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Research Article

Modernization of the SC-INT subchannel thermal-hydraulic code*

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Abstract

The article presents the main results of the work cycle on modernizing the source code of the SC-INT computer program designed for subchannel thermal-hydraulic calculations of the water-cooled nuclear reactors cores. The mathematical description of the program is briefly provided, including the method of allocation of control volumes in space, the discrete analog of the basic conservation laws forming the system of nonlinear equations, as well as the method of its solution. The path passed on the internal modernization of the program is described in detail: ejection of outdated Fortran programming language constructions, transition to structure-oriented approach of writing source code, development of modular architecture, as well as implementation of the alternative numerical algorithm for solving the main system of nonlinear equations using the PETSc library. As an example of the SC-INT program capabilities, which appeared after the above described modernizations, the results of thermal-hydraulic calculation in fine-mesh subchannel approximation of a full-scale VVER-1000 reactor core are presented. The core under consideration is assembled from fuel assemblies of different designs: with and without installed «Vikhr» and «Progonka» type intensifier grids. It is demonstrated that the residuals on the main coolant parameters achieved in the simulation of the full-scale core match in order with the corresponding values characteristic for calculations of small-scale experimental fuel assembly models. Thermal-hydraulic calculations of full-scale cores in the subchannel approximation opens the possibility for development of coupled program complexes designed for improved estimation of the parameters of multiphysics processes in the cores of water-cooled nuclear reactors.

Keywords

control volume method, core, software architecture, subchannel analysis, thermal-hydraulic calculation, VVER

Introduction

Throughout the history of nuclear energy development, there has been continuous improvement of programs used for modeling of multiphysics processes in nuclear reactors. Despite the low popularity of the Fortran programming language in the field of commercial software development, this programming language is the main tool for developing new and supporting existing programs for high-performance computing in the academic environment, as well as in

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various industrial sectors. It is worth noting that the ongoing modernization of this class of programs over time can in most cases be classified as external changes that expand the provided functionality (for example, by adding new physical models), rather than as internal changes that affect exclusively the source code architecture. As a result, the software architecture may not correspond to modern programming practices adopted in commercial software development.

This article presents the results of the cycle of works carried out by specialists from the Department of Thermalphysical Research of the National Research Center «Kurchatov Institute» since 2020 to modernize the source code of the SC-INT program in the Fortran. The SC-INT program (rights holder JSC «TVEL») is designed for performing steady-state subchannel thermal-hydraulic calculations of the cores of water-cooled nuclear reactors. The SC-INT program is a development of the SC-1 program (Oleksyuk 2002): the main direction of modernization was to expand the scope of physical application of the program by adding models that take into account the influence of installed heat and mass transfer intensifier grids on coolant parameters (Kobzar et. al 2015). In 2023, the procedure of the certification of the SC-INT program in Rostekhnadzor was successfully completed (Attestation certificate 2023).

However, this article focuses not on substantiating the scope of physical application of the SC-INT program, but on significant changes in the internal structure of the source code, that led to the speedup of the program, as well as the convenience of its use as a research tool by specialists who are not the main developers of the program. The first part of the article is devoted to the mathematical description of the program, then the chronology of the modernization of its source code is presented, and finally, the results of calculation of a demonstration problem, which is VVER-1000 reactor full-scale mixed core, are presented.

The results of the cycle of works presented in this article were obtained within the framework of the contract with JSC «TVEL».

General description of the SC-INT program

The SC-INT program is based on a one-fluid model, according to which conservation laws are considered not for each phase separately (liquid, gaseous, etc.), but for some homogenized fluid, the characteristics of which depend on the mass and volume fractions of each phase. Equations for modeling the behavior of two-phase coolant in the one-fluid model are obtained based on the combination of conservation equations written separately for each phase (Butterworth and Hewitt 1977), which, in particular, are presented in the approximation of phase pressure equality in (Avramova and Salko 2016). When combining and further discretizing the differential equations written in the two-fluid model, we naturally obtain quantities that characterize the flow and parameters of the homogenized fluid.

The mathematical model of the SC-INT program has the following assumptions.

