect collisions on early stages and to correct technological, design and engineering documentation; to perform polyvariant calculations to define the efficiency of separate nodes and the scheme in whole; to reason technical and design solutions and to evaluate the fission and nuclear materials during all the stages of the technological process including the in-process one. Currently the integrated system of models and codes is being developed for consistent simulation of heterogeneous processes and phenomena that are required to consider under calculating maintaining and reasoning the safety of CNFC technologies. The integrated system includes the existing and newly developed models and codes intended to describe technologic processes and apparatus, nuclear and radiation safety, ignition criteria, combustion, construction and engineering system behavior under critical loading and so on. The use of modern computational systems allows to perform associate calculations with date exchange between different codes from simple engineering to CFD-codes and to provide the solution of the complex problem of CNFC technology simulation.
1. Introduction
There is no doubt nowadays that the the nuclear power industry needs process codes to be developed, which simulate not only the reactor operation, but also the nuclear fuel technology at all stages of its production and processing. The need for such codes is especially pressing for developing the innovation production technologies, when there are no ready-made solutions for the entire range of processes, and serious scientific research is needed in respective areas. The process simulation is hoped to reduce the cost and duration of physical and chemical experiments, replacing them with a computational experiment, at least partially.

The task of fuel reuse in the course of closing the NFC involves the construction of multiple variants of the process and their comparative evaluation in order to find the optimal solution from the point of view of economics, ecology and safety of the created production process. The use of mathematical simulation in this search allows to automate the calculation, avoid many errors in routine calculations, accumulate, process a large number of solutions and determine the best option.

The most important tasks in the development of nuclear fuel cycle technologies are to ensure the nuclear, radiation and process safety of the complex facilities, including the production of the end part of the CNFC, as well as to ensure the control of nuclear materials. Currently, the process safety at radiochemical plants is substantiated mainly by special tests that simulate the process conditions or by operating experience of similar industries. This approach involves spending a sufficiently large amount of time and resources, which makes it quite expensive. In addition, the approach has many limitations since it is impossible to conduct dangerous experiments to test a large number of emergency situations, especially for newly developed radiochemical processes that have no analogues.

Multiple tasks of the challenge and heterogenous data that are necessary to obtain by calculation in the development and further operation of radiochemical plants has led to the need to create a system of codes for simulation, optimization, monitoring, control and justification of the process safety. The consistency of the mathematical models used, specially developed solution methods and data exchange formats allow to optimize the use of computing resources and provide the necessary accuracy and adequacy of modeling, regardless of the current operational process parameters.

2. Software package VIZART for balance calculations of process circuits
The balance calculation is carried out to determine the typical parameters of process operations, such as flow rates, composition of materials and elements, acidity, density, etc., as well as characteristics specific to radiochemical processes - isotopic composition, radioactivity, heat release of main products and process wastes. The obtained data can be used for a comparative analysis of various process circuits, for assessing the practicability and feasibility of the proposed process solutions in terms of the scope and activity of radioactive waste (for example, assessing the economic acceptability of a technology option in terms of the cost of handling waste from SNF processing).

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 (figure 1) 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 [1, 2]. The models basis is adjustable, which allows creating and editing existing software blocks corresponding to individual operations and processes, almost simultaneously with conducting research in the relevant areas.
A set of specialized algorithms (dispatchers) has been developed to calculate the parameters of process circuits, allowing to carry out a through calculation of the material flow parameters throughout the entire process circuit and parameters of process operations, with taking into account the mutual influence of the process circuit components. Depending on the type of the problem being solved, two main simulation models are considered: stationary and dynamic. It is possible to make calculations both in stationary and in dynamic mode for the same process circuit, which is provided by means of an object-oriented approach used in the VIZART software. A special feature of the simulation in the VIZART software is tracking not only substance and element compositions of material flows, but isotopic compositions as well, which provides the possibility of calculating the activity and heat release. In this case, a special module calculates the evolution of components isotopic composition depending on the process duration.

