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VALIDATION OF PWR-RELEVANT MODELS OF SUBCHANFLOW USING THE NUPEC PSBT DATA

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Abstract

At the Institute for Neutron Physics and Reactor Technology (INR) of the Karlsruhe Institute of Technology (KIT) investigations are devoted to the further development and qualification of sub-channel and system codes. A new sub-channel code named SUBCHANFLOW is being developed and validated at INR. It is a modular code programmed in Fortran-95 with dynamic memory allocation, use of SI-units and including many fluids like liquid metals and water, helium and air. The current validation work is focused on PWR relevant phenomena using the NUPEC PSBT benchmark data for void fraction and critical power. In this contribution, the main features of SUBCHANFLOW are described and the status of the validation is presented.

1. Introduction

At INR current investigations are focused on the further development and qualification of numerical design and safety tools including multidimensional thermal hydraulic codes at different scales (subchannel and fuel assembly level). After a critical review of legacy subchannel codes, it was decided to develop a modern and modular subchannel code based on the COBRA-family [1,2,3]. The new code is called SUBCHANFLOW [4]. Since the programming work is almost finished, emphasis is now put on the stepwise improvement and validation of the physical models. In addition SUBCHANFLOW is the subchannel code of choice for the coupling with deterministic and Monte Carlo neutronic codes for improved design studies and safety evaluations. This kind of research is continuously increasing worldwide. In order to ensure the prediction accuracy of such codes, it is necessary to validate it with respect to experimental results. The Karlsruhe Institute of Technology (KIT) is involved in development and validation of the SUBCHANFLOW code for the analysis of LWR and innovative reactor cores. It can be used to investigate the thermal hydraulic behavior of reactor fuel assemblies of PWR and BWR at subchannel and fuel assembly level.
An extensive validation of the BWR- and PWR-relevant models of SUBCHANFLOW was performed using the BWR BFBT Benchmark data [6] and the PWR PSBT Benchmark [7]. A large number of experiments were performed by NUPEC to investigate the pressure drop, void fraction and DNB of different PWR bundle geometries and subchannel types for different thermal hydraulic conditions i.e. mass flux, inlet subcooling, pressure and radial and axial power profiles.
In this paper, the main features of SUBCHANFLOW are presented followed by the description of the tests performed at the PSBT facility. In addition, the modeling issues to represent the numerous tests for SUBCHANFLOW simulations are outlined and the comparison of the code predictions with the measurements are presented and discussed. Finally the conclusion and further work are given.

2. Short description of the subchannel code SUBCHANFLOW

SUBCHANFLOW is a thermal hydraulic subchannel code developed for the simulation of fuel rod bundles and cores of light water and innovative reactor systems being developed at KIT/INR [4]. The code can handle both rectangular and hexagonal fuel bundles and core geometries. Both single and two phase flow conditions in reactor cores can be described solving a system of three balance equations for stationary and transient flow situations. The bases for the source code are the legacy subchannel programs COBRA-IV-I [1] and COBRA-EN [2]. Hereafter the main features of SUBCHANFLOW will be shortly described. To take profit of validated empirical correlations, the general trend to describe the two phase flow in a more mechanistic way i.e. simulating the processes on a micro-scale basis e.g. separate conservation equations for liquid droplets, films or vapor bubbles is not followed here.

2.1 Programming and Data Structure

Contrary to the old methods of data management like Fortran equivalence, swapping to hard disk and Fortran COMMON structure, SUBCHANFLOW consists of a global data structure centralized in one single Fortran module. All arrays are dynamically allocated depending on input data, which is problem specific. Physical models such as for the thermo-physical properties of the coolant and solid materials are written in separate modules. The portability of the code is assured by avoiding functions that depend on operating systems. Consequently SUBCHANFLOW can be compiled under WINDOWS, LINUX or other UNIX systems without problem. A standard Fortran 95 compiler is always required.
The input deck is designed as a text based “user interface” using comprehensive keywords and simple tables. A manifold output is created for different post processing tools e.g. to generate simple curves or more extensive three dimensional diagrams. In opposite to the majority of subchannel codes, SUBCHANFLOW uses rigorously SI units internally in all modules.

2.2 Code numerics

The numerical solver is based on the pressure difference method of COBRA-IV-I and COBRA-EN. It is a fully implicit up-wind approach without Courant time step limitation. In the numerical solution, each external iteration step proceeds axially level by level starting from the bottom. Hence strictly upward flow can be handled, only. For strongly buoyant driven flows convergence will not be obtained.
In the frame of the implicit scheme two systems of linear equations at each axial level need to be solved for the enthalpy and axial pressure gradients.