1. Only steady-state flows are considered.
2. The exchange of energy and momentum between neighboring control volumes caused by turbulent pulsations is calculated using a standard approach for subchannel programs, described, in particular, in the review work (Liuet. al 2020). According to this approach, a turbulent diffusion coefficient is introduced as the ratio of the average amplitude of fluctuations of transverse mass velocity to the average mass velocity in the axial direction. Empirical correlations depending on the geometric characteristics of rod bundles are used to calculate this coefficient.
3. Turbulent shear stresses are not calculated directly.
4. Viscous friction at liquid-liquid boundaries is not calculated directly.

The control volume method is used to discretize the original system of differential equations – in the transverse direction, the computational domain is divided into subchannels, in the axial direction – into layers. The intersections of subchannels and axial layers create a set of control volumes. Fig. 1 shows a three-dimensional image of two neighboring control volumes, located in the j-th axial layer and having subchannel indices i and ik (the index ik denotes a subchannel that is a neighbor to the i-th subchannel through its k-th hydraulic connection).

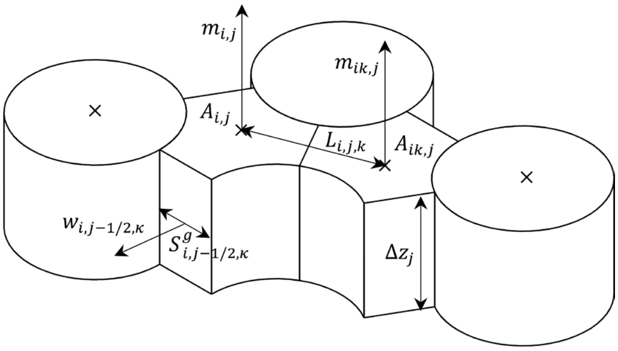

Figure 1. Two adjacent regular control volumes: A is the cross-sectional area, m^2; Δz is the height of axial layer, m; L is the center-to-center distance, m; m is the mass flow rate in the axial direction, kg/s; S^g is the interrod gap, m; w is convective transverse mass flow rate per unite length, kg/(ms).

As a result of integrating the differential equations over the introduced control volumes, the following system of nonlinear equations is obtained.

Discrete analog of the mass conservation equation:

$$m_{i,j} - m_{i,j-1} + \Delta z_j \cdot \sum_{k=1}^{N_k^i} w_{i,j-1/2,k} = 0 \qquad (1)$$

Discrete analog of the energy conservation equation:

$$\begin{gathered}
[m \cdot h]_{i,j} - [m \cdot h]_{i,j-1} + \Delta z_j \cdot \sum_{k=1}^{N_k^i} [w \cdot h]_{i,j-1/2,k} = \\
\Delta z_j \cdot \sum_{r=1}^{N_r^i} q^l_{i,j-1/2,r} + \Delta z_j \cdot \sum_{w=1}^{N_w^i} L_{i,j-1/2,w} \cdot \tilde{R}_{i,j-1/2,w} \cdot \left(T_{iw,j-1/2} - T_{i,j-1/2}\right) + \\
\Delta z_j \cdot \sum_{k=1}^{N_k^i} \lambda_{i,j-1/2,k} \cdot S^g_{i,j-1/2,k} \cdot \frac{T_{ik,j-1/2} - T_{i,j-1/2}}{L_{i,j-1/2,k}} + \\
\Delta z_j \cdot \sum_{k=1}^{N_k^i} w^T_{i,j-1/2,k} \cdot \left(h_{ik,j-1/2} - h_{i,j-1/2}\right)
\end{gathered} \tag{2}$$

where h is the specific enthalpy, J/kg; λ is the thermal conductivity coefficient, W/(m·K); q^l is the linear heat rate, W/m; $\tilde{R}$ is the averaged heat transfer coefficient through an unheated wall located between two control volumes, W/(m^2·K); T is temperature, K; w^T is the turbulent transverse mass flow rate per unit length, kg/(m·s).

In the right-hand side of equation (2), the terms respectively account for the energy generation from fuel rods, energy exchange through an unheated heat-conducting wall, energy exchange due to thermal conductivity and turbulent transverse mass flow rates.

