COUPLING OF THE CFD CODE ANSYS CFX WITH THE 3D NEUTRON KINETIC CORE MODEL DYN3D FOR VVER APPLICATIONS

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The CFD code ANSYS CFX has been coupled with the neutron-kinetic core model DYN3D. ANSYS CFX calculates the fluid dynamics and related transport phenomena in the reactor's coolant and provides the corresponding data to DYN3D. In the fluid flow simulation of the coolant, the core itself is modeled within the porous body approach. DYN3D calculates the neutron kinetics and the fuel behavior including the heat transfer to the coolant. The physical data interface between the codes is the volumetric heat release rate into the coolant. In the prototype that is currently available, the coupling is restricted to single-phase flow problems. In the time domain an explicit coupling of the codes has been implemented so far.

Steady-state and transient verification calculations for a small-size test problem confirm the correctness of the implementation of the prototype coupling. The test problem was a mini-core consisting of seven real-size VVER-1000 fuel assemblies. Comparison was performed with the DYN3D stand-alone code. In the steady state, the effective multiplication factor obtained by the DYN3D/ANSYS CFX codes shows a deviation of 0.2 pcm from the DYN3D stand-alone solution. The transient test case simulated the withdrawal of the control rod from the central fuel assembly at hot zero power in the same mini-core. Power increase during the introduction of positive reactivity and power reduction due to fuel temperature increase are calculated in the same manner by the coupled and the stand-alone codes. The maximum values reached during the power rise differ by about 3 MW at a power level of 240 MW. These differences are caused by the use of different flow solvers.

After this verification a steady-state full power calculation for a full VVER-1000 reactor was carried out in order to show the applicability of the new code system to real problems. A CFX grid consisting of about 1.3 10^6 nodes was created. The main difference to a pure DYN3D calculation with its 1D thermal hydraulic model is the presence of a lateral coolant flow at a velocity in the order of 1 cm/s from the circumference of the core centre. It is driven by the acceleration of the liquid in the centre due to the stronger heating. This flow increases the exchange of heat in the lateral direction by advection and leads to a 'smearing' of the step-like temperature profile that has been found in a pure DYN3D calculation.

1. Introduction

Analyses of postulated reactivity initiated accidents (RIA) in nuclear reactors are carried out using 3D neutron kinetic core models. The feedback is usually calculated using 1D thermal hydraulic models for channel flow, partly with the possibility of cross flow between theses channels. A different possibility is the use of subchannel codes for the determination of the feedback. The code DYN3D developed at Forschungszentrum Dresden-Rossendorf is an example for a 3D neutron kinetic core model. In its basic version, the code contains models for the solution of the 3D neutron

diffusion equation in two energy groups for fuel assemblies with rectangular and hexagonal cross section [1]. Recently the code was extended to an arbitrary number of energy groups. Further, a simplified transport approximation for the flux calculation was implemented for fuel assemblies with quadratic cross section [2].

DYN3D has been coupled to the 1D system codes ATHLET and RELAP5 to conduct adequate analyses if the interaction of the reactor core with the plant components has to be taken into account [3].

Computational Fluid Dynamics (CFD) codes are widely used in industrial applications for single phase flows, e.g., in the automotive or aircraft industries. For several years these codes have been applied also to fluid dynamical processes in nuclear reactors. One of the main nuclear CFD applications is the simulation of single-phase coolant mixing processes in the reactor pressure vessel (RPV) of pressurized water reactors (PWR). Big efforts were put into the validation of the results of such calculations [4, 5, 6, 7]. The application of CFD for multiphase systems is not yet mature. Safety analyses related to nuclear light water reactors require reliable simulations for different scenarios including two-phase flow situations. The development and validation of models for the simulation of the different types of two-phase flow conditions is underway [8].

The CFD code ANSYS CFX [9] is the reference CFD code of the German CFD Network in Nuclear Reactor Safety. One of the goals of the co-operation inside this network is the development of CFD software for the simulation of multi-dimensional flows in reactor cooling systems. This includes the above mentioned work on two-phase flow problems as well as the coupling of different simulation technologies. In the frame of the coupling activities an interface between ANSYS CFX and the system code ATHLET is under development [10]. A second topic is the coupling of the CFD code ANSYS CFX with the 3D neutron kinetic core model DYN3D, which is described in this paper.