In the external iteration loop the following calculations are performed:

- Heat conduction for solid structures (rod, heater) for all levels
- At each axial level:
  - Turbulent cross flow mixing,
  - Enthalpy equation,
  - Axial/lateral momentum equation (axial pressure gradient, lateral mass flow),
  - Mass conservation equation (axial mass flow),
  - Thermo-physical properties, state equations of working fluids, and
  - Empirical model equations e.g. constitutive relations.

All transients are based on a steady state calculation done before

2.3 Physical Models used in the present simulation

The main physical models implemented in SUBCHANFLOW are summarized here after.

- **Fluid dynamics system of equations:** A three equation two phase flow model i.e. a mixture equation for mass (1), momentum (2),(3) and energy (4) balance is used. The constitutive relations are expressed as mixture equations for wall friction and wall heat transfer as well as a slip velocity relation. Many available empirical correlations can be implemented anytime if needed e.g. regarding pressure drop, heat transfer, void generation, etc.

$$A_i \frac{\Delta X_j}{\Delta t}(\rho_{ij} - \rho_{ij}^n) + (m_{ij} - m_{ij-1}) + \Delta X_j \sum_{k\in i} e_{ik} w_{kj} = 0 \quad (1)$$

$$\frac{\Delta X_j}{\Delta t}\left(m_{ij} - m_{ij}^n\right) + m_{ij} U'_{ij} + \Delta X_j \sum_{k\in i} e_{ik} w_{kj} U'^{*}_{kj} =$$
$$= -A_i\left(P_{ij} - P_{ij-1}\right) - g A_i \Delta X_j \rho_{ij} \cos\theta - \frac{1}{2}\left(\frac{\Delta X f \Phi^2}{D_h \rho_l} + K v'^{*}\right)_{ij} | m_{ij} | \frac{m_{ij}}{A_i} - f_T \Delta X_j \sum_{k\in i} w'_{kj}(U'_{ij} - U'_{nj}) \quad (2)$$

$$\frac{\Delta X_j}{\Delta t}(w_{kj} - w_{kj}^n) + \left(\overline{U}'_{kj}\, w_{kj}^* - \overline{U}'_{kj-1}\, w_{kj-1}^*\right) = \frac{s_k}{l_k}\Delta X_j P_{kj-1} - \left(K_G \frac{\Delta X v'^{*}}{sl}\right)_{kj} | w_{kj} | w_{kj} \quad (3)$$

$$\frac{A_i}{\Delta t}\left[\rho''_{ij}\left(h_{ij} - h_{ij}^n\right) + h_{ij}\left(\rho_{ij} - \rho_{ij}^n\right)\right] + \frac{1}{\Delta X_j}\left(m_{ij} h_{ij}^* - m_{ij-1} h_{ij-1}^*\right) + \sum_{k\in i} e_{ik} w_{kj} h_{kj}^* =$$
$$= \sum_{r\in i} P_r \Phi_{ir} q''_{rj} - [\sum_{k\in i} w'_{kj}(h_{ij} - h_{nj}) + \sum_{k\in i} C_k s_k (T_{ij} - T_{nj})] + \sum_{r\in i} r_Q \Phi_{ir} q'_{rj} S \quad (4)$$

Where:

A : axial flow area

ρ : $\alpha\rho_v + (1-\alpha)\rho_l$ (mixture density)

ρ_n : mixture density at the end of the previous time step (or at the beginning of the current one)

m : mixture axial mass flowrate

w : mixture crossflow rate

ρ_l : liquid density

ρ_v : vapor density

α : void fraction

g : gravity acceleration

P : pressure

θ : inclination of the channels with respect to the vertical

f : friction factor

ϕ_2 : two-phase friction multiplier

K : pressure loss coefficient for grid spacers or grid plates

f_T : transverse momentum factor

v' : effective specific volume for momentum transport
U' : effective momentum velocity

h : $xh_v + (1-x)h_l$ (mixture flowing enthalpy)
Φ_{ir} : fraction of the heated perimeter P_r
h_n : enthalpy at the end of the previous time step
h_l : liquid enthalpy
h_v : vapor enthalpy
x : flowing steam quality,
q'' : heat flux from a fuel rod into the fluid, assumed uniform around the rod circumference
q' : linear power generated in a rod
w' : turbulent cross flow
T : temperature
n = l+l'-1: index of the channel adjacent to channel i through gap k
h_{ij}* : flowing enthalpy at axial level j assumed as the donor cell enthalpy
h_{kj}* : flowing enthalpy
C_k : thermal conductance in lateral directions
r_Q : fraction of the fission power generated in a fuel rod, that enters the coolant directly.