Discrete analog of the axial momentum equation:

$$\begin{gathered}
\left[\frac{m^2 \cdot v}{A}\right]_{i,j} - \left[\frac{m^2 \cdot v}{A}\right]_{i,j-1} + \Delta z_j \cdot \sum_{k=1}^{N_k^i} \left[w \cdot \frac{m \cdot v}{A}\right]_{i,j-1/2,k} = \\
-V_{i,j} \cdot g \cdot \rho_{i,j-1/2} - V_{i,j} \cdot \frac{p_{i,j} - p_{i,j-1}}{\Delta z_j} - \\
V_{i,j} \cdot \left(\left[\frac{\lambda_f}{d_{hy}}\right]_{i,j-1/2} + \frac{\xi^{loc}_{i,j-1/2}}{\Delta z_j}\right) \cdot \frac{1}{2} \cdot \left[\frac{m^2 \cdot v}{A^2}\right]_{i,j-1/2} + \\
\Delta z_j \cdot \sum_{k=1}^{N_k^i} K^T \cdot w^T_{i,j-1/2,k} \cdot \left(\left[\frac{m \cdot v}{A}\right]_{ik,j-1/2} - \left[\frac{m \cdot v}{A}\right]_{i,j-1/2}\right)
\end{gathered} \tag{3}$$

where d_{hy} is the hydraulic diameter, m; λ_f is the friction factor, relative units; K^T is an empirical coefficient responsible for the similarity of turbulent exchange of momentum and energy, relative units (in the article, it is taken equal to1.0); p is the pressure, Pa; v is the specific volume, m^3/kg; ξ^{loc} is the local resistance coefficient, relative units.

In the right-hand side of equation (3), the terms respectively account for the action of the gravitational force, the force caused by the pressure gradient, losses due to friction and local resistances, as well as the exchange of momentum due to turbulent transverse mass flow rates.

Discrete analog of the transverse momentum equation, obtained as a result of integration over control volumes of transverse hydraulic connections:

$$\begin{gathered}
\left[L \cdot w \cdot \frac{m \cdot v}{A}\right]_{i,j,k} - \left[L \cdot w \cdot \frac{m \cdot v}{A}\right]_{i,j-1,k} = \\
-V_{i,j,k} \cdot \frac{p_{ik,j-1/2} - p_{i,j-1/2}}{L_{i,j-1/2,k}} - \\
V_{i,j,k} \cdot \frac{\xi^w_{i,j-1/2,k}}{L_{i,j-1/2,k}} \cdot \frac{1}{2} \cdot \left[\frac{w \cdot |w| \cdot v}{\left(S^g\right)^2}\right]_{i,j-1/2,k}
\end{gathered} \tag{4}$$

where ξ^w is the resistance coefficient to transverse flow, relative units.

Numerical solution algorithm of the SC-INT program

The resulting system of equations (1)–(4) is nonlinear with respect to the vector of unknowns, consisting of axial mass flow rate, enthalpy, pressure, as well as transverse convective mass flow rate. It is worth noting that the above system of equations contains values of the main variables in intermediate nodes relative to the main computational grid. These values are determined using the appropriate interpolation schemes in the SC-INT program.

The necessary geometric characteristics A, S^g, d_{hy}, L, Δz are set by the program user in the input file.

To close the above-described system of equations, expressions are needed for determining the thermophysical properties of the coolant, friction factors, resistance coefficients, turbulent transverse mass flow rates, heat transfer coefficients, etc. A comparison of sets of empirical correlations used in various Russian subchannel programs, including SC-INT, for calculating the closure relations is presented in article (Vertikov et. al 2025).

The presented system of nonlinear equations in the SC-INT program is solved iteratively. On each iteration, the unknown quantities are sequentially found for each axial layer. When moving to the next axial layer, turbulent transverse mass flow rates are calculated according to the corresponding correlations. Next, a system of linear equations is solved to find the distribution of coolant enthalpies within this axial layer. After that, for each control volume within this axial layer, the thermophysical properties of the coolant are updated, and other closure relations are calculated. The next step is solving the linear equations system to find convective transverse mass flow rates. This system is obtained by combining the continuity equation (1) and the momentum equations (3)–(4). Next, the values of axial mass flow rates are corrected. The final step is correcting the pressure drops in the transverse direction on the previous axial layer.