2. Coupling of ANSYS CFX and DYN3D

2.1. Coupling Approach

The coupling approach is based on the selection of best-in-class software tools for the simulation of each of the phenomena to be described by the coupled codes. For this, the module predicting the coolant flow within DYN3D is replaced by a fully three-dimensional CFD simulation using ANSYS CFX. A detailed and spatially resolved modeling of the whole reactor core down to the fuel pin level in the CFD code is not feasible for practical applications at present and in the foreseeable future. It is possible to achieve acceptable computation times only by modeling the reactor core as a porous region. This reduced resolution of the structures in the core affects the thought location of the interface between the CFD code and the neutron kinetics core model. An incorporation of the bare neutron kinetics model of DYN3D only, as it was done in the internal coupling of ATHLET and DYN3D [11], is not possible because the heat transfer from the fuel pins to the coolant cannot be calculated by ANSYS CFX due to the above mentioned restrictions. Therefore, it was decided to define the physical data interface at the level of the volumetric heat release rate into the fluid. The CFD code ANSYS CFX calculates the fluid dynamics in the reactor coolant inside the core. It provides the velocity, temperature, density and boron concentration fields to DYN3D. Based on these parameters DYN3D determines the nuclear power, calculates the fuel temperature distribution and the heat transfer to coolant. The volumetric heat source is given back to ANSYS CFX. It should be noted that in the current prototype, the coupling is restricted to single-phase flow conditions. Especially the division of the heat source into different parts (immediate evaporation vs. convective heating) and the two-phase flow treatment in the porous body approach are subject to further investigations.

2.2 Implementation of the Coupling

In the coupled calculation, ANSYS CFX acts as the master program; DYN3D is implemented as a set of subroutines. ANSYS CFX uses its own memory management system for the array data handling while DYN3D uses dynamical arrays available in FORTRAN 90. Direct data exchange between these two standards is not possible. In the connecting subroutine of the two programs the relevant DYN3D data are transferred into the CFX memory management system before sending them to the CFX solver. In a similar way CFX data to be transferred are converted to FORTRAN 90 arrays.