- **Heat conduction:** Heat conduction in the fuel pellet and within the cladding material is solved by a fully implicit finite difference method. Axial heat conduction can be considered, if necessary. The temperature dependent material properties of different fuels (UO_2 and UO_2PuO_2) are implemented following the approach used in the TRACE code [9]. As cladding materials Zircaloy and stainless steel (316 SS), heater materials (Boron Nitride), Inconel-600 are programmed. In addition, a simplified model of electrical heaters of the BFBT benchmark can be chosen. The rod model can easily be extended, improved and modified thanks to the modular structure of code.

- **Heat transfer:** Relevant heat transfer modes along the boiling curve are described by the combination of different heat transfer models with similar logic to the one of RELAP4/MOD5 [8]. Single phase wall heat transfer is described by the Gnielinski correlation used also in the TRACE code [9].

$$h_{\text{coef}} = \frac{\text{Nu} \bullet k}{D_h} \bullet \left(\frac{\text{Pr}}{\text{Pr}_w} \right)^{0,11} \tag{5}$$

$$\text{Nu} = \frac{\left(f/2 \right)(\text{Re}-1000)\,\text{Pr}}{1+12.7\left(f/2 \right)^{1/2}\left(\text{Pr}^{2/3}-1 \right)} \tag{6}$$

$$f = \left(1,58 \bullet \ln(\text{Re}) - 3,28\right)^{-2} \tag{7}$$

Where:
Pr : Prandtl number (Pr_w Prandtl number wall)
Re : Reynolds number
Nu : Nusselt number
k : thermal conductivity

D_h : hydraulic diameter

f : friction factor

- **Void generation models:** The void fraction is calculated by the Armand (8) correlation. For sub-cooled boiling the Unal (9) model is used.

$$\alpha = x \bullet v_g \frac{0.833 + 0.167 \bullet x}{v_l (1 - x) + x \bullet v_g} \tag{8}$$

$$\Delta T = a \bullet \frac{q_W''}{h_{coef}} \tag{9}$$

Where:
v : specific volume (v_g gas; v_l liquid)
q_w'' : heat flux
h_{coef} : heat transfer coefficient

- **Pressure drop:** The single phase friction is modeled by the Blasius (10)correlation. For two phase flow the Armand two-phase multiplier is used (11-13). The influence of spacer grids is considered by defining appropriate pressure loss coefficients recommended by the benchmark team.

$$f = a \,\mathrm{Re}^b + c \tag{10}$$

o for turbulent flow:
a = 0.32 b = -0.25 c = 0

o for laminar flow
a = 0.64 b = -1.0 c = 0

$$\Phi^2 = \frac{(1-x)^2}{(1-\alpha)^{1.42}} \qquad (0 < \alpha < 0.6) \tag{11}$$

$$\Phi^2 = 0.478 \frac{(1-x)^2}{(1-\alpha)^{2.2}} \qquad (0.6 < \alpha < 0.9) \tag{12}$$

$$\Phi^2 = 1.73 \frac{(1-x)^2}{(1-\alpha)^{1.64}} \qquad (0.9 < \alpha < 1.0) \tag{13}$$

- **Critical heat flux:** The critical heat flux is calculated by a combination of a modified Barnett and the Babcock&Wilcox-2 correlation as used in COBRA-IV-I [1]. The following table explains the correlations in three different pressure regions. The transition between the regions is described by a simple linear interpolation. The correlation does not take into account the special design of the used spacer grid.