For the convergence of the outer iteration cycle, conditions on the residuals of enthalpy, axial mass flow rate, and transverse convective mass flow rate must be met. In future versions of the SC-INT program, it is planned to add the ability to track changes during iterations of user-specified quantities – thermal engineering margins, local coolant parameters at a specific point of the calculation model, etc.

As options for solving the linear systems, there is either the iterative Gauss-Seidel algorithm, historically implemented in the SC-1 and SC-INT programs, or an algorithm using the PETSc library (Balay 2023), which compared to the original one has the following advantages:

- allows performing calculations with non-uniform axial meshing;
- allows performing calculations with an increased maximum allowable number of hydraulic connections for a subchannel up to six;

- shows better convergence speed and stability when performing calculations of large fragments of cores (a cluster of seven adjacent fuel assemblies, a 60-degree symmetry sector).

Development of a modular architecture for the SC-INT program

The previous sections provided a brief mathematical description of the SC-INT program and the numerical algorithm used to solve the main system of nonlinear equations. The cycle of works performed by the authors of the article pursued the following goals:

- speedup in performing both multivariant validation calculations and calculations of large-scale fragments of nuclear reactors cores;
- increasing the speed and convenience of further program modification during research work (implementation of new correlations for calculating closure relations or alternative numerical algorithms).

At the first stage of this cycle of works, the use of «common blocks» was abandoned by transferring the corresponding variables to a single module. However, it is worth noting that this change was purely «cosmetic», nothing changed in terms of the presence of global state in the program– individual subroutines and functions still worked with a single set of global variables that could be modified anywhere and at any time. The presence of global state is, from a modern perspective, an example of bad software architecture, since it prevents either the compiler or the developer from dividing the program into a finite number of separate entities capable of performing a specific, intended functionality in isolation. In the first case (from the compiler's point of view), this leads to the inability to use some optimizing properties. In the second case (from the software developer's point of view), this leads to the already mentioned difficulties in modernization and testing of the program.

The second stage of source code modification involved more significant changes compared to the above, namely, the transition to a structure-oriented approach and a modular architecture of the SC-INT program. For this reason, the following steps were taken during the preliminary stage. Firstly, the Git version control system was connected, and the version of the SC-INT program at the current stage was designated as «v1.0». Secondly, a test suite covering a significant part of the functionality of the SC-INT program was developed. It included verification and validation tests (more about validation of subchannel programs is written in work (Oleksyuk and Vertikov 2025; Vertikov et. al 2025)), as well as research and design problems performed in the past using older versions of the SC-INT and SC-1 programs.

The rejection of the global state involved several stages. Initially, the approximate program call tree was searched for so-called «leaves», i.e. program units from which no other subroutines or functions are called. In the SC-INT program, such «leaves» were functions for calculating closure relations according to specific empirical correlations. The source code of these functions was modernized to meet the criteria of the so-called purity (the keyword «pure» in the Fortran). Pure functions must be deterministic, i.e. obtain the same results when receiving the same arguments and not have side effects, which include modification of global variables, input and output operations, etc. At the same time, the language constructs of the Fortran-77 standard, which were declared obsolete in newer standards (90/95 and 2003), were being phased out. Further, based on the developed functions, data structures were designed for convenient exchange of information between different program units.

At the next stages, the above procedure was applied not to the «leaves» of the tree, but to the «branches» on which they are located, and so on to the «root», which is the main program. At each stage, the data structures were adapted, which required adjusting the code developed earlier.

The second stage was completed with the release of version «v1.3». The developed modular architecture made it possible to perform multivariant calculations in parallel mode, in particular, when conducting validation, to calculate various experimental states in parallel.

As a demonstration of the acceleration achieved, the calculation times for 167 experimental states in which a departure from nucleate boiling was recorded on the 37CT-1.3-BASE experimental model (Kobzar and Oleksyuk 2019) are presented below for two versions of the program. In both versions of the program, the value of 0.1% was adopted as the convergence criterion for the outer iteration cycle for transverse convective mass flow rate. In single-threaded mode, the time for version «v1.0» was ~260 seconds, and for «v1.3» ~125 seconds. For version «v1.3» in multi-threaded mode, the times were 70, 45 and 30 seconds for 2, 4 and 8 threads, respectively. Calculations were performed on a personal computer with an «Intel Core i5-10600KF» processor.

