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ADAPTATION OF SUBCAL SUBCHANNEL CODE FOR SQUARE-LATTICE ROD BUNDLES USING PSBT BENCHMARK

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Abstract. Subchannel analysis is a commonly used approach for simulating heat transfer and coolant flow in nuclear reactor cores. This paper presents the adaptation of the SUBCAL computational code, originally developed for reactors with a triangular lattice, to configurations with a square lattice. Geometry-dependent computational relations, models and correlations were identified and analyzed based on the research. The selected relations for the square lattice were implemented into the SUBCAL code, and the computational model was optimized for the recalculation of the PSBT benchmark. Verification of the proposed changes was carried out by evaluating the results of the benchmark recalculation against experimental data and through code-to-code comparisons with results from other participating organizations. These modifications and the recalculated PSBT benchmark represent the starting point for validating the SUBCAL code for this type of analysis.

Keywords: subchannel analysis, SUBCAL, PSBT benchmark, boiling crisis, void fraction.

1. Introduction

Thermohydraulic analysis of the core is an integral part of the safety evaluation of nuclear reactors. It is performed to verify and optimize safety margins and operating limits. Accurate determination of local coolant parameters is necessary, for example, to calculate the critical heat flux, to determine the boiling crisis margin, or to predict the fuel temperature. One of the methods used to simulate heat transfer and coolant flow in the reactor core is subchannel analysis. The method of subchannel analysis was developed for the purpose of calculating the thermohydraulic parameters of the medium flowing through the rod bundle. The rod bundle is divided into a large number of interacting parallel subchannels. The required thermohydraulic parameters (e.g. flow velocity or temperature) are calculated as mean values for the subchannels through the solution of a system of differential equations describing fluid flow and heat transfer within and between them. Thus, subchannel analysis is a special type of so-called lumped parameter computational approach [1].

Computational tools employing subchannel analysis have been under development since the 1960s [2]. One such tool is the SUBCAL subchannel code [3], which is being developed and used in the Czech Republic. The development of the SUBCAL subchannel code was originally initiated by Chemcomex and is currently being continued by UJP. The SUBCAL code is used for thermohydraulic calculations of the core of VVER nuclear reactors operating in the Czech Republic. For these types of reactors, i.e. reactors with triangular rod bundle geometry, the code is approved for use by the SÚJB (Nuclear Regulatory Body of the Czech Republic). However, with the planned construction of new nuclear units in the Czech Republic, it is necessary to start taking steps to adapt, optimize and validate the SUBCAL code for calculations of PWRs with square-lattice rod bundles.

The system of differential equations of conservation laws, which underlies the subchannel analysis method, is implemented in the SUBCAL code in a general form, independent of the lattice geometry. This system of equations is complemented by computational models and correlations that ensure its solvability and simultaneously enhance the physical interpretation of the problem being solved. These are precisely the relationships that are derived either experimentally or theoretically for specific conditions and geometries. This applies, for example, to models of cross-flow resistance, critical heat flux correlations, or relationships describing frictional resistance. To demonstrate the applicability of the SUBCAL code for computations involving square-lattice rod bundles, the PSBT benchmark [4], described in Section 2, was recalculated using the code. The code modifications made and the selection of models and correlations are further described in Section 3.

2. Benchmark description

The international OECD/NRC PWR subchannel and Bundle Tests (PSBT) benchmark, based on the NUPEC experimental database, was created mainly to support the development of subchannel codes. This benchmark was chosen because it is internationally recognized, relatively easy to access, and provides one

