SKETCH-N/ATHLET coupled calculations using the boundary conditions plugin

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Abstract. The paper describes recent developments in the multi-physics coupling scheme between the SKETCH-N nodal neutronics code and the best-estimate thermohydraulic code ATHLET v3.2. The boundary conditions plugin was implemented. The verification and validation were performed using the transient of the Kalinin-3 international Benchmark. The simulation results using the boundary conditions plugin show good agreement with experimental data and calculations performed by using SKETCH-N/ATHLET direct calculations. The calculations of the transient "Switch off of one MCP (Main Coolant Pump) at nominal power" is performed applying a simple core thermohydraulic model without taking into account inter-channel mass transfer.

1. Introduction
The development of multi-physics coupling between neutronics and thermohydraulic codes began already at the end of the last century. Since the computing power at that time was limited, such codes could not provide higher level of nodalization and precision. At present, coupled calculations are very widespread and allow user to prepare highly accurate modelling for almost all types of nuclear reactors and nuclear power plants [1–11]. The main idea of coupled calculations is to conduct modelling as accurate as possible, considering the largest possible number of phenomena, while keeping an acceptable computation time [12]. Active work is underway on the definition and resolution of multi-physical benchmarks [13 – 15] and the creation of the high-fidelity fast neutronics pin-by-pin codes [16].

However, if the certain data given, many calculations can be simplified, for example, by replacing the modeling of the primary or secondary reactor loop with the boundary conditions. When solving such problems, it is often necessary to specify tables with a large amount of data as the boundary conditions, which is problematic to transfer to the ATHLET input file. For this kind of simplifications, it was decided to develop a boundary conditions plugin that allows transferring data from tables written in text files directly to the ATHLET variables.

To verify the correctness of usage of the boundary conditions plugin, the international Kalinin-3 benchmark problem was chosen [14]. The experiment described in this benchmark is an asymmetric process of shutting down one (of the four) MCP at nominal power. The experimental data described in the benchmark allow validating the coupled simulation result. Since previous work [17] related to the
creation of the SKETCH-N/ATHLET coupled scheme deals with the same problem, the calculation results can also be verified with previous coupled solution.

2. Used codes

2.1. SKETCH-N
SKETCH-N [17], as the further development of the finite-difference code SKETCH, is designed to solve the diffusion equation in Cartesian [18, 19] and hexagonal [20] geometries for one-, two- or three-dimensional models with an arbitrary number of neutron energy groups and groups of delayed neutrons. For spatial discretization in Cartesian geometry, polynomial, semi-analytical and analytical nodal methods with a quadratic representation of transverse leakage can be used. The grid mesh for Cartesian coordinates is arbitrary. For hexagonal geometry, a polynomial nodal method is developed based on the conformal mapping of a hexagon into a rectangle.

The program has the interface subroutine based on the PVM (Parallel Virtual Machine) library can be used to link the program to external thermal-hydraulic system codes such as TRAC. SKETCH-N also has its own thermohydraulic module SKAZKA.

2.1.1. Cross-section library. The macro- and micro cross sections obtained by the UNK [21] calculations depend on the state variables of the fuel assembly. The SUBSET-XS [22] program is used to perform an approximation on these cross-sections using the combination of multidimensional polynomials and spline on burnup. The significant terms for a given accuracy are selected from an array of multidimensional polynomials automatically by the program.

The applied library of neutron-physical characteristics of the different types of fuel assemblies depends on the following parameters:

- fuel burnup: 0 – 60 MWday/kgHM (Heavy Metal);
- coolant density: 0.4 – 1 g/cm3;
- coolant temperature: 293 – 600 K;
- fuel temperature: 293 – 1800 K;
- boric acid concentration: 0 – 3 000 ppm.

2.2. ATHLET
ATHLET (Analysis of THermal-hydraulics of LEaks and Transients) [23] – thermohydraulic best-estimate code developed by the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) for the analysis of operational conditions, abnormal transients and all kinds of leaks and breaks in nuclear power plants. The ATHLET v2.1A code is certified in Russia for carrying out calculations of stationary and transient modes in water cooled reactors [24]. In the past, ATHLET was already successfully coupled with several other neutronics codes [3, 25 – 26]. The code gives the possibility to calculate the whole spectrum of design basis and beyond design basis accidents (without core degradation) for PWRs, BWRs, SMRs and future Gen IV reactors.