As can be seen from the presented times, there are deviations from the «ideal» scenario, in which using N threads leads to an N-fold acceleration of the program's operation. This deviation is due to the fact that the parallel program region is exclusively the one within which the main system of nonlinear equations is solved, while the region for reading data from the program's input file, and, most importantly for the problem under consideration, the region for writing calculation results to the output file, operate in single-threaded mode. In the considered variant, the total amount of time spent by the program on writing calculation results is approximately 10 seconds. Taking this time into account leads to an approximately sixfold acceleration when using eight threads compared to the initial fourfold one.

The third stage of the SC-INT program modernization involved the implementation of a module for solving the main system of nonlinear equations using the PETSc library, which provides a wide range of methods for solving systems of linear algebraic equations and preconditioners. The main reason for the need to develop an alternative numerical algorithm was its unsatisfactory convergence speed in problems with large spatial dimensions (60-degree symmetry sectors and full-scale cores of VVER-type reactors). For example, the mesh of a full-scale VVER-1000 reactor core consists of 107,580 subchannels through which coolant flows, directly involved in the effective cooling of fuel rods. Moreover, this number can be increased by adding subchannels that model coolant leaks between the peripheral row of fuel assemblies and the reactor baffle, as well as leaks through guide and instrumentation tubes. In the axial direction, usually from 60 to 100 layers are allocated. Thus, the total number of control volumes of the main computational grid in such problems is on the order of 10^7. The version of the SC-INT program, in which the numerical algorithm using the PETSc library was first implemented, was named «v2.0».

Demonstration calculation of VVER-1000 reactor full-scale core

The test problem, the calculation results of which are presented to demonstrate the capabilities of the SC-INT program for simulating coolant flow within large-scale core fragments, is the core of the VVER-1000 reactor of Unit 4 of the Balakovo NPP at the initial moment of the 18th fuel campaign. This campaign is characterized by the fact that fuel assemblies of various designs are located within the core.

The per-assembly cartogram of the core is presented in Fig. 2. In this figure, for each assembly, its number, relative inlet flow rate in accordance with the CFD calculation (modeling of the non-uniformity of