Correlation	Pressure (bar)	Mass flow rate (kg/m^{2}s)
Modified Barnett (14), (15), (16), (17)	p < 50	190 ≤ G ≤ 8409
Barnett (18), (19), (20), (21)	70 ≤ p < 90	
B&W2 (22), (23), (24), (25)	p ≥ 103.4	1020 ≤ G ≤ 5430

$$q''_{crit} = (80126.6049) \bullet \frac{A + B(h_f - h_i)}{C + x_L} \tag{14}$$

$$A = 0.7477 \bullet D_h^{0.052} G^{0.663} \left[1 - 0.315^{(-0.329 D_e G)}\right] \bullet \left(\frac{2066883.6}{h_{evap}}\right) \tag{15}$$

$$B = \left(6.18011 \bullet 10^{-8}\right) D_h^{1.445} G^{0.691} \tag{16}$$

$$C = \left(2.27101 \bullet 10^{-2}\right) D_h^{0.0817} G^{0.5866} \tag{17}$$

$$q''_{crit} = (80126,6049) \bullet \frac{A + B(h_f - h_i)}{C + x_L} \tag{18}$$

$$A = 205.2518 \bullet D_h^{0.68} G^{0.192} \left[1 - 0.744^{(-0.189 D_e G)}\right] \tag{19}$$

$$B = \left(3.1519 \bullet 10^{-5}\right) D_h^{1.261} G^{0.817} \tag{20}$$

$$C = 184.1242 \bullet D_h^{1.415} G^{0.212} \tag{21}$$

$$q''_{crit} = (3.15459) \bullet \frac{C \bullet \left[\left(0.3702 \bullet 10^{8}\right)\left(4.3603 \bullet 10^{-4}\right) G\right]^{B} - \left[4.8209 \bullet 10^{-2} \bullet G\left(h_i - h_f\right)\right]}{\left[12.710\left(2.2521 \bullet 10^{-3}\right) G\right]^{A}} \tag{22}$$

$$A = 0.7118 + \left(3.0064 \bullet 10^{-8}\right) P - \left(137.9 \bullet 10^{5}\right) \tag{23}$$

$$B = 0.8340 + \left(9.9320 \bullet 10^{-8}\right) P - \left(137.9 \bullet 10^{5}\right) \tag{24}$$

$$C = \left(1.1550 - 16.0248 \bullet D_h\right) \tag{25}$$

Where:

x_L : heated length
D_e : wetted diameter
G : Mass flow rate
h_{evap} : evaporation enthalpy
h_f : fluid Enthalpy
h_i : inlet enthalpy

- **Cross flow:** The turbulent lateral mixing in SUBCHANFLOW is parameterized by flow rate and geometry dependent formulas. The Roger Tahir model (26), which does not need any additional parameter is used in combination with a flow regime dependent multiplier (Beus, [3]). Void drift is not included and the mixing is calculated without mass exchange.

$$w'_{kj} = 0,0018 \bullet \mathrm{Re}^{-0,1} \bullet \left(\frac{S_{kj}}{d} \right)^{0,106} \bullet \left(\frac{D_h}{S_{kj}} \right) S_{kj} \bullet \bar{G} \tag{26}$$

Where:
$\bar{G}$: Average axial mass flux
S : gap
d : diameter of rod

- **Transport and thermo-physical properties of working fluid:** For coolant properties and state functions the IAPWS-97 formulation is used.

- **Boundary conditions treatment:** As boundary condition the total flow rate is selected. The flow is automatically distributed to the parallel channels depending on the friction at the bundle inlet. Temperature at inlet and pressure at the outlet are prescribed as boundary conditions.

3. Description of the NUPEC PSBT Experimental Data

The experiments performed at the PSBT test facility were performed to generate an extensive data base for the validation of physical models of thermal hydraulic simulation tools such as CFD, subchannel and system codes describing PWR-relevant safety phenomena e.g. pressure drop, void fraction and critical power. For this purpose typical subchannel geometries (corner, lateral and central) as well as fuel assembly design were selected for the experiments. In **Figure 1** the layout of the PSBT test facility is shown, where the central part is the test bundle. The facility was designed for a maximal pressure of 19.2 MPa and a maximal coolant temperature of 362°C that permits to perform tests representative for PWR conditions [5].