2.1. Stationary calculations
The calculation of the material balance in the stationary mode is used to prepare the source data, justify the feasibility of process solutions, access the volume, activity and types of radioactive waste. In this case, the reagent consumption is calculated per unit mass of the input flow, for example, per 1 ton of processed SNF, with taking into account return flows of process media, for example, nitric acid or process water. The calculation results are given in the tabular form (figure 2) containing flow parameters at all nodes of the process circuit: volumetric and mass flow rates, chemical, elemental and isotopic composition, as well as specific activity, heat release and other parameters of products specific to radiochemical processes.
Automating the calculation of material balance reduces the amount of routine manual calculations and the time to prepare the source data. Dynamic environment to prepare the calculation scheme and a possibility to change the parameters of the user interface allows considering a significant number of different variants of process solutions and, accordingly, choosing the most optimal variant of the process circuit.

- identify collisions of processes at the early stages of development;
- optimize the process circuits for RW volumes and product quality;
- prepare source data for the facilities and equipment design when NFC technologies are developed;
- take into account the operating time of Pu, Np, Am and Cm under the specified conditions of the stationary cycle;
- take into account the scope of work in progress (scrap, filters, etc.);
- take into account non-returnable losses.

2.2. Dynamic calculations
The source data set for each node of the process circuit during dynamic calculations include the duration of the operation, the frequency and volume of downloads, the expenses of material flows, the equipment performance, and the duration and complexity of operations that require human presence (“service operations”). As a result of the calculation, a cyclogram of the equipment operation is built, with necessary volumes of intermediate tanks and storage facilities and the need for replicating devices determined, the accumulation of fissile materials in intermediate tanks and storages, heat generation and activity in the process devices estimated, and the necessary number of main process personnel determined (figure 3). Dynamic calculations are applied to:

- assess and optimize layout solutions of the production lines in terms of performance requirements, consistency of redistribution, the production dynamics for intermediate and final products;
- assess the accumulation of fissile and nuclear materials in various process areas, in intermediate repositories and vessels, which is the source data for assessing the safety and compliance with non-proliferation criteria;
- assess the volumes and types of generated RW;
- account for FM decomposition (for example, 241Pu) and accumulation (for example, 241Am) during storage and processing;
- analyze workload of the main process personnel.
2.3. Dynamic calculations

The VIZART software includes a specialized subsystem that allows optimization of process parameters by mathematical methods. First, a process model is built, then the optimized parameters and the target function are selected. Integral parameters calculated in the simulation used as optimization criteria, for example, the performance of the production line.

The CNFC technology is possible to be optimized in several areas:

- optimization of the production line layout with changing the set of process nodes and procedures;
- optimization of the production line layout for the performance and material flow processing time;
- optimization of process modes of operations in order to achieve the general requirements of the Proryv PD.

An example of a solution of the optimization problem with the help of the VIZART software is given in figures 4 and 5, which show a solution to minimize the time needed for production of raw pellets of MNUP fuel fabrication module with the set parameters of the boundary grinding time and the limited size of powder granules. The nitrides grinding duration affects the size of the powder granules, which are to be sent for regrinding if they do not meet the specifications, i.e. it has a non-linear effect on the overall duration of the process of obtaining raw fuel pellets. The overview of the target function is shown in figure 4(b).
The duration of nitride grinding was optimized to provide the minimum process duration while meeting the necessary powder quality.

3. Mathematical models of processes

The course of a chemical process is determined by a variety of factors - from the operating mode parameters (temperature, pressure, flow rate of working fluid, etc.) and the characteristics of the material flow (composition, density, structure, etc.) to the design parameters of the equipment, where these processes are implemented. In the ideal case, computer models of processes should take into account the influence of all these parameters on the characteristics of the final and intermediate products, as well as the course of the process itself should be considered. Therefore, the mathematical descriptions of such processes are complex systems of differential and/or algebraic equations connecting the parameters of the material flow and process parameters in time. The development of a process model should be based on a theoretical understanding of the process and extensive experimental information that is not available or insufficient for most of innovative processes being a part of the SNF processing, fuel fabrication/refabrication and radioactive waste management technologies. Data on the properties of substances containing radionuclides are also incomplete. Therefore, the development of models based on fundamental physicochemical ratios is a challenging and time-consuming task, requiring to obtain large amounts of experimental data [3, 4]. Empirical and semi-empirical models are often developed for practical purposes, based on the available information about the process. The areas of applicability and the factor values shall be determined for such models.