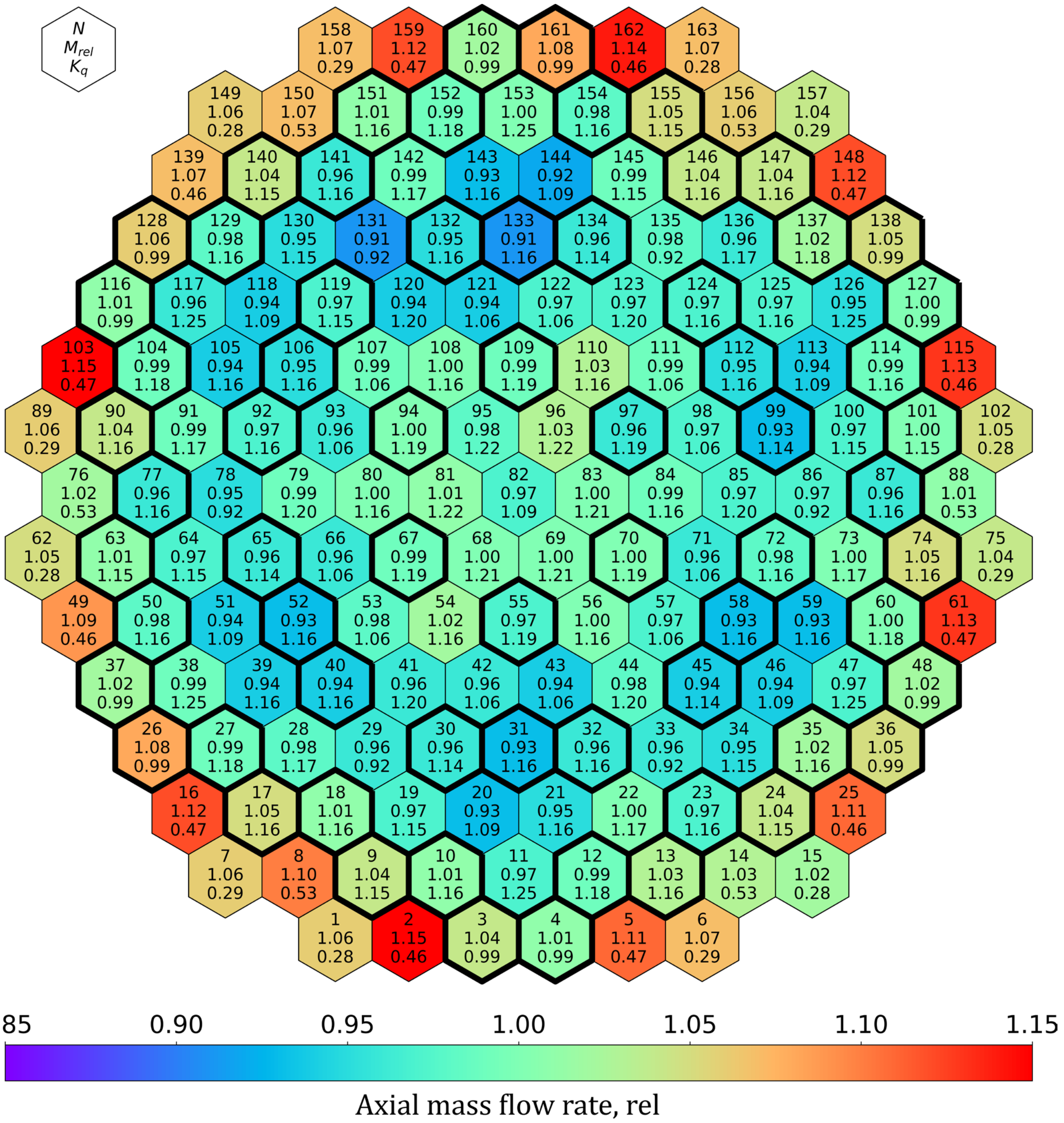

Figure 2. Cartogram of the VVER-1000 reactor core of the fourth power unit of the Balakovo NPP at the initial moment of the 18th fuel campaign.

coolant flow distribution at the core inlet is carried out, in particular, in work (Krapivtsev and Solonin 2021)), as well as its relative power in accordance with the neutron-physical calculation using the KASKAD software suite (Lizorkin et. al 2015) are marked. Also on this cartogram, the TVS-2M with installed «Vikhr» and «Progonka» type heat and mass transfer intensifier grids designed by OKB «GIDROPRESS» (Perepelitsa 2020) are marked with bold boundaries. All assemblies of this type are fresh.

The problem under consideration is characterized by the presence of significant convective transverse flows due to the presence of inlet non-uniformity in the flow distribution and hydraulically unequal fuel assemblies.

The calculations were performed using the reactor's nominal operating parameters. Realistic fuel-pin power density profiles obtained from the KASKAD software suite were used. The calculation model is divided axially into 60 layers, which matches the level of detail of the fuel-pin axial power density profiles.

To demonstrate the effectiveness of the numerical algorithm implemented in the third stage of the program modernization, two calculations were performed: using an algorithm based on the PETSc library and using an algorithm from the SC-1 program.

Fig. 3 shows for both calculations the changes in the process of the external iteration cycle, which ended upon reaching the specified maximum permissible number of iterations of 2500, the values of the three main residuals – enthalpy, axial flow rate and transverse convective flows. As can be seen from this figure, the implemented numerical algorithm demonstrates a significantly improved convergence rate – the residual for transverse convective flows closely approached the corresponding value specified during the demonstration of the effectiveness of parallel calculations on small-rod fuel assembly models. The following PETSc library options were used: the «conjugate residuals method» was used for solving the linear equations system, and the «successive over relaxation preconditioning» served as the preconditioner. The PETSc calculation was run on the personal computer described above, taking approximately 12 hours.

