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DEVELOPMENT OF A COUPLING SCHEME BETWEEN MCNP AND COBRA-TF FOR THE PREDICTION OF THE PIN POWER OF A PWR FUEL ASSEMBLY

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ABSTRACT

In the frame of multi-physics activities at Forschungszentrum Karlsruhe, different coupling schemes between 3D transport and 3D subchannel thermal hydraulic codes are being developed and tested. Such methods are needed to improve the design methodologies and the prediction of local safety margins for both LWR and innovative reactors. Since the iterative solutions are time consuming, these developments are predestined to be carried out in a super computing environment. Recently the coupling of MCNP and COBRA-TF has been developed and tested in a Linux-Cluster. The aim of this investigation was the pin-power prediction of a PWR-fuel assembly taking into account the thermal hydraulics/neutronics feedbacks in the nuclear data. A master program consisting of shell scripts and FORTRAN routines was developed to supervise the execution of the modules as well as to synchronize the tasks to be performed at each time step. First of all the coupled MCNP/COBRA-TF was applied to predict the pin power of a PWR fuel assembly in a Linux Cluster. Converged results were achieved after 8^{th} iterations. Since the CPU-time was rather large, a relaxation method was implemented to speed-up the convergence of the coupled solution. It could be demonstrated that the implemented relaxation method led to a considerable CPU-time reduction. Further investigations are necessary to formulate the coupling scheme in a more general purpose sense i.e. independently of a specific fuel assembly configuration and to be applied for whole core calculations.
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Key Words: MCNP, COBRA-TF, coupling, pin power calculation, high performance computing

1. INTRODUCTION

Increased activities worldwide are focused on the improvement of numerical reactor simulations in both multi-physics and multi-scale domains. Since modern core loadings are becoming more complex e.g. due to the extensive use of MOX-fuel, burnable poisons, increased burn-up and enrichment, etc. sophisticated design and safety evaluation tools are necessary to realistically describe the physics of such cores. These methods are essential to demonstrate that the new fuel assembly and core designs fulfil the safety requirements and economic expectations. Several

international benchmarks and investigations have been performed to explore the prediction capability of 3D deterministic and Monte Carlo methods and to identify needs for further improvements [1, 2, 3]. An additional trend is the development of different coupling schemes between neutronics and thermal hydraulic codes at various levels of spatial resolution. In [5, 6, 7] the coupling of 3D transport with CFD codes are realized and tested. Recently, different coupling schemes between Monte Carlo and subchannel codes have been developed [8, 9, 10]. Moreover, coupling schemes between MCNP and CFD codes were also developed and tested in [11, 12]. Due to the nature of CFD and Monte Carlo solutions, they are CPU-intensive already as stand-alone solutions. The situation becomes worse once these codes are run in coupled mode due to the iterative approach and the needed high histories and cycle number to get converged results with sufficient statistics. Consequently, the investigations at Forschungszentrum Karlsruhe are focused on the coupling between 3D transport and Monte Carlo with subchannel codes (COBRA-TF) with the goal of pin power prediction of PWR and BWR fuel assemblies. In [13] a coupling procedure between THREEDANT and COBRA-TF within the modular KAPROS-system was developed. The predicted 3D pin power of the PWR fuel assembly was validated by MCNP-simulations[14]. Based on the previous work a new procedure was developed to couple MCNP and the 3D subchannel thermal hydraulic code COBRA-TF. The coupled system MCNP/COBRA-TF was applied to predict the pin power of a fresh PWR UO2-fuel assembly. A short description of the coupling scheme and related issues are provided here. The convergence behaviour of the coupled system was also investigated. To accelerate the convergence a relaxation method was implemented leading to a considerable reduction of the CPU-time.

2. DEVELOPED COUPLING APPROACH

The coupling scheme between MCNP and COBRA-TF was developed aiming to predict the 3D-pin power of a PWR fuel assembly [14]. It consists mainly of the following parts: a) master program for the supervision of the execution and data transfer between involved modules, b) a spatial mapping between the neutronics and the thermal hydraulic domain and c) interface modules to manage the data transfer from the neutronics to the thermal hydraulic part and vice versa.

2.1. The master program

A master program was developed that automatically supervises, organizes and controls the execution of the coupled programs including the interface modules. It is a shell script including many sublevel shell scripts, interface routines such as mc2cobra or cobra2mc. The sublevel scripts e.g. mc2cobra or cobra2mc includes Fortran routines to perform different tasks at each time step of the coupled solution before passing the data from one module to the other. Two versions of the master programs were developed to run the coupled systems MCNP4/COBRA-TF and MCNP5/COBRA-TF in serial and in parallel application, respectively. In Figure 1, the sketch of the master program for the parallel option is shown. In this frame the resource management and job scheduling are realized with the LoadLeveler (LL).