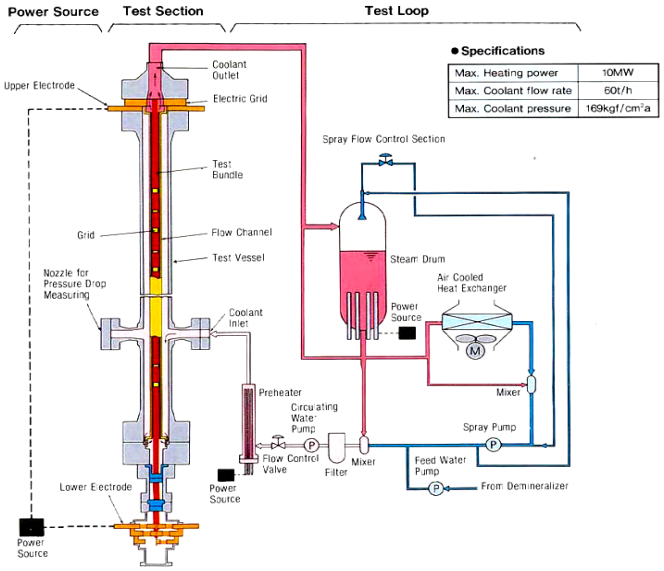

Figure 1: PSBT Subchannel Types considered for the Experiments

Table 1 Geometrical characterization of the different bundle arrangements

	5x5	**6x6**	**5x5 (guide tube)**
Number of fuel simulators	25	36	24
Number of guide tubes	0	0	1
Fuel simulator diameter	9,5 mm	9,5 mm	9,5 mm
Guide tube diameter	0 mm	0 mm	12,24 mm
Inner wall-to-wall-distance	64,9 mm	77,5 mm	64,9 mm
Bundle length	3658 mm	3658 mm	3658 mm

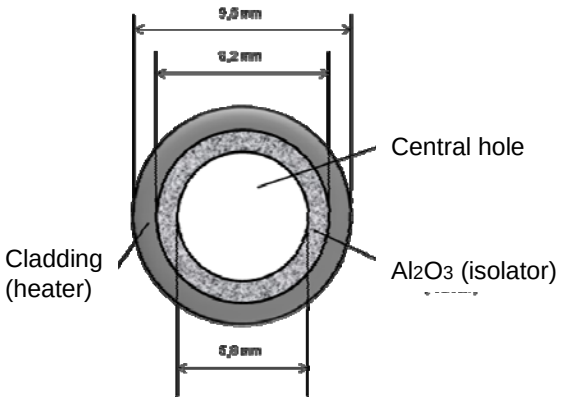

Figure 2 Geometry and material composition of fuel rod simulator

3.1 PSBT Void Fraction Tests

The PSBT tests consist of single subchannel and fuel assembly tests of different pin arrangement, thermal hydraulic conditions and shape of the axial power profile. The tests are performed for both steady state and transient conditions [5]. The experimental investigations were focused on measurements of the void generation, and pressure drop which are important safety-relevant parameters. The obtained data are appropriate for the validation of subchannel and CFD codes, and system codes. Parameter ranges representative of PWR are considered regarding pressure, coolant velocity and coolant temperature. In the test section, not only single subchannels, **Figure 3,** but also various bundles containing 25 till 36 fuel rod simulators and one guide tube, **Figure 4**.

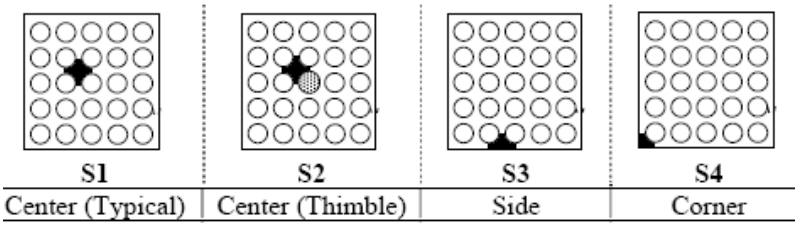

Figure 3 PSBT Subchannel types considered for the Experiments

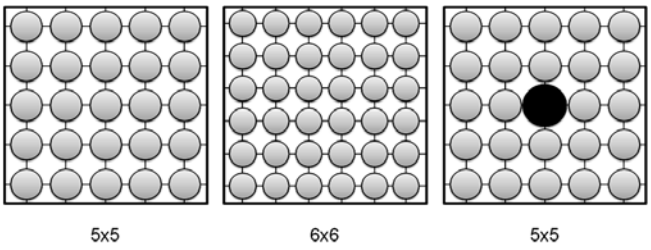

Figure 4: PSBT Bundle Type B5, B6 and B7 considered in the Experiments

3.2 PSBT Critical Power Tests

The second phase of the OECD PSBT benchmark is focused on the prediction of the critical power under steady-state and transient conditions. Different bundle geometries (A, B, C and D) were introduced in the test section for the DNB tests, see **Figure 5**. In total 9 test series were performed (0, 1, 2, 3, 4, 5, 6, 7, 8, 11T, 12T and 13) using different axial power profiles (constant, cosine shape). The test series 11T and 12T are transient tests while the others are steady state tests [5].