The need to develop detailed models of the processes is determined by the tasks of selecting and optimizing the process regimes. They are also necessary to analyze the process risks and emergency modes [3].

A library of process models is created to simulate CNFC processes, where local process models are implemented in the form of modules which software interface allows them to be used either independently or as part of a process circuit, and the type of user interface depends on the use case. At the same time, the library of these models can be used both as a part of the balance calculations of the VIZART software package and in the simulation of the software package KOD TP. The entire set of data required for the calculation is stored in a specialized database and is available for modification and addition using the interactive user interface when preparing a specific calculation option (figure 6). At the moment, the library of the complex includes over 30 detailed mathematical models of MNUP fuel fabrication/refabrication processes, processing of SNF of fast reactors and radioactive waste management. A set of missing information is identified the course of developing physicochemical models of processes, to determine and verify the model parameters, check the
sufficiency of the mathematical description of processes, calibrate and determine the range of the model applicability, and develop pilot programs.

Figure 5. Independent calculation of the crystallizer mathematical model in the VIZART software.

Thus, detailed physical (chemical) -mathematical models of processes are necessary to:

- determine the permissible ranges of operating modes and monitored parameters;
- determine the service life of the equipment and the frequency of replacement of process units (equipment components);
- calculate weight and dimensional characteristics of the equipment or individual nodes;
- optimize the process modes;
- assess risks in emergency modes;
- describe transient modes (startup/ shutdown).

In addition, data of mathematical descriptions of the processes are used to create simplified models that are necessary when developing simulation models of process nodes with control systems (KOD TP), and to specify calculated coefficients for the balance model of the VIZART software.

4. Software complex KOD TP (Process Optimization and Diagnostics Code)

KOD TP is designed, first of all, to simulate the operation of the process circuit in order to study the performance, manageability and optimization of both individual processes, nodes and installations, and the process interfaces, as well as control and monitoring systems. In order to implement of the KOD TP, mathematical models of processes are reduced to recurrent digital ratios to enable them to be solved in real time, corrected to consider the influence of real equipment and supplemented by models of auxiliary equipment (tanks, pumps, valves, etc.), which are integral components of the chemical production. In addition, models of the control and monitoring systems of these process units are included [5], individual models are combined into complex simulation models of automated process installations and assembled into a single software package for simulating the operation of both individual production sections and the entire process circuit [6]. The calculating KOD TP being developed allows to carry out simulation modeling of the future production operation taking into account the APCS functions in real time, to ensure the delivery of test effects to the process simulation models and record their responses according to the identified variables (figure 7). Using the
calculation results obtained with the KOD TP, it is possible to reduce the number of design errors significantly when choosing regulating devices, actuators and sensors, to ensure high-quality development and pre-setting of algorithms based on a computational and not industrial experiment.

The results of calculations using the KOD TP allow to:

- coordinate of the operation of units and installations in a single process circuit for material flows and parameters (modes) of processes;
- assess the applicability of control, diagnostics and monitoring algorithms (APCS model of process nodes);
- assess changes in the output parameters of flows and products when a disturbance is introduced into the circuit and a return of processes to a stationary mode using control systems;
- train engineering and technical personnel on process control and equipment maintenance, including for emergencies and equipment failure in real time (figure 7);
- develop electronic management procedures (automated sequences of operator actions when performing process operations as per existing manuals and operating guidelines) (figure 8).

Currently, electronic procedures for the carbothermal synthesis line (CTS) have been developed in accordance with the model calculations in the KOD TP, which allowed to identify collisions in the documents (instructions and operation manuals) before installing and performing start-up and adjustment of the equipment (figure 8).

Figure 6. Computational experiments in KOD TP.
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5. Imitation (kinematic) model of production lines
The imitation model is designed to study the interconnected performance, efficiency, monitoring and controllability of production in the virtual environment under start-up, transient, and stationary conditions in the form of kinematic models with real time or advanced process visualization.