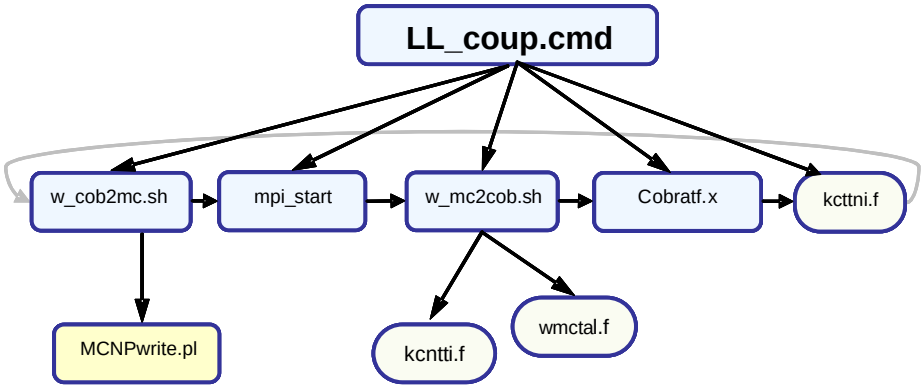

Figure 1 Master program for the automatic execution of MCNP5/COBRA-TF

2.2. Description of the coupling procedure

- **LL_coup.cmd**: It is a L**oadLeveler** command file which first defines the job type and the path, etc. Then the script driving the coupling is written inside the command file which calls other sub-level shell scripts. It starts the execution and controls the number of iterations to be done. There is a loop of iteration numbers to repeat the neutronics/TH calculations. The script calls other scripts in a certain sequence and gives them the proper numbering. The sequence is shown in Figure 1. At the end of the loop there is an if-statement which examines an indicator of the convergence. If the convergence criterion is met, the loop is broken and the shell **LL_coup.cmd** exits.
- **w_cobra2mc.sh**: This shell is called by the main script and represents the cobra2mc interface. It gets the file needed to write a new MCNP input and executes the Perl script, "MCNPwrite.pl". This PERL-script extracts the thermal data from the COBRA-simulation, writes the cell temperatures in the cell block, selects the cross section identifiers from a table of available temperatures and generates "pseudo"-materials of higher and lower temperature ACE-files. It then writes them in the material block of the MCNP input.
- **mpi_start.sh**: It is the lunch-script that executes the **mcnp5.mpi** command (MCNP5 executable). It ends with end-of-line statement, "**eol**". The next shell script will wait until the MCNP5 job is finished.
- **w_mc2cobra.sh**: It executes two FORTRAN programs. The first is "**wmctal.f**" which reads the "**mctal**"file from MCNP and the second is "**kcntti.f**" which builds the input file (deck.inp) of COBRA-TF. It also renames the results extracted from MCNP. The "**wmctal.f**" normalizes the 3D power to the linear heat rate expressed in [w/m]. Then the "**kcntti.f**" transforms the results from 1/4th to 1/8th of the FA according to the spatial mapping and reads a skeleton file (struc.dat) of the COBRA-TF input file (deck.inp) and copy it to deck.inp with the updated values obtained from "**wmctal.f**" at each iteration step.

- **cobratf.x**: It is the executable of the COBRA-TF code.
- **kcttni.f**: This program is executed within the driving shell script. It extracts the TH results, transforms them to the 1/4th of FA (MCNP model) and applies the relaxation technique if needed. In addition, it monitors the convergence of the thermal parameters. To do so, the relative parameter variation such as of the fuel temperature $\Delta T_f / T_f$ between the actual and last iteration is calculated and compared with a predefined convergence criterion. The "**kcttni.f**" program writes the results of the convergence checking in an auxiliary file. The driving script examines if the convergence is reached or not.
- The iterative approach is initiated with a thermal hydraulic solution with an assumed axial power profile.

2.3. Spatial mapping between Monte Carlo and thermal hydraulics

A fixed spatial mapping between the neutronic and the thermal hydraulic part of the fuel assembly models was defined. In Figure 2, the radial discretization of the computational domain in MCNP and COBRA-TF is shown. Based on this radial representation, the neutronic nodes have to be mapped to the thermal hydraulic ones i.e. a correspondence between both has to be established and programmed to facilitate the data transfer between both codes during the iteration procedure. It means that for example the radial and axial pin power predicted in MCNP has to be passed to the COBRA-TF code according to the mapping scheme so that COBRA-TF can take into account the right heat source of each axial pin node, see Figure 3. Since the radial discretization of the neutronic part (MCNP) differs from that of the thermal hydraulic part, additional work has to be done before transferring the data from the thermal hydraulic to the neutronic part to take into account feedbacks correctly. In Figure 4 , the different meshing of the MCNP and COBRA-TF is shown. The data have to be processed properly considering the MCNP meshing. This is important for the parameters predicted in thermal hydraulic subchannel domain.