3. Plugin description
As mentioned above, the boundary conditions plugin for the SKETCH-N/ATHLET coupled codes was created to simplify the computational models when the necessary data is available. A schematic description of the plugin logic is shown in Figure 1.
As can be seen from the figure, the plugin works as follows: the required data is read, then the special GCSM signals in ATHLET are accessed, which allow controlling the processes and variables in the thermohydraulic code. Data from the text file is transferred directly to the GCSM signal values. The procedure for accessing and transferring data is performed at each time step of the calculation, giving the values of the boundary conditions for the thermohydraulic code as part of the coupled codes.

In this work, the Kalinin-3 benchmark was calculated. Boundary conditions in the form of temporary tables were taken on the basis of previous calculations [13] and represent a text file with the conventional names of the signals and the time distribution of the value corresponding to this signal.

4. Models

4.1. Neutronic model
The neutronic model consisted of 163 fuel assemblies corresponding to the fuel assemblies installed in the reactor. The core loading of the reactor is presented in [17]. Each fuel assembly in the model was split by 24 axial layers, including the upper and lower reflectors. The thermal power was calculated in 20 height layers and, before transferring information from SKETCH-N to ATHLET, they were recalculated to the capacities in 10 axial layers. The side reflector of the core was also taken into account in the model.

4.2. Thermohydraulic model
The thermodynamic computational model consisted of 163 channels connected from above through an ATHLET branch object in which a constant pressure was maintained. At the inlet to each fuel assembly, using a plugin, the pressure, flow rate and temperature corresponding to the given fuel assembly were given as boundary conditions. A schematic representation of the model in ATHLET code is shown in Figure 2.
Figure 2. Schematic representation of the ATHLET model.

Also, as can be seen from the figure, heat conduction volumes were specified in each channel, corresponding to the gas gap in the centre of the fuel element, the fuel pellet, and the fuel element cladding. It was taken into account that each fuel assembly has 312 fuel elements. In contrast to the previous work, convective mass transfer between fuel assemblies was not taken into account in the thermohydraulic model.

5. Results

The results of comparing the distribution of the power release at the beginning of the process described in the Kalinin-3 benchmark are presented in Figure 3. Each picture represents the distribution of the calculated Kq deviation from the experimental values in percent.

Similarly, Figure 4 shows the deviations of the calculated Kq values from the experimental ones at the end of the process.

As can be seen from the figures, at the beginning of the process, Kq differ only in an overloaded fuel assembly; an assumption based on these differences was made in [17]. At the end of the process, the errors in calculating Kq increase with the presence of the plugin by approximately 1% in some fuel assemblies.
Figure 3. Relative deviation of $K_\alpha$ (Calculation vs Experiment), at the beginning of the process %: (a) – SKETCH-N/ATHLET calculation without plugin, (b) – SKETCH-N/ATHLET calculation with plugin.

Figure 4. Relative deviation of $K_\alpha$ (Calculation vs Experiment), at the end of the process %: (a) – SKETCH-N/ATHLET calculation without plugin, (b) – SKETCH-N/ATHLET calculation with plugin.

Figures 5 and 6 show the number of nodes depending on the $K_\nu$ relative error from the experimental data and SKETCH-N/SKAZKA calculations at the beginning and the end of the process using the boundary conditions plugin and without using it respectively.
Figure 5. The number of nodes depending on the Kv relative error from the experimental data and SKETCH-N/SKAZKA calculations (Using the boundary conditions plugin): (a) – at the beginning of the process, (b) – at the end of the process.

Figure 6. The number of nodes depending on the Kv relative error from the experimental data and SKETCH-N/SKAZKA calculations (Without the boundary conditions plugin usage): (a) – at the beginning of the process, (b) – at the end of the process.

As can be seen from the Figures 5 and 6, when using the boundary conditions plugin, the number of nodes with the higher Kv relative difference values decreased, which indicates that the average Kv error also decreased for both SKETCH-N/SKAZKA and experimental data comparisons. Also Kv relative differences smaller in comparison with the SKETCH-N/SKAZKA calculations because of SKAZKA takes the same boundary conditions data as an input data for the plugin.

6. Conclusion
The work presented the results of the development of the boundary conditions plugin for a coupled SKETCH-N/ATHLET codes. The plugin allows to simplify calculation models if the necessary data is available. The results of comparing the calculations of the full-scale model of the VVER-1000 reactor in the SKETCH-N/ATHLET coupled scheme and the calculations of the simplified model in the SKETCH-N/ATHLET coupled scheme using the plugin with experimental data showed approximately similar results, which justifies the possibility of using the plugin when calculating this benchmark. It is also necessary to carry out similar tests using the plugin on other reactor experiments.
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