It's worth noting that a set of similar problems, such as fuel cycle moments, can also be solved in parallel using SC-INT. However, in this case, it's important to keep in mind that the main limitation in solving large-scale linear system equations is not the processor frequency, but the RAM bandwidth. Therefore, if the bandwidth is insufficient, running multiple large-scale fragment calculations in parallel may slow down the calculation.

Fig. 4 shows the axial dependences of the average coolant flow rate for seven fuel assemblies arranged in a horizontal row (see Fig. 2). In the lower part of the core, the leveling of the inlet non-uniformity is observed, and in the upper part of the core – the consequence of the presence of intensifier grids in some assemblies. This image demonstrates the complexity of the thermal-hydraulic processes occurring in the core, for the correct modeling of which the SC-INT program can be used after the modernization.

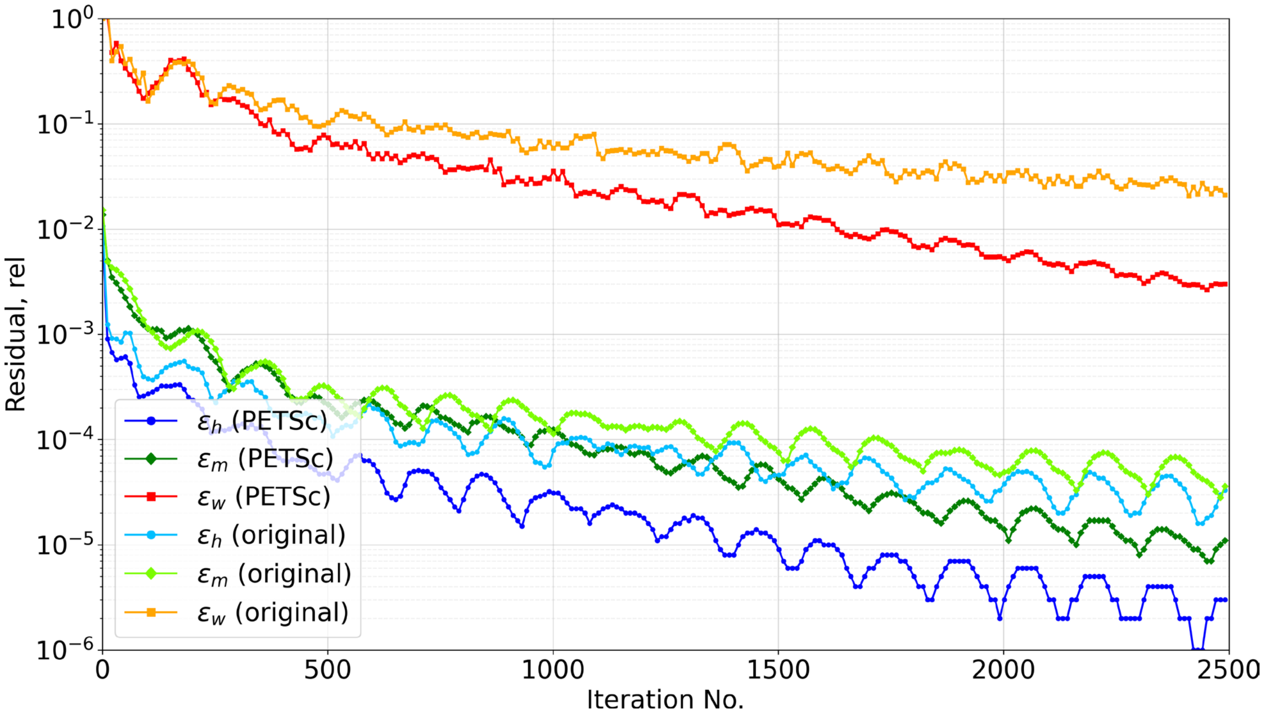

Figure 3. Change in residual values during the external iteration cycle.