73	74	75	76	77	78	79	80	81
64	65	66	67	68	69	70	71	72
55	56	57	58	59	60	61	62	63
46	47	48	49	50	51	52	53	54
37	38	39	40	41	42	43	44	45
28	29	30	31	32	33	34	35	36
19	20	21	22	23	24	25	26	27
10	11	12	13	14	15	16	17	18
1	2	3	4	5	6	7	8	9

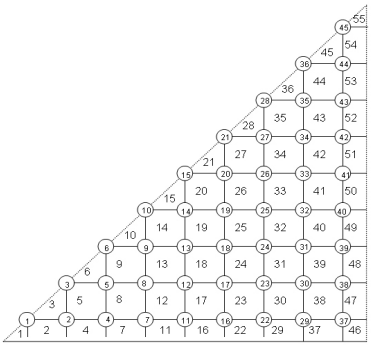

Figure 2 Spatial representation of the neutronic computational domain in MCNP (left) and of the thermal hydraulic domain in COBRA-TF(right)

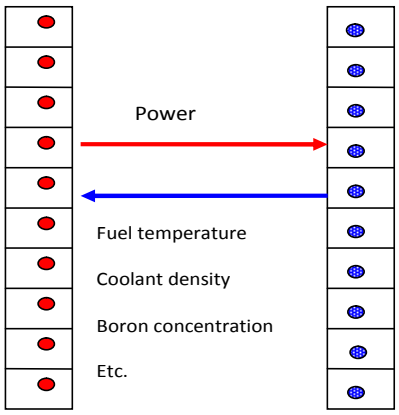

Figure 3 Axial mapping of the neutronic and thermal hydraulic part for data exchange

In MCNP, volume averaged values of the feedback parameters are needed. For each axial level, a volume averaged fuel temperature, cladding temperature and coolant density were derived from the COBRA-TF results. For the calculation of the coolant temperature and density the four subchannels surrounding a fuel pin were considered.

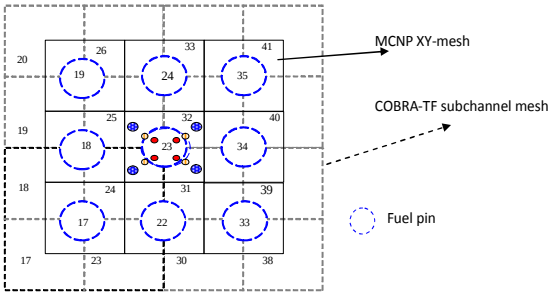

Figure 4 Mesh overlay between the thermal hydraulic and neutronic domain

2.4. Convergence testing

A method to check the convergence of the thermal hydraulic parameters was implemented in the program "**kcttni.f**". The relative parameter variation between two iteration steps, i.e. the current and the last one, is calculated according to the equation (2.1). It gives the relative deviation of a parameter e.g. fuel temperature (T_f) considering the actual (i) and previous iteration (i-1):

$$\Delta T_f / T_f = \frac{T_f^{\,i} - T_f^{\,i-1}}{T_f^{\,i}}, \qquad (2.1)$$

Two convergence methods are used. In the first one, the variations of local parameters in each cell of the computational domain are calculated online. In this case, for example the variations of

the fuel and coolant temperatures as well as density in all 810 cells are predicted. Then, the maximal relative parameter variation is searched and compared with the predefined criterion, e.g. 0.006, as follows:

$$(\Delta T_f / T_f)_{\max} \leq 0.006 \tag{2.2}$$

In case of the second method, the variations of the node average parameters of all axial nodes of the fuel assembly are calculated externally. Afterwards the maximal variation is identified and compared with the criterion. If the maximal variation is less than or equal to the convergence criterion, then it is assumed that the coupled solution is converged and the simulation is terminated.

2.5. Treatment of temperature dependence of the cross section for MCNP

In coupled simulations it is important to consider the thermal hydraulics feedback mechanisms mainly due to the material density and temperature effects on cross sections. There are different ways to account for such effects e.g. online generation of cross section data using NJOY [16] or a priori generation of nuclear data with NJOY for the whole range of state parameters and pseudo-material approach [17]. Different interpolation methods of the temperature dependent nuclear data for isotopes of interest at a desired temperature were tested for the coupling scheme: linear and square root weighting of the temperature of two cross section sets. In the latter method the weighting factor (for T_1) is given by the relation:

$$w_1 = \frac{\sqrt{T_2} - \sqrt{T}}{\sqrt{T_2} - \sqrt{T_1}} \tag{2.3}$$

Where T is the actual temperature, T_1 is the lower temperature of isotope of interest and T_2 is the higher temperature of the isotope of interest. The weighting factor for T_2 is expressed by $w_2=1-w_1$ since the sum of both fractions is equal to unity. To consider these effects in the coupled simulations, the MCNP input needs to be modified at each time step.

In [4], it was shown that for a single pin rod problem the K_{eff} –deviation is more than 2σ (two times the standard deviation) between the square root interpolation of two ACE files (200 K interval) and the ACE file from JEFF-31at exact temperature. On the contrary the deviation is only 1σ for linear interpolation. The standard deviation was 10^{-4}. But when using the square root interpolation method in connection with temperature intervals of only 50 K instead of 200 K the K_{eff} –deviation was reduced to a value less than 1σ.