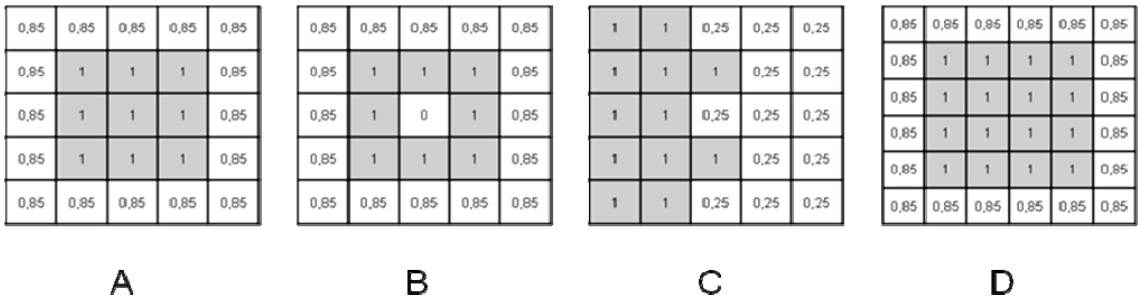

Figure 5: Bundle type with corresponding radial power profile for DNB tests

For the DNB tests, thermocouples were positioned in the inner surface of the fuel rod simulators, Figure 2 of the inner radial part of the bundles at different axial planes, located in the upper part of the bundle. During the test conduction, the bundle power was continuously increased till a sharp cladding temperature increase of 11 K was measured indicating that DNB has happened at the thermocouple position where it was observed. The exact position of the thermocouples can be found in [5]. It is important to mention that the measurement error amounts 1% for the pressure and power, 1.5 % for the mass flow rate and 1K for the temperature.
The DNB transient tests (11T and 12T) were selected in such a way that they are representative for postulated PWR scenarios such as pressured decrease, increase of coolant temperature, reduction of mass flow rate and power increase.

4. SUBCHANFLOW Post-test calculations of PSBT Experiments

An extensive validation of the SUBCHANFLOW models using the data of the DNB tests described in the OECD/NEA PSBT Benchmark was investigated in [7].

4.1 Modeling of the PSBT Tests in SUBCHANFLOW

For the analysis of the thermal hydraulic bundle behavior with subchannel codes it is primordial to develop a simplified representation of the test section (input deck) taking into account the geometrical, material and operational peculiarities of each test. Since many tests (steady state and transient) have been investigated with SUBCHANFLOW, the modeling of one bundle geometry will be outlined hereafter as example for all others. The first step developing a model is to perform a radial nodalization of the bundle defining the numbering of the subchannel, the gaps and the fuel rods as it is shown in **Figure 6** for the 5x5 PWR bundle. In **Figure** 6 a radial nodalization of the PSBT bundle is shown, where the subchannel and pin numbering of SUBCHANFLOW is indicated. In total three subchannel types (I, II, III) are present, for which the flow area, heated and hydraulic parameters were introduced in the input decks for the 36 subchannels. The spacer grids of different types were considered by a given loss coefficient, only. Axially the bundle was subdivided in 24 segments of equal height. The fuel rod simulator was subdivided radially as follows: Isolator in 6 mesh points, cladding in two mesh points.

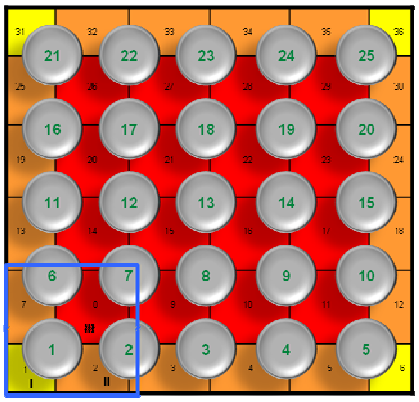

Figure 6: Radial nodalization of the bundle

The thermal hydraulic conditions at core inlet (mass flow rate, coolant temperature) and outlet (pressure) as well as the radial and axial power profiles of each test were considered in the post-test simulations with SUBCHANFLOW.

4.2 SUBCHANFLOW Simulation of Void Fraction Tests

Many steady state void fraction tests were simulated with SUBCHANFLOW for single subchannel types (S1, S2 S3 and S4) and for different fuel assembly types using the model described above. As can be seen in **Figure 7** and **Figure 8** the predicted void fraction for the single subchannel S1 and S2 agree well with the measured data.