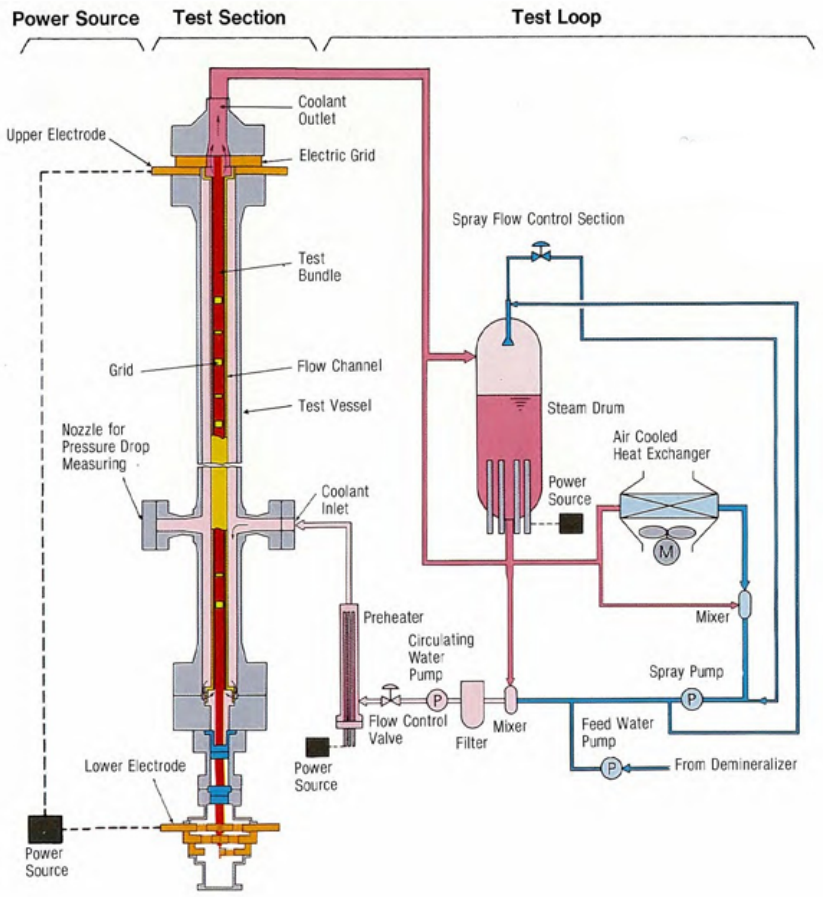

FIGURE 1. System diagram of NUPEC PWR test facility [4].

of the few opportunities to compare a large number of codes on many different experimental tasks. An advantage of this benchmark is that it uses experimental bundles rather than full-scale assemblies, making it a suitable first step for adapting SUBCAL to this type of calculation. The benchmark compares void fraction values and boiling crisis characteristics obtained from measurements at the NUPEC test facility with corresponding results calculated by participating organizations using various computational codes, including several CFD and system codes in addition to subchannel codes. The benchmark is divided into two phases, each of which includes several exercises.

Phase I – Void Distribution Benchmark

- *Exercise I-1*: steady-state single subchannel
- *Exercise I-2*: steady-state bundle
- *Exercise I-3*: transient bundle
- *Exercise I-4*: pressure drop

Phase II – DNB Benchmark

- *Exercise II-1*: steady-state fluid temperature
- *Exercise II-2*: steady-state DNB
- *Exercise II-3*: transient DNB

2.1. NUPEC TEST FACILITY

The NUPEC experimental facility is designed to be able to simulate the operating conditions of PWRs with a square fuel lattice. The design pressure is 19.2 MPa and the design temperature is 362 °C, but the range of conditions commonly used for experimental measurements is given in Table 1 below.

Quantity	Range
Pressure	4.9–16.6 MPa
Mass velocity	550–4150 $\mathrm{kg\,m^{-2}s^{-1}}$
Inlet coolant temperature	140–345 °C

TABLE 1. Range of NUPEC PWR test facility operating conditions [4].

The basic functional units of the facility are the high-pressure and high-temperature recirculation loop, the cooling loop, the instrumentation and the data recording system. As can be seen in Figure 1, the main components of the recirculation loop are the test section, the circulation pumps, the heater and the steam drum, which acts as a pressurizer. The test section can be modified to test both the coolant flow through the experimental rod bundle and through a single subchannel. The experimental rods are electrically heated.