3. TESTING THE COUPLING SCHEME

3.1. Problem Definition

To test the coupling scheme a D3 model of a PWR fuel assembly (FA) was developed. The FA-data and geometrical details are taken from [15]. The fuel assembly consists of 300 fuel pins and 24 control rods. The control rod guide tubes are filled by water and will be referred afterward as water rods. The active fuel rod length amounts 390 cm and the fuel rod pitch is 1.27 cm long. The Zircaloy-4 cladding thickness is 0.0064 cm and the outer fuel rod diameter amounts 0.95 cm. The diameter of the fuel pellet is 0.822 cm meaning that the gap is smeared with the fuel pin (hot conditions). The water rod tube inner and outer diameter is 1.1127 and 1.235 cm. The fuel is UO_2 with a U-235 content of 4 wt % at BOC conditions.

3.2. Developed models

The MCNP model consists of a quarter of the fuel assembly which is shown in Figure 5. The active FA-length is divided into 10 nodes i.e. 10 axial planes of 81 zones each. Each radial zone in the x-y-plane consists of 3 cells where every zone is a universe representing a fuel rod or water rod position. The fuel rod consists of fuel, cladding and moderator cells. The water rod zone consists also of three cells. Each cell has its own temperature and material cards. In total, there are 2430 cells representing the active length of the fuel assembly. Two additional axial nodes represent the axial reflector layers of 30 cm length. Each reflective plane is a lattice filled by two universes, each one consisting of three cells. One universe corresponds to the fuel rod positions (fuel density of 10E-15 i.e. vacuum) and the other one to the water rod positions.

The material data for the top/bottom reflector are taken by averaging the data of the top/bottom node of the active length. The reflective zones are shown in Figure 5, central part.

In the cell block, the cell temperatures and water densities must be changed every coupling step. In the material block, every fuel and water cell of the active length has its own material card whose XS identifier has to be changed according to the cell temperature. To account for temperature change, assigning of ACE files of the nearest temperature is done for water cells since the coolant temperature range is short and pre-generated files of 10 K intervals exist. For fuel cells, interpolation of two ACE sets performed when the difference in temperature is more than 5 K. For the cladding, one data set at 600 K is used for all cladding cells. Since cell temperatures are updated every time step, MCNP will automatically consider the Doppler broaden in elastic scattering cross-sections. Due to symmetry considerations only one eighth of the FA is modeled by COBRA-TF, see Figure 2. There a total of 55 subchannels (seven subchannel types) and 45 fuel rods including the water rods are present in the model.

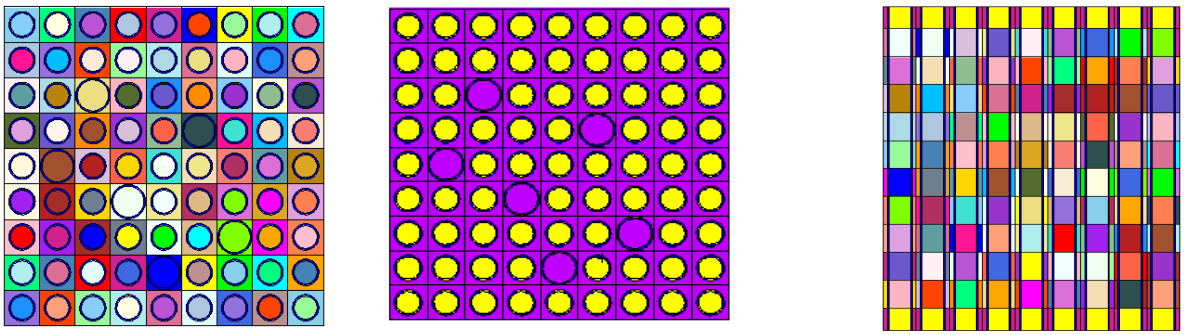

Figure 5 MCNP FA-Model: x-y lattice of active and reflector zone, y-z cross section

Each subchannel type is characterized by a flow area, hydraulic and heated diameters. In this problem the inlet mass flow rate for the FA, the coolant temperature at the FA-inlet and the pressure at the FA-outlet are given boundary conditions.

3.3. Results of coupled simulation

The coupled system MCNP/COBRA-TF was applied in a serial (MCNP4/COBRA-TF) and a parallel (MCNP5/COBRA-TF) environment using the FA-model presented before. The MCNP4/COBRA-TF was executed Linux cluster using only one processor. The simulation was terminated after ten iterations. For this simulation the number of histories per cycle was set to 100,000 using 200 escaped and 300 active cycles. The computation time for the coupled simulation was about 180 hours, obtaining standard deviations for the tallies with less than 0.7 % relative errors for individual cells. In **Figure 6**, the evolution of the linear power during the first eight iterations is shown. The coupled simulation starts with a cosine-shaped profile. During the iteration steps this profile of the linear power changes. The linear power peak moves to the bottom part of the FA since the moderator there is denser. The initial profile changed during the further iterations, oscillating at the beginning and with decreasing variation later on.