The imitation model consists of:
- 3D models of the main process equipment of the production lines, hoisting machinery and line transport equipment located indoors;
- a calculation cyclic graphs for the equipment operation with detailed information to the production units and process operations (VIZART software);
- a calculation balance model of material flows, including the composition of fissile materials flows VIZART software);
- calculation models of processes, including the APCS (KOD TP).
Design documents for equipment and detailed design documents, flow charts of production processes are generated based on the process description, as well as descriptions of production flows are provided. Information for production lines in terms of cyclograms of the equipment operation, supplied fluid, input and output flows is obtained via an integration solution from the VIZART software. As a result, a simulation model of production processes is obtained at the simulation start, taking into account the design parameters from the VIZART software and design limitations of the equipment.

In order to create a real time simulation model of the entire production process, including control and management systems, process models in the KOD TP software are supplemented with prepared visualization scenarios of process modes, including situations that go beyond the main process parameters. It allows a visual demonstration of the ongoing processes with the equipment. The KOD TP gives a start signal and transmits the necessary parameters to the visualization subsystem of the kinematic model. The visualization script is launched based on the parameters data (figure 10). All scenarios are formed with taking the criticality into account. This approach allows the simulation model in conjunction with the KOD TP to operate in real time.

Application of the simulation model:

- analysis, calculation, optimization and confirmation of the possibility:
  - to increase the performance of production lines;
  - to expand the range of processed or manufactured products;
- optimization of the number of staff;
- training the operating personnel (part of virtual simulators), including the elaboration of repair work (planned and emergency);
- simulation of emergency situations;
- development of information materials for the general public;
- development of process mode visualization scenarios for training technical personnel.
6. **The system of models and codes to justify the process safety.**

An analysis of the types of hazards at radiochemical plants shows that the safety analysis is a complex task of mathematical simulation. Most data needed for calculations to justify the safety of process facilities with existing models and codes can be obtained today from calculations of the material flows parameters using the VIZART software and mathematical models of processes. Consequently, when the process models are developed, calculations in the VIZART software package in combination with neutron-physical codes and codes for calculating the stress and the structure behavior can be used to substantiate the nuclear, radiation, fire and explosion safety technology.

In order to assess the nuclear, radiation and fire-explosion safety of processes within the framework of the Proryv PD, the mathematical models of the processes are being elaborated, with taking into account the geometry and design features of the equipment where these processes occur:

- development of gas/hydrodynamic models of multiphase systems has been started, which allows determining stagnant zones in the devices and accumulation of nuclear materials there, as well as justifying some structural features of the equipment (examples of simulating the dilution device and centrifugal extractor are given in figure 11 and figure 12);
- development of models for calculating the thermophysical process parameters has been started, with taking into account the flow heat generation, heat exchange with the fluid and reagents, and considering the device preheating;
- the radiation loads on process reagents and equipment items in the solvent device of the PDEC PM have been calculated, with a possibility of through calculations using the VIZART software and neutron-physical codes to substantiate the radiation safety demonstrated;
- there started activities on defining the criteria for igniting various process fluids and modeling processes to analyze the fire and explosion safety of the processes.

![Figure 11. Solution device. Uranile nitrate concentration field.](image-url)
In addition, a database of boundary process and equipment parameters is being developed, as well as critical characteristics of material flows in the processes.

7. Conclusion

At present, an integrated system of models and codes is being developed as part of the Proryv Project direction for consistent simulation of heterogeneous processes and phenomena that are to be taken into account when calculating and analyzing the safety of CNFC technologies. The models and codes to be developed are already used in the development of technologies for the closing interfaces of the CNFC (preparation of the source data for the design and construction of equipment). Calculation models allow detecting collisions at early stages and making changes in process, design and engineering documentation; carrying out optimization calculations in order to identifying the performance of individual nodes and the entire circuit; justify technical, design and engineering solutions, as well as evaluating the content of nuclear materials at all process, including work in progress.

Both existing and newly developed models and codes are used for the tasks of justifying the process safety of the system being developed, in order to describe processes and devices, nuclear and radiation safety, criteria for ignition, combustion, behavior of structures and engineering systems under critical loads etc.

The use of specialized codes for solving specific problems and the development of interaction interfaces between them in solving compex problems can significantly reduce the time and amount of computation and optimize the use of computing resources. The use of modern computing systems allows arranging related calculations with data exchange between various software tools - from engineering to CFD-codes, and ensuring that the complex problem of simulating the CNFC technology is solved.

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