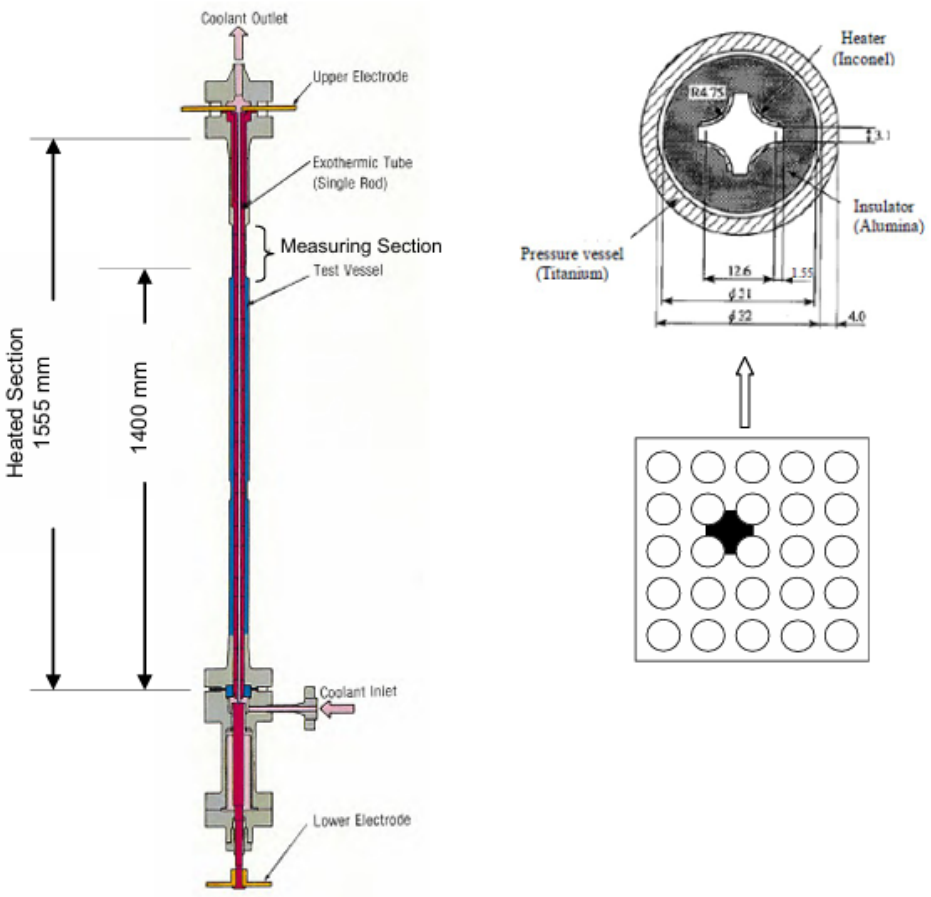

Figure 2. Test Section for central subchannel void fraction measurement [4].

2.2. Void Distribution Benchmark

In the first phase of the benchmark, the void fraction measurements were performed for the rod bundle with a square lattice and for a single subchannel. The determination of the void fraction was carried out by measuring the density in the measuring positions of the test section. The density of the flowing coolant was measured using the gamma ray attenuation method. In this method, the medium under study is located in a position between the gamma ray source and the detector. The reconstruction of the density distribution, or the void fraction, was performed using a CT scanner.

The test section of the experiment with a single subchannel was modified to measure the characteristics of the main types of subchannels – central, central with thimble, side and corner. For all modifications of the single subchannels, 1 555 mm of their length was heated and the section for measuring the void fraction was located 1 400 mm from the beginning of the heated section. The inlet nozzle controlling the coolant flow was located just below the heated section. The upward direction of the coolant flow reflects the design of PWRs. Figure 2 illustrates the modification of the test section for testing a single subchannel and the cross section through this section for the case of a central subchannel between four heated rods.

A bundle of experimental electrically heated rods with 5×5 arrangement was used to simulate the coolant flow through the fuel bundle. The total heated length of the experimental bundle was 3 658 mm. The void fraction was measured in three positions at distances of 2 216 mm, 2 669 mm and 3 177 mm from the beginning of the heated section. The coolant was fed horizontally into the pressure vessel through the inlet nozzle at the bottom of the test section. Figure 3 illustrates the modification of the test section for testing the bundle and the cross section of the test vessel.

The void fraction was measured for all four types of single subchannels in the steady state (one test series for each type). The measurement of the void fraction in the experimental bundle was carried out in both steady state and transient conditions. Different types of transients were applied: power increase, flow reduction, depressurisation, temperature increase. The resulting void fraction at each of the three measurement positions was given as the average of the values from the four central subchannels in the centre of the bundle. Three types of rod bundles were used for these measurements – the main differences were the different axial and radial power profiles. The specific design details of the bundles and the specification of the test series (specified via pressure, mass flux, power, inlet temperature) are given in reference [4].