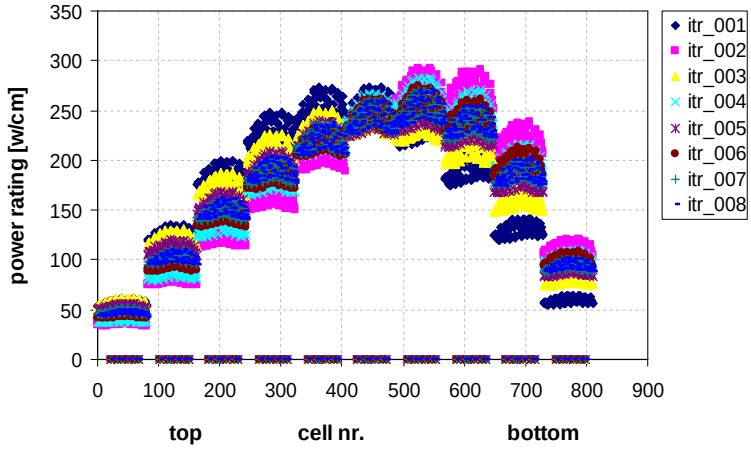

Figure 6 Predicted axial linear power during the iterations of MCNP4/COBRA-TF

The pin power distribution predicted by MCNP4/COBRA-TF within the fuel assembly is shown in Figure 7. It is worth to mention that the power generation shows a peak in the lower FA-part where the colder coolant is entering the FA and hence it is denser. The maximum pin power is located in the fourth axial node.

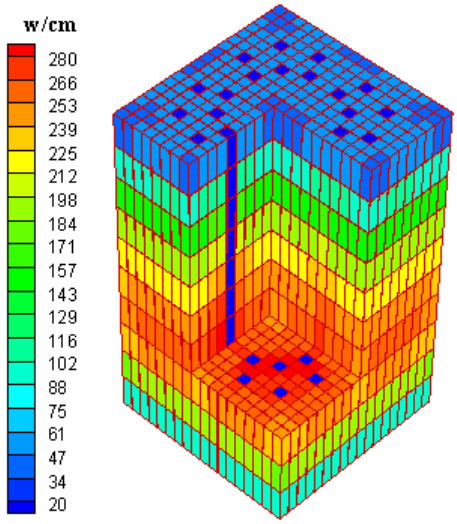

Figure 7 Predicted pin power distribution within the PWR-fuel assembly with MCNP4/COBRA-TF

The same problem was also investigated with MCNP5/COBRA-TF using the same number of histories and cycles as before but 20 parallel processors. In this case the coupled system needed only 12.5 hours for the ten iterations compared to the 180 hours of the MCNP4/COBRA-TF simulation. The standard deviation was also less than 0.7 % of relative error. The predicted linear power profile is very similar as the one shown in Figure 7. The evolution of the predicted fuel temperature exactly follows the power profile. The maximum temperature is also predicted at the fourth axial node. The coolant density is highest at the FA-bottom where cold water is entering the FA. It gradually decreases along the FA-height. The clad temperature of the different pins show different profile than the fuel temperatures as expected. The maximum cladding temperatures are predicted at node 5 and 6 i.e. around the middle of the FA.

3.4. Convergence behavior of the coupled system

The convergence behavior of the coupled system was extensively studied. The TH-parameter variation at individual cells and at the axial node was introduced. Based on the first method, the convergence can be checked and the coupled runs terminated. The latter one is applied externally specifically to study the convergence and is applied as well for local and node average powers. In the latter method e.g. the fuel temperature of the 81 pins was averaged at each axial level. Then its variation was calculated during the iterations steps. The fuel temperature, as well the power, experience the largest variation compared to other TH parameters during the iterations. It means that the coolant temperature converged earlier than the fuel temperature. The reason for

that may be because the fuel temperatures show a large variation in both axial and radial direction within the FA compared to the coolant and cladding temperature. Therefore the fuel temperature was selected to investigate the convergence behavior as in Figure 8.

- **Temperature convergence**

The variation of the individual cell fuel temperatures (**local variations**) as predicted by the first method is illustrated in Figure 8 in dependence of the iteration steps. Note that every point represents the maximal parameter variation at each iteration step. The coupled run was stopped after the convergence criterion (0.54 % < 0.6 %) was met i.e. in this case after the 8th iteration. In addition the node-wise variation of the fuel temperature (**node average variation**) was studied as convergence criterion. As can be seen in Figure 8, the node-wise variation of the fuel temperature converged faster than the other method based on the local fuel temperature. These curves indicate that integral values converge faster than the local values. Furthermore, the coupled simulation was continued after the 8th iteration step even though the convergence criterion was met to check the stability of the convergence. It can be seen there that only the node averaged fuel temperature variation fulfill the convergence criterion. The local variation of the fuel temperature shows an oscillatory behavior since the fuel temperatures varies strongly in the radial direction leading to oscillations.