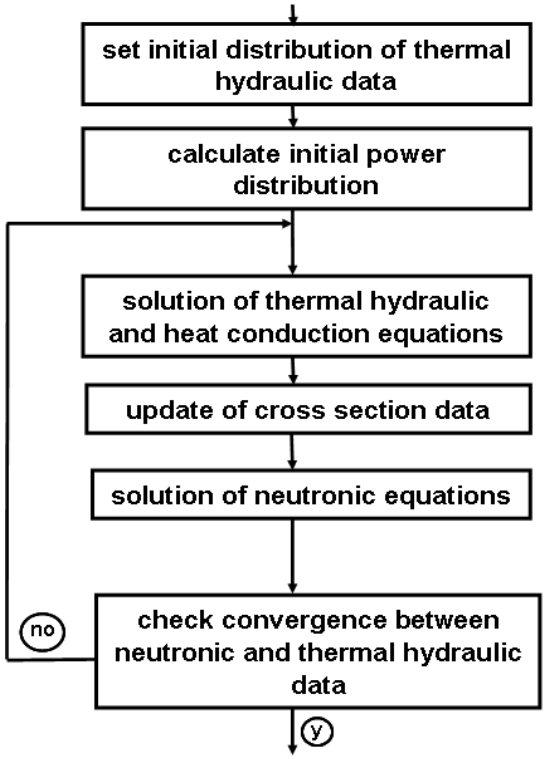

Fig. 1 Standard iteration scheme in DYN3D for steady-state calculations

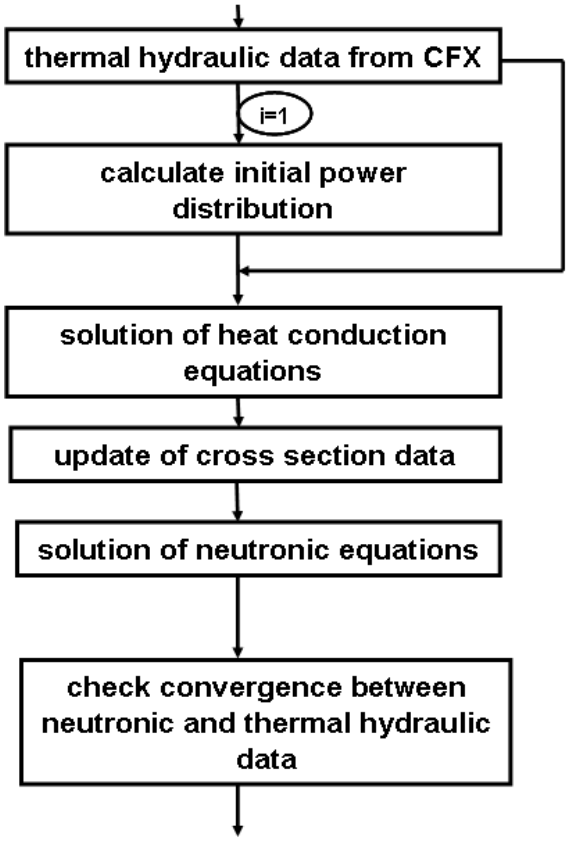

Fig. 2 Iteration scheme in ANSYS CFX / DYN3D for steady-state calculations (DYN3D part)

A 3D volume mesh-to-mesh transfer of field quantities between ANSYS CFX and DYN3D had to be implemented taking into account the largely different mesh resolutions used in the two codes. A 3D-volume mesh-to-mesh transfer for arbitrary data fields was implemented in CFX. The conservation of the data during transfer is properly ensured. The DYN3D coarse nodalisation is represented by a separate, coarsely meshed zone in CFX. The developed transfer code works independently. The coarsely meshed zone is also available for post-processing DYN3D data in CFX-Post. Both zones co-exist side-by-side in CFX.

Altogether 40 new subroutines were written in the CFX part for the implementation of the coupling. All coding was done at the user programming interface, so that no custom solver of CFX was needed. In the DYN3D part five new subroutines were written; changes were introduced into nine existing subroutines. All DYN3D routines were compiled together with the CFX-specific coupling routines, and all were linked into a single shared library that is loaded by CFX at run time and controlled purely by user input.

For steady-state calculations an iteration scheme between ANSYS CFX and DYN3D was implemented. Figs. 1 and 2 show the steady-state iteration scheme in DYN3D and in the coupled ANSYS CFX/DYN3D code (DYN3D part). As can be seen, the iteration scheme was slightly modified in the coupled calculation. DYN3D is called from CFX, solves the heat conduction and the neutron-kinetic equations and sends the results back to CFX ("i" stands for the actual number of iteration). Further, it should be noted that in the DYN3D stand-alone case the thermal hydraulics is brought to convergence at each iteration step before going to the solution of the neutron-kinetic equations. In the coupled code calculation the approach is different: DYN3D is called at the end of each iteration step of ANSYS CFX. In this way, the number of iterations between the codes increases, but this implementation requires less total computation time as the dominant part of the computation time is spent for ANSYS CFX.

The convergence in a steady-state DYN3D stand-alone calculation is based on assessments of the following variables:

- change of the effective multiplication factor
- maximum change of node-wise fuel temperature (average)
- maximum change of node-wise coolant density

The same criteria are assessed inside DYN3D during coupled code calculations. The density data are those obtained from CFX. In this way the convergence criteria available in both codes remain unchanged. The steady-state calculation is finished only when the corresponding criteria are fulfilled in both codes.

At the current stage of the implementation no iteration between ANSYS CFX and DYN3D is carried out during transient calculation. An explicit coupling approach is applied. DYN3D is called after ANSYS CFX has finished the calculation for the current time step. The time step size is identical for both codes. An extension to a semi-implicit coupling with iterations between the codes within each time step is planned to be implemented. It is also planned to implement an adaptive time step control for both solvers based on their specific needs.