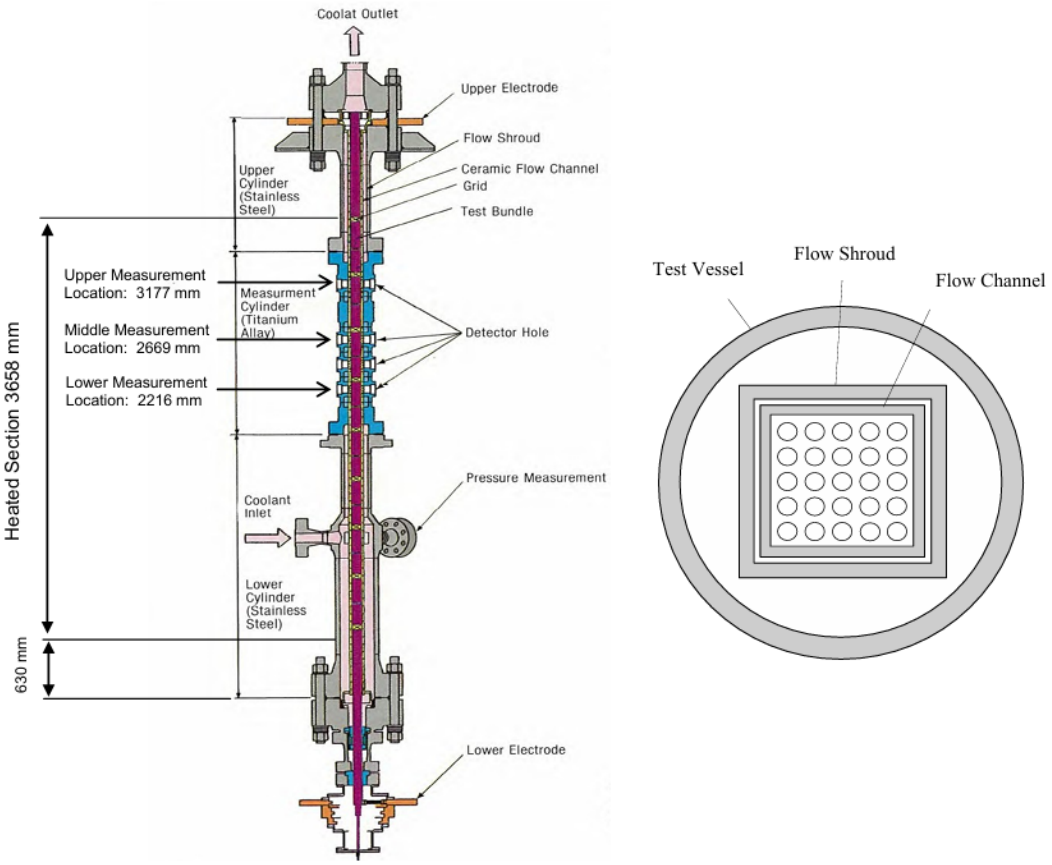

FIGURE 3. Test Section for rod bundle void fraction measurement (left); Cross-section of test vessel (right) [4].

2.3. DNB Benchmark

In the second phase of the benchmark, experiments aimed at determining the boiling crisis were performed only on rod bundles. The arrangement of these measurements corresponds to the schematics in Figure 3, and the heated bundle length was 3 658 mm. In addition to the 5×5 bundles, 6×6 rod bundles were also used to determine boiling crisis characteristics. The method of gradual increase of power was used in the measurements. The power was increased in small steps, each step being consistently monitored and recorded using thermocouples at set positions on the inner surface of the heated rods. If there was a temperature increase of more than 11 °C, the critical heat flux density was confirmed to have been reached.

DNB was investigated as well as the void fraction in steady-state and transient conditions. Under steady-state conditions, the objective was to determine the rod bundle power at which a boiling crisis would occur for given values of pressure, mass flux, and inlet temperature. For benchmarking purposes, a total of six test series were performed and evaluated under steady-state conditions using five different rod bundles. In the case of transients (power increase, flow reduction, depressurisation, temperature increase), the objective was to determine the time at which a boiling crisis occurs. Two test series were performed and evaluated under transient conditions, each on one type of bundle. The specific design details of the bundles and the specifications of the test series (specified via pressure, mass flux, power, inlet temperature) are given in reference [4].

3. Subchannel model

The development of the SUBCAL code was initially focused on the computation of fuel bundles with a triangular lattice geometry, which was reflected in the implementation of correlations and experimentally derived physical models. The recomputation of the experiments performed within the PSBT benchmark was intended to demonstrate the feasibility of using the SUBCAL code for subchannel analysis of flow in bundles with a square lattice. The computational model was developed according to the SUBCAL code user manual [5] and the PSBT benchmark specification [4].

3.1. Geometry modelling

The method of specifying the bundle geometry in SUBCAL code is very general and independent of the lattice type. All the data necessary for constructing the geometric model were obtained from the PSBT benchmark specification document [4] or could be derived from the information contained therein.

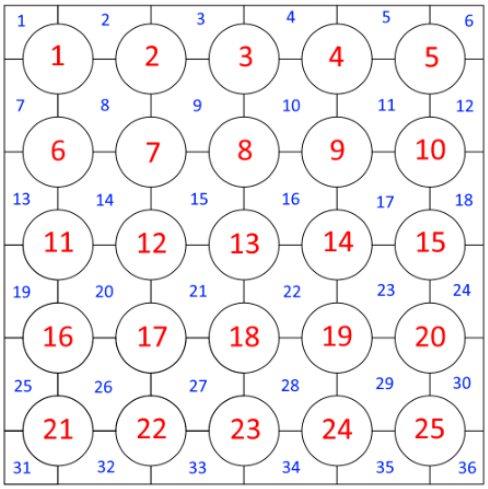

Figure 4. Schematic of 5×5 rod bundle division into subchannels (blue – subchannels; red – rods).