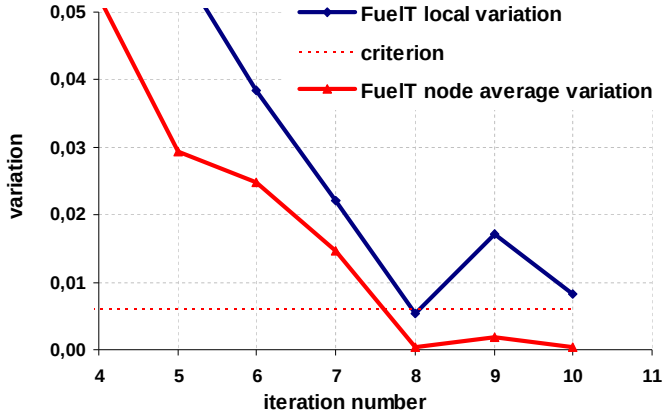

Figure 8 Convergence behavior of fuel temperature of MCNP4/COBRA-TF

The same investigations of the convergence behavior were performed with the MCNP5/COBRA-TF obtaining similar results as given in Figure 9.

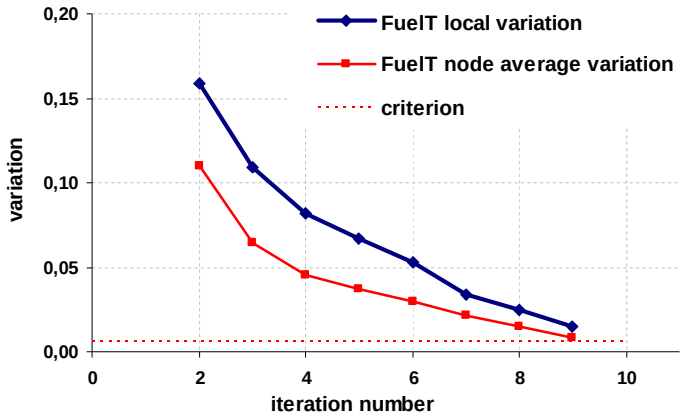

Figure 9 Convergence behavior of fuel temperature of MCNP5/COBRA-TF

- **Power convergence**

In addition to the fuel temperature convergence check, the convergence of the fuel assembly power was investigated. In Figure 10, the power convergence as predicted by MCNP4/COBRA-TF is presented. It can be noted that the power converged slower than the fuel temperature and it shows a slightly oscillatory behavior. At iteration 8 the power variation was very close to the criterion. But only the parameter variation based on the node variations went below the criterion (0.01) except for uppermost node.

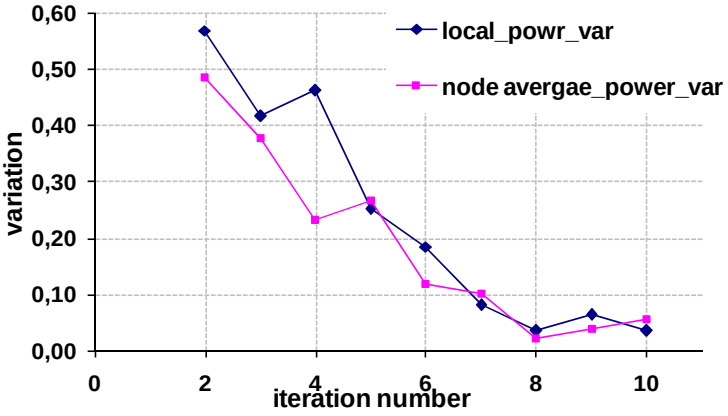

Figure 10 Convergence behavior of power of MCNP4/COBRA-TF

In addition to the investigation of the convergence behavior of the two coupled systems, a comparison of the main parameters predicted by MCNP4/COBRA-TF and MCNP5/COBRA-TF was performed. Both coupled systems predicted a very similar FA-averaged linear power. Deviations at certain axial levels were not larger than 0.036 between both simulations. The standard deviations, relative error, varied between 0.0027 and 0.007. The CPU time needed by MCNP4/COBRA-TF was 180 hours for 10 MC/TH iterations compared to 12/16 hours of CPU time for MCNP5/COBRA-TF. If a larger number of particles is required e.g. for a big problem or to get better statistics the CPU-time will increase, too. For example a MCNP5/COBRA-TF run was performed for 5x105 histories per cycle and using 500 active cycles and 200 escaped cycles.

It took 55 hours for a converged solution. If this problem had to be simulated with MCNP4/COBRA-TF, it would take several weeks. This emphasizes the need to develop techniques to accelerate the convergence. Such a method will be presented and discussed in the next chapter.

4. IMPROVING THE CONVERGENCE OF MCNP/COBRA-TF

Since the CPU time of the coupled solution is rather high, a relaxation method was implemented with the goal of speed-up the convergence behavior. This method consists in weighting the results of the actual simulation step with the ones of the previous step by applying weighting factor ***w*** ($0 \leq w \leq 100$). The parameters of two iteration steps i.e. iteration ***i-1*** and ***i*** are related to each other by the following relation:

$$T_{f,i,weighted} = \frac{(100 - w) \cdot (T_{f,i-1}) + w \cdot (T_{f,i,calculated})}{100} \qquad (4.1)$$

This method was implemented in the subroutine **kcttni.f** and it was applied to the thermal hydraulic parameters. Since the appropriate value for the weighting factor is unknown, it has to be selected carefully after some parametric investigations on a case by case basis. An optimal value for ***w*** was selected which minimizes the oscillation of the parameter variation and show a fast convergence behavior. It was studied first of all outside the coupling procedure and then it was implemented in the coupled scheme.