Neither the iteration scheme nor the convergence criteria were changed in the ANSYS CFX code.

3. Verification

The selection of the case for testing the implementation and for the verification of the coupling was based on the following considerations:

- fast running problem
- small size problem
- not unrealistic case
- comparison of calculation results with standard DYN3D calculation should be possible

It was decided to create a mini-core consisting of seven real size VVER-1000 fuel assemblies (Fig. 3). The flow rate through this mini-core was set to 812 kg/s, the inlet temperature is 280 °C.

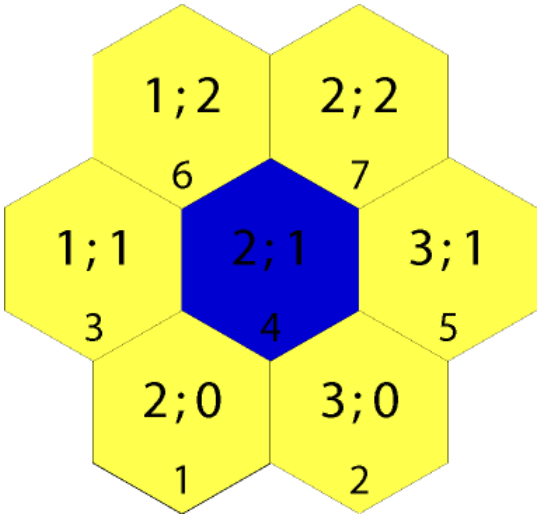

Fig. 3 Scheme of the mini-core

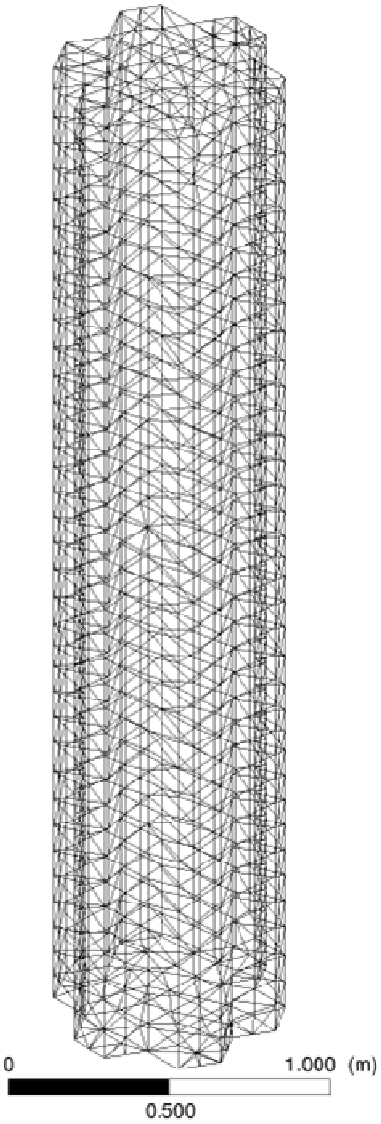

Fig. 4 ANSYS CFX calculation grid of the mini-core

As usual, the resolution of the DYN3D grid is one node per fuel assembly in radial direction. 14 nodes were used over the height. The height of the nodes was set unequal in order to test the correctness of the mesh-to-mesh-transfer algorithm. The CFX calculation grid contains 18,000 nodes (Fig. 4).

3.1. Steady-State Problem

For the verification of the steady-state calculation procedure, the power of the mini-core was set to 120 MW. This ensures an average heat-up of about 27.5 K.

Fig. 5 shows the convergence of the effective multiplication factor in both calculations. The number of iterations is higher in the coupled calculation. This is due to the above mentioned different iteration scheme, where the neutron-kinetic module is called at every iteration step in CFX. In the stand alone version of DYN3D, the neutron-kinetic module is called only when the thermal

hydraulics has reached convergence. Here, the internal thermal hydraulic iterations are not counted. The resulting K_{eff}-values differ by 0.2 pcm, only.