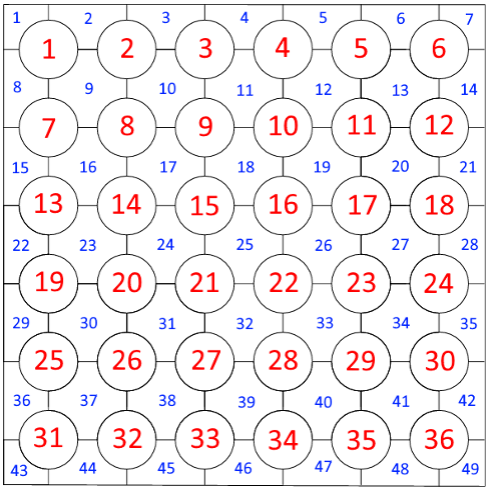

Figure 5. Schematic of 6×6 rod bundle division into subchannels (blue – subchannels; red – rods).

For the first part of the benchmark, computational models of four types of single subchannels had to be created. Since the SUBCAL computational code requires specifying at least two subchannels, each single subchannel was divided into halves and each half was specified as a separate subchannel. The two adjacent subchannels thus created were entered with half the dimensional parameters – flow area, wetted perimeter and heated perimeter. Additionally, the rods were specified in such a way that each of the adjacent subchannels contained only half the area compared to the original experimental configuration. As a result, only half the amount of coolant was heated by half the thermal power. The heated length of 1 555 mm was divided into 150 axial sections, with non-uniform axial step sizes chosen so that the output file would include a point at the 1 400 mm measurement coordinate.

The specification of geometric and power parameters for the rod bundle modelling followed the standard procedure commonly used in the SUBCAL code. Most of the rod bundles used in the benchmark measurements had 5×5 lattice configurations. As illustrated in Figure 4, the computational models of all such bundles were divided into 36 subchannels (only the basic types – central, side, corner).

One test series from the second phase of the benchmark was measured on a bundle of 6×6 rods. The model of this bundle was divided into 49 subchannels, as shown by the schematic in Figure 5.

The total heated length of 3 658 mm was the same for all bundles and was divided into 245 axial sections in the computational models. The length of the axial steps was again chosen to be non-uniform so that the desired values could be read in the output from three measuring positions with axial coordinates of 2 216 mm, 2 669 mm and 3 177 mm. The definition of spacer grids in the SUBCAL code input file is carried out by assigning point resistances (loss coefficients) at specific axial positions. Since the actual spacer grids in the experimental rod bundles are not point-like, two typical approaches are used to define the position of the resistances. Point resistances are either placed at the axial coordinate of the bottom edge of the spacer grid, or at its axial center. In this case, due to the size of the spacer grids, the option of placing the resistances at the axial centers was chosen.

3.2. Specific computational relations

Adaptation of the code to the computation of square-lattice rod bundles was implemented mainly through the choice of specific relations and models that depend on the geometry of the bundle. The selection of relations and the optimization of the computational settings were not only based on general research, but inspiration was also drawn from benchmark evaluations [6, 7]. The benchmark evaluation included a questionnaire in which some participants reported the correlations and models used for the analysis of each problem set. Some settings and model choices were taken directly from the questionnaires and documentation for the subchannel codes developed for the square geometry involved in the benchmark.

To recalculate the benchmark, the computational correlations and models that required adjustment or replacement were identified – namely the critical heat flux correlation, the cross-flow resistance model, the frictional resistance model, and the turbulent mixing coefficient. Within the SUBCAL code, certain relations could be modified directly through the input file, whereas others, which were hard-coded, required adjustment or new implementation within the source code in collaboration with the developers.

The choice of the critical heat flux correlation was a key step in the development of the computational models for the second phase benchmark exercises. In the SUBCAL code, the choice of correlation and specification of the DNBR calculation is made by the user in the input file. However, the list of commonly used

correlations from which the code user can choose is limited to correlations designed for the triangular lattice or for specific VVER reactor fuel types. It was therefore necessary to find and implement into the code a suitable, publicly available correlation used for the analysis of square-lattice rod bundles. Considering applicability, availability, and the feasibility of implementation, the EPRI correlation [8] was chosen for use in the benchmark recalculation. This correlation was also used by several benchmark participants (e.g. in the SUBCHANFLOW or MATRA code) and according to the evaluation [7], very good results were obtained with it.

In the SUBCAL code, the model implemented for calculating the friction factor is designed for a triangular lattice. This model had to be replaced in the source code. The previous model for calculating the friction factor was defined in the SUBCAL code in the single-phase region by the general relationship

$$\xi = a_1 \mathrm{Re}^{a_2} + a_3 \,, \tag{1}$$

where coefficients a_1, a_2 and a_3 are constants. Many of the models available and used in subchannel analysis have this form and differ only in the constants. For the SUBCAL code, the use of either the McAdams or Blasius correlation was considered. Both take the general form 2 and were applied by some of the benchmark participants. However, the model from the literature [9], where the constants are computed for a particular geometry, was ultimately considered more appropriate. For the rod bundles from the benchmark, the constants $a_1 = 0.153$, $a_2 = -0.18$ and $a_3 = 0.0$ were calculated and used based on the given design properties (e.g. rod diameter or rod pitch).

Cross-flow occurs between adjacent subchannels. In the SUBCAL code, the resistance to this cross-flow is given by relation

$$f = A \cdot \mathrm{Re}^B + C \,, \tag{2}$$

where coefficients A, B and C are constants entered by the user in the input file. This general relation can be applied to both triangular and square lattice. Therefore, it was proceeded to determine the coefficients according to Idelchik [10], which is common for the calculations performed by the SUBCAL code. The determination of the coefficients was carried out according to the relations for the square lattice, using the values of the geometrical parameters of the rod bundles, namely the rod pitch and diameter. The following coefficient values were calculated for the benchmark rod bundles and used in the computational model: $A = 3.151$, $B = -0.2$ and $C = 0$.

The choice of the value of the turbulent mixing coefficient was made on the basis of the information provided by the benchmark participants in the questionnaires. The coefficient values used in the subchannel codes for recalculating the benchmark exercises ranged from 0.04 to 0.06. Within this range, the effect of the coefficient on the results of each benchmark task was tested in the SUBCAL code. There was no significant effect on the void fraction values and deviations in the boiling crisis identification. The resulting turbulent mixing coefficient was set to 0.045 for recalculation of all benchmark exercises by the SUBCAL code.

4. Results

The SUBCAL computational code was used to recalculate all tasks from the PSBT benchmark with the exception of Exercise II-1. The measurements made in Exercise II-1 can be used to optimize the turbulent mixing coefficient, which was not performed due to time and resource constraints. The results of the calculations performed using the SUBCAL code were then evaluated by comparing them with experimental data obtained on the NUPEC facility. In addition, the results were also analysed against the results of the calculations performed by the other subchannel codes involved in the benchmark. The code-to-code evaluation was mainly performed according to the statistical variables, mean errors and standard deviations, introduced in the benchmark evaluation [6, 7].

4.1. The first phase – void fraction

The void fraction values were subtracted from the SUBCAL code output files in axial coordinates corresponding to the measurement positions. In the bundle exercise, the final void fraction value was obtained as the average of the values from the four central subchannels. In the diagram in Figure 4, these are the subchannels numbered 15, 16, 21 and 22. The relative error of the experimental measurement of void fraction, as declared in the benchmark specification document, is 3 %. In the result graphs, the measurement error is represented by an error band or an error bar of ±6 % of the maximum possible void fraction value.

For the first exercise, the graph in Figure 6 shows the results of all test series. The value of the void fraction in four types of separate subchannels was predicted and for each of them, one test series was performed (i.e. Test series 1 – central; Test series 2 – central with thimble; Test series 3 – side; Test series 4 – corner). The horizontal axis indicates the experimentally measured void fraction value and the vertical axis the void fraction value predicted by the SUBCAL code. It can be observed that in the region of lower values of the void fraction, the SUBCAL calculation over-predicts the results compared to the experiment. Conversely, in the higher steam content regions, the results tend to be under-predicted. In the benchmark evaluation [6] for some subchannel codes, a similar trend can be observed. However, in the case of this exercise, the results obtained by the different codes are quite heterogeneous.

For the bundles at steady-state conditions in the second exercise, the prediction of the void fraction values

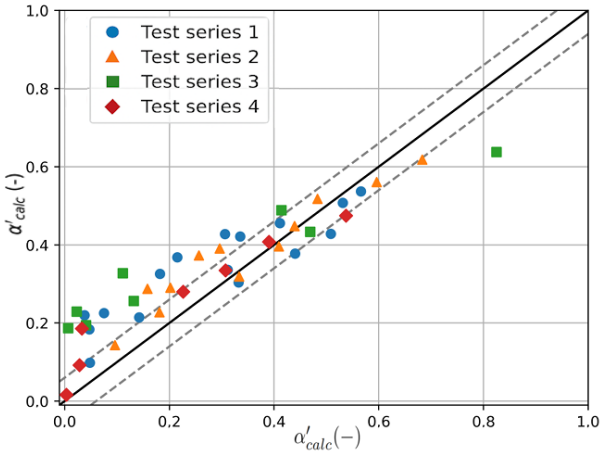

Figure 6. Void fraction determined by the SUBCAL code for a single subchannel in the steady-state.

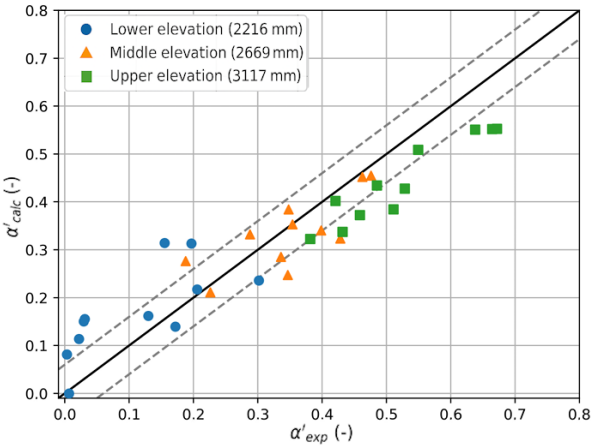

Figure 7. Void fraction determined by the SUBCAL code for the bundle in steady-state condition – test series number 8.

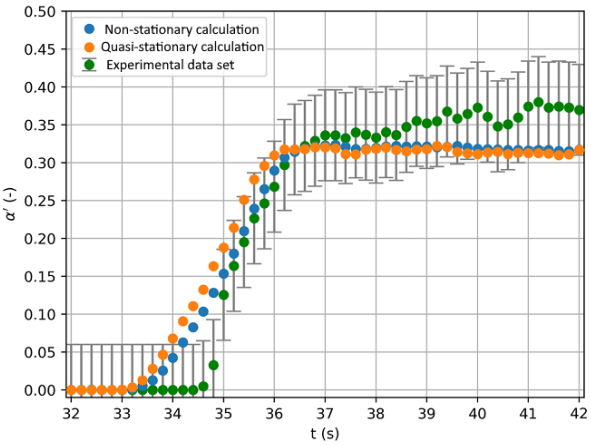

Figure 8. Void fraction for the test series 7T – power increase.

was evaluated in the same way as for the single subchannels. All available test series were recalculated with the SUBCAL code. As can also be observed in the representative graph in Figure 7 (all graphs are available in reference [11]), in the lower measurement position, where lower values of the void fraction were achieved, the results are generally rather over-predicted by the SUBCAL code in all series. The tendency to over-predict the results in the lower position was observed for most of the computational codes involved in the benchmark evaluation [6]. In contrast, in the upper measurement position, the SUBCAL results are under-predicted and differ from the experimentally measured values more than the results of other codes.

Overall, however, no cases were identified in the second exercise where the results obtained by the SUBCAL code deviated significantly from the calculations performed by the codes involved in the benchmark. This was also verified using statistical variables – mean error and standard deviation. The values of mean errors and standard deviations determined for the SUBCAL code calculations were in all test series at the level of the values obtained from the analysis of the results of the other subchannel codes in the benchmark evaluation [6].

In the third exercise, the void fraction values were analyzed during four transients – depressurisation, flow reduction, temperature increase and power increase. With the SUBCAL code, the calculations were performed in two ways, a quasi-stationary and a non-stationary approach. The void fraction was read for the upper measurement position only, because according to the benchmark evaluation [6], the experimental measurements in the lower and middle positions showed significant instabilities. The results of this exercise were processed only graphically and no statistical evaluation was performed. The graph in Figure 8 represents one of the recalculated transients. The complete results of the recalculation of the third exercise by the SUBCAL code are available as graphs in Reference [11].

From the plots of all test series, it was observed that the values calculated by the SUBCAL code and the other subchannel codes follow the general shape of the waveform of the experimentally measured data. In the illustrative example shown in Figure 8, most of the values obtained by the SUBCAL code calculation were within the error bars of the void fraction measurement. However, in the code-to-code comparison, no significant differences were observed between the calculations performed by the SUBCAL code and the subchannel codes involved in this PSBT benchmark exercise. The difference between the non-stationary and quasi-stationary calculation of transients by the SUBCAL code was almost negligible in most cases.

4.2. The second phase – DNB

In the second phase, tasks II-2 and II-3 were recalculated with the SUBCAL code. Using EPRI correlation, the power at which the first occurrence of a boiling crisis was registered was determined in Exercise II-2

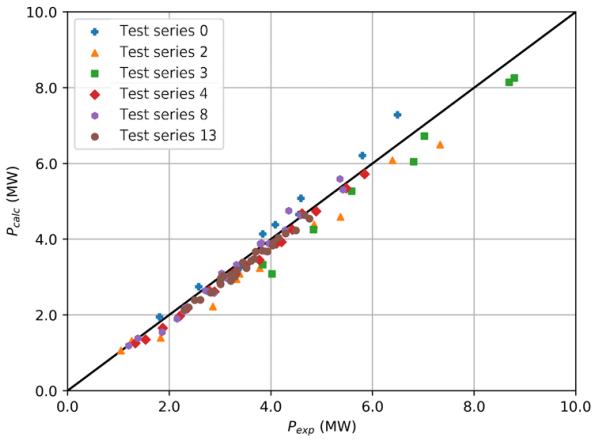

FIGURE 9. DNB prediction results for steady-states.

for the specified steady-state conditions. The determination of this power was performed for each mode by iterating the power to a DNBR value equal to one. An identical correlation was used in Exercise II-3, where the time of occurrence of the boiling crisis was determined for the transients. In this case, a standard non-stationary calculation was performed and the time step at which the DNBR value determined by the EPRI correlation reached 1.0 was identified in the output file.

A total of six test series of steady-states were experimentally measured and recalculated by the SUBCAL code to determine the power at which the boiling crisis is identified. The graph in Figure 9 shows the results of all series. Each point is assigned the power value obtained from the experimental measurements by the coordinate on the horizontal axis and the power value predicted by the SUBCAL code by the coordinate on the vertical axis. In most cases, the SUBCAL code predicted reaching a boiling crisis at a lower power than experimentally measured. Type-matched graphs are available in the second phase benchmark evaluation [7] for all codes involved. Visual comparison of these graphs with the plot in Figure 9 revealed no regimes in which the SUBCAL code's results were significantly different from those of the other subchannel codes. The values of mean error and standard deviation were also compared and it was observed that the SUBCAL code calculations are also on par with the other subchannel codes.

In Exercise II-3, two test series consisting of four transients – power increase, flow reduction, depressurization, and temperature increase – were experimentally measured and recalculated by the SUBCAL code. The results are presented in Table 2 including the mean error, with the order of the results corresponding to the order of the transients in the previous list. The largest deviation from the experimental value can be observed for the test series 12T in the case of the third process, i.e. depressurization. The boiling crisis was not reached within the specified range of the transient process, and therefore the process was extrapolated to a longer time period. The assignment of the transients corresponded to experiments in which the device was switched off after reaching the boiling crisis to avoid damage. This did not provide too much opportunity to over-predict the code results.

Test series	t_{exp} [s]	t_{calc} [s]	ME [s]
11T	106.7	106.0	**−1.8**
	52.9	51.4	
	88.8	87.1	
	140.6	137.4	
12T	86.6	87.2	**0.5**
	55.0	51.2	
	143.8	148.5	
	128.8	129.2	

TABLE 2. DNB prediction results for transients.

5. CONCLUSIONS

In connection with the planned construction of new nuclear power units in the Czech Republic, the SUBCAL code is also expected to be used for core calculations of reactors with a square lattice. Therefore, it is necessary to adapt the code to this new configuration. In addition, it must be demonstrated that the results calculated by the SUBCAL code for a square lattice meet the required standards. As part of the assessment and validation of the code for square-lattice geometry, the PSBT benchmark was recalculated. A review of the commonly used relations and models dependent on the bundle geometry was first carried out. Primarily, models found in the available literature were considered; however, in industrial applications, it is expected that for specific types of fuel assemblies, some models will be provided directly by the supplier.

The results obtained with the SUBCAL code throughout the PSBT benchmark calculations demonstrated a high level of consistency with those of other participating subchannel codes. Although the predictions for single subchannels in Exercise I-1 were less accurate, SUBCAL performed well in all exercises involving full rod bundles, which is more relevant since single subchannel cases are not typical in subchannel analysis. In steady-state and transient conditions, as well as in void fraction and boiling crisis predictions, the results were similar to those of other reliable codes focused on the square lattice. In some test series, SUBCAL was even among the most accurate. These results confirm that SUBCAL can be successfully used for square-lattice bundle calculations and meets the required standards.

For further optimization and to obtain data for validation, it will be necessary to verify the accuracy of the calculations not only on benchmark tasks but also using operational data. However, the modifications made based on the literature review during the PSBT benchmark recalculation provide an important foun-

dation for the future development of the SUBCAL code adapted to the requirements of newly introduced technologies.

List of symbols and abbreviations

f Cross-flow resistance [–]
P Power [MW]
t Time [s]
α' Void fraction [–]
ξ Friction factor [–]
Re Reynold's number
exp Experimental (subscript)
calc Calculated (subscript)
A, B, C Constants
a_1, a_2, a_3 Constants

CFD Computational Fluid Dynamics
DNB Departure from Nucleate Boiling
DNBR Departure from Nucleate Boiling Ratio
EPRI Electric Power Research Institute
ME Mean error
NRC Nuclear Regulatory Commission
NUPEC Nuclear Power Engineering Center
OECD Organisation for Economic Co-operation and Development
PSBT PWR subchannel and Bundle Tests
PWR Pressurized Water Reactor
VVER Water-Water Energetic Reactor (WWER)

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