For these investigations, the reference solution is represented by the coupled solution without relaxation method i.e. with w=100. It converged after the 8th iteration meaning that the parameter variation was below the convergence criterion of 0.006.

First of all, several weighting factors were applied externally to the first two iterations using the node average fuel temperatures as the parameter. The so obtained axial fuel temperature distribution is compared to the one of the reference solution in Figure 11. Different weighting factors (30, 50, 60 and 80 %) were used. It can be seen that the weighting factors of 50% and 60% are closer to the reference solution than the values of 30 and 80 %.

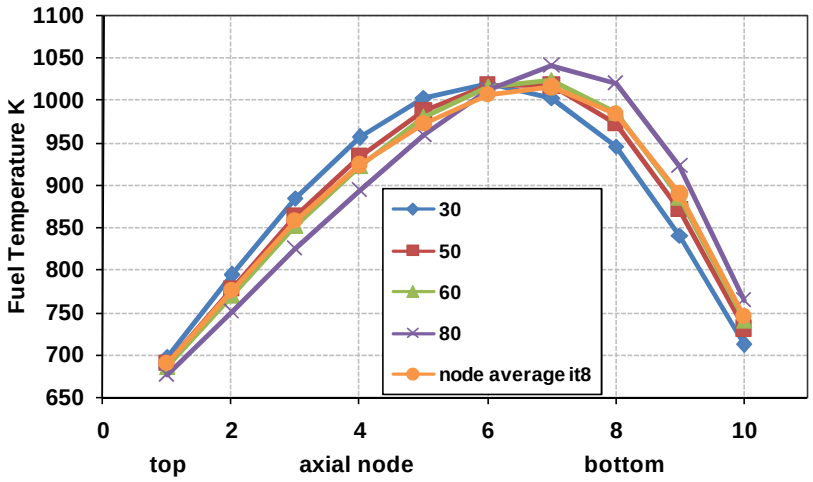

Figure 11 Testing of several weighting factors

Based on this results the weighting factor of ***w=50*** was selected to be implemented in the coupled solution.

Two MCNP5/COBRA-TF simulation cases were investigated using this weighting factor and different number of particles and escaped and active cycles for MCNP5.

In the first case, 100 thousands particles per cycle and a total of 500 cycles with 200 cycles to be escaped were used. In the second case, 300 thousands particles per cycle and a total of 600 cycles with 300 to be escaped were used. For case 1, the total number of histories was 50 million histories where 30 million histories are active. The predicted linear power for this case is shown in Figure 12. The simulation converged at the iteration number 5. It is apparent that the oscillation of the results becomes smaller with increasing iteration number. These oscillations are around the converged solution and smaller compared to the ones of the oscillations without relaxation. The standard deviation (relative error) varied from 0.27 % to 0.63 %. The local variation in fuel temperature was 0.5 % at iteration 5 which is below the criterion. The local power variation was 1.8 %. An additional case was studied for a weighting factor of 85 with numbers of histories and cycles like in the case 1 for comparison purposes.

For case 2, the number of histories was increased to 180 millions and half of the cycles were escaped so that the number of active histories is 90 millions. The relative errors were reduced to values between 0.15 % and 0.36 %. The fuel temperature converged at the 6th iteration. The local variation in fuel temperature was 0.45 % at iteration 6 which is below the criterion. The power variation was 2.4 %.

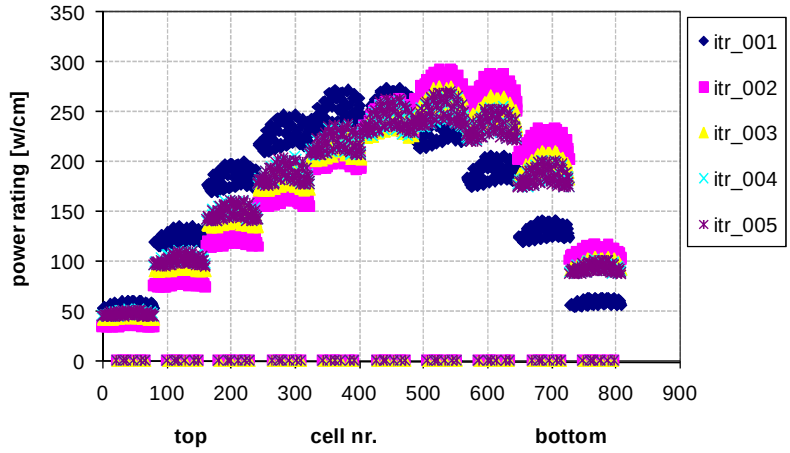

Figure 12 Evolution of the predicted axial linear power during the iterations of MCNP5/COBRA-TF

In Figure 13, a comparison of the convergence behavior of the three cases is shown. It is worth to mention that the increase of the histories did not contributed to a faster convergence (case2). However it shows a more stable convergence behavior and almost no oscillations compared to the case with fewer histories (case 1). For ***w= 85,*** the coupled solution did not fulfill the convergence criterion until the iteration 10.