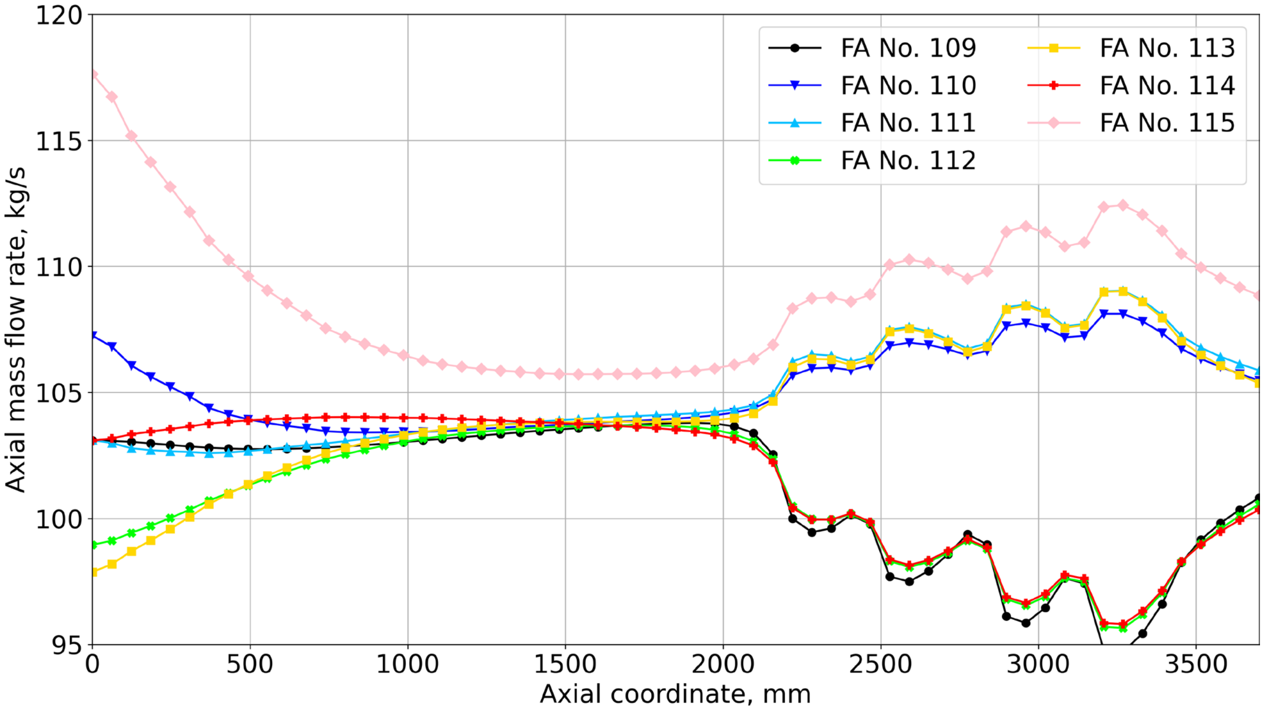

Figure 4. Dependence of the average coolant flow rate over the fuel assembly on the axial coordinate.

Conclusion

The modernization of the subchannel thermal-hydraulic program SC-INT described in the article allowed simultaneously increasing the convenience of working with the source code and improving the performance of the program as a whole. As a result of the completed cycle of works, the transition to a structure-oriented approach was made, a modular software architecture was developed and implemented, and the outdated Fortran constructs were abandoned.

The achieved convenience of working with the source code will accelerate further modernization of the program, for example, the implementation of the ability to calculate dynamic processes or the implementation of a two-fluid model for more precise modeling of two-phase flow. Moreover, already at this stage, specialists who are not the main developers of the program can effectively modernize individual sections of the source code within the framework of research work, for example, when implementing mechanistic models of heat transfer crisis (Zubkov et. al 2025).

The ability to perform thermal-hydraulic calculations of full-scale cores of water-cooled nuclear reactors, achieved using a numerical algorithm based on the PETSc library, makes it possible to obtain a realistic coolant flow parameters and the corresponding distribution of thermal margins. In the future, based on the results of modeling full-scale cores, it is possible to develop a methodology for substantiating thermal engineering reliability with a significantly smaller number of assumptions and with significantly more scope for justified reduction of conservatism compared to the approaches currently used. Also, the results of such calculations can be used to interpret the readings of thermocouples of the in-reactor control system. For further increasing the performance of the SC-INT program when modeling large-scale fragments of cores, the implementation of a numerical algorithm that allows performing a single calculation in parallel mode is necessary.

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