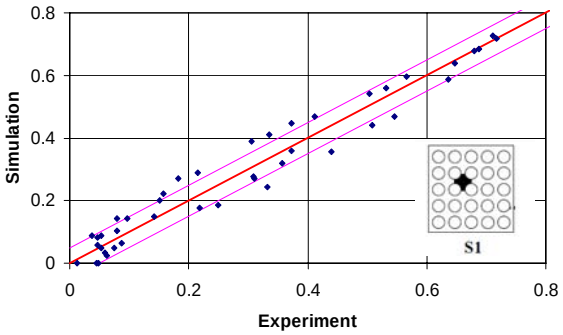

Figure 7: Comparison of predicted and measured void fraction for the test S1

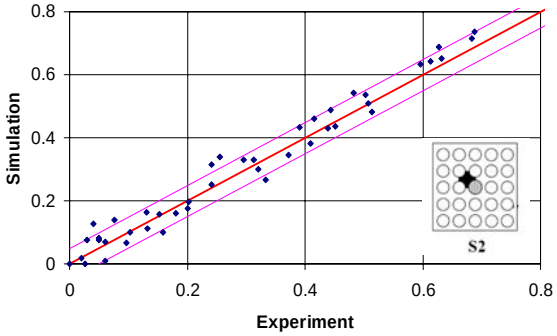

Figure 8: Comparison of predicted and measured void fraction for the test S2

The SUBCHANFLOW predictions for the bundle tests compared to the experimental data for two axial positions of the bundle (lower and upper) is given in **Figure 9**, **Figure 10** and **Figure 11**. For the lower and middle levels, SUBCHANFLOW tends to over-predict the void fraction for several tests while for the upper level the agreement is very good, i.e. within the 10 % error band. For the upper level, the comparison of the predictions and the data are much better than for the lower part for the majority of tests. It has to be noted that the void fraction was measured in the four central subchannels of the

bundle. These simulations were performed using a simple mixing coefficient in the frame of the equal mass mixing model to account for the mixing vane spacers.

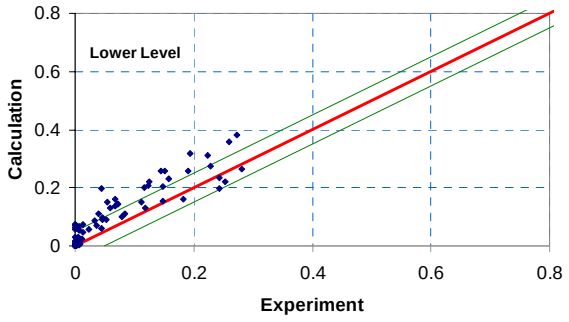

Figure 9: Comparison of predicted and measured void fraction for the test set S5

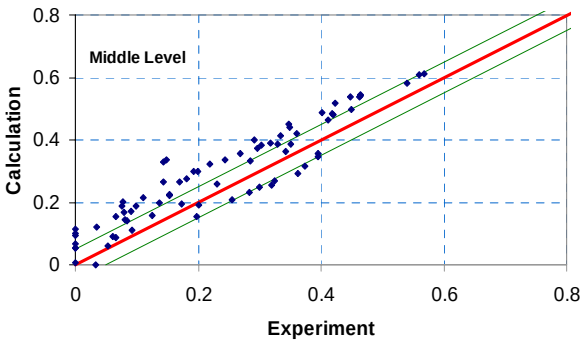

Figure 10: Comparison of predicted and measured void fraction for the test set S5

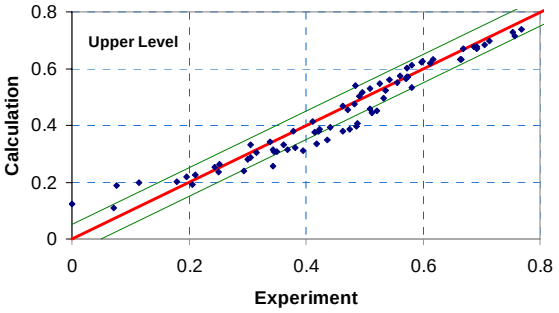

Figure 11: Comparison of predicted and measured void fraction for the test set S5

4.3 SUBCHANFLOW Simulation of Critical Power Tests

At the PSBT facility seven steady state test sets (**0, 1, 2, 3, 4, 5, 6, 7, 8, and 13)** were performed to measure the critical power under thermal hydraulic conditions representative for postulated PWR transients. The measured parameters were the critical power and sometimes the axial position. For these SUBCHANFLOW simulations, the bundle power was stepwise increased till somewhere a sudden cladding temperature escalation was detected indicating that critical power was reached. To assess the quality of the predictions compared to the measured data the relative deviation, the empirical averaged, and the standard deviation were used. This was done for all above mentioned test sets. For example the test set 0 includes around 70 experiments that were simulated with SUBCHANFLOW.