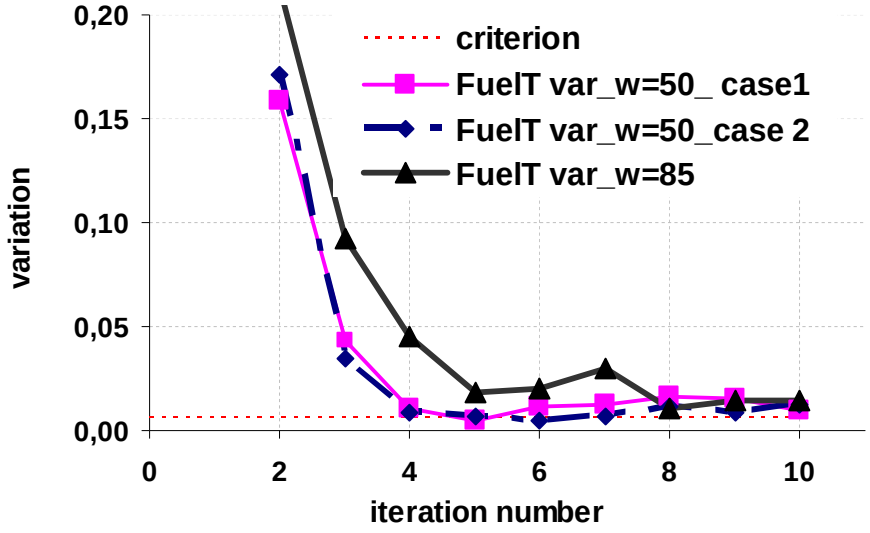

Figure 13 Comparison of the convergence behavior of MCNP5/COBRA-TF using different *w*

The linear power predicted based on the node- and cell-averaged parameter showed a similar convergence behavior as the fuel temperature, Figure 14. However the variations of the linear power are more pronounced than the one of the fuel temperature.

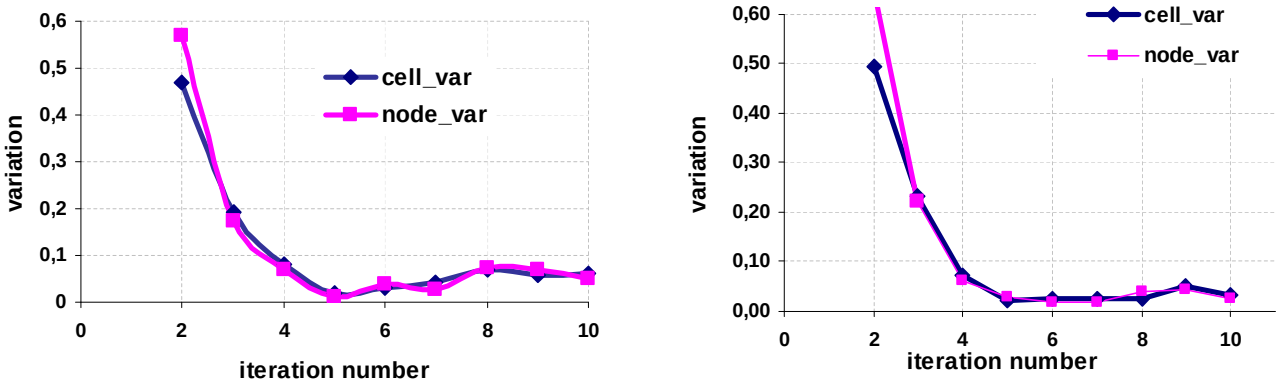

Figure 14 Power convergence with less histories (left) and more histories (right)

Based on these investigations, it can be stated that the coupled solution shows a good convergence behavior for weighting factors between 50 and 60 applied to both methods (node and cell). Converged results were obtained already after the 5-6th iteration meaning after about 6.25 hours instead of 12.5 hours.

5. CONCLUSIONS

A new coupling scheme for MCNP and COBRA-TF has been developed and applied for the prediction of the pin power of a PWR fuel assembly. In this approach a coupled

neutronics/thermal hydraulic solution is achieved iteratively. Both the mapping scheme and the treatment of the temperature dependence of nuclear data are key issues for the coupled solution. The needed nuclear data for the relevant materials and isotopes at representative range of temperature were generated in advance using the NJOY system. Appropriate interpolation methods were used to get the nuclear data for the actual temperature prevailing at each iteration step within the 3D pin-by-pin fuel assembly nodalization. The predicted 3D pin power distribution of the fuel assembly is physical sound. Finally different methods to speed-up the convergence behavior of the iterative coupled solution were investigated and an appropriate weighting factor was selected. The implemented relaxation technique led to a considerable reduction of the CPU time. Despite these promising results, further investigations are necessary for example to formulate the coupling scheme in a more general framework for different fuel assembly configuration. For envisaged whole core simulation with the coupled system additional effort will be necessary on both MCNP and subchannel codes in connection with the exploitation of high performance computers.

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