4.3.1 Steady state critical power tests

In Figure 12 the comparison of all simulated test of Set 0 with the SUBCHANFLOW predictions are exhibited. It can be seen that calculated critical power is close to the measured ones i.e. within 10 % of error margin for most of the test. Only for few tests the deviations of the predictions from the data are inside the 30 % error band. Detailed investigations have shown that the largest deviations are found for pressure of about 100 bar. The results are almost insensitive to the mass flux and the inlet temperature.

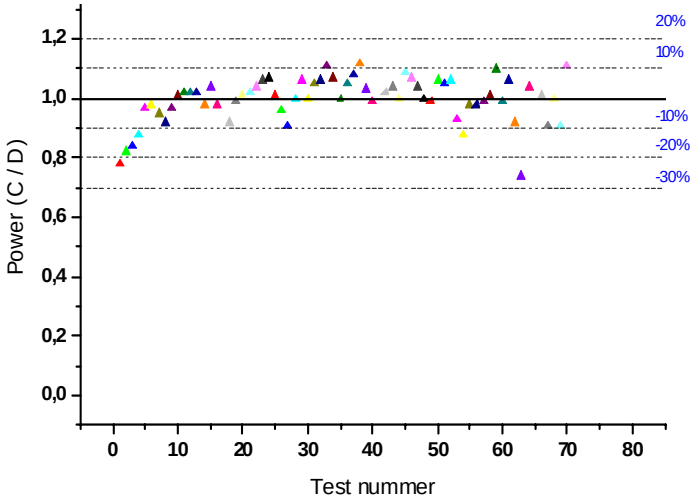

Figure 12 Comparison of predicted (C) and measured (D) critical power for the PSBT Test Set 0

The Test Set 4 consists of the same bundle arrangement 5x5 but with a more realistic axial power profile (cosines shaped) compared to the Set 0. In total 76 tests were analysed with SUBCHANFLOW. In Figure 13 a comparison of the SUBCHANFLOW predictions with the data of the Test Set 4 is shown. It can be observed there that SUBCHANFLWO tends to under predict the critical power. Part of the predictions lies within the 10 %, the 20 % and the 30 % of error margin. On the contrary to the Test Set 0, the results are insensitive to the bundle pressure and also to the mass flux and inlet temperature.

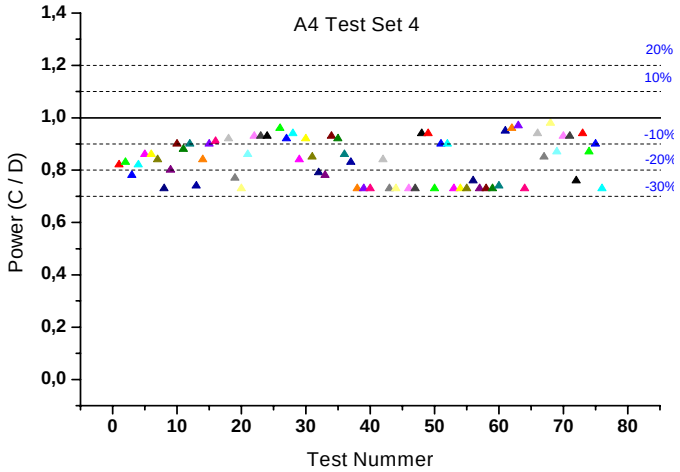

Figure 13 Comparison of predicted (C) and measured (D) critical power for the PSBT Test Set 4

5. Conclusion

The comparison of the simulations with the experimental data has shown that SUBCHANFLOW is able to predict the measured pressure drop, void fractions, and DNB in an acceptable manner for Test with high pressure values. For pressure intervals between 50-70 bars and 90-100 bars, the simulations showed predictions with deviations from experimental tests of up to 30% due to imprecise approximations of the interpolations. In future versions of SUBCHANFLOW additional correlations will be implemented and validated e.g. the implementation of lookup procedure for the prediction of CHF to cover a large range of operating parameter.

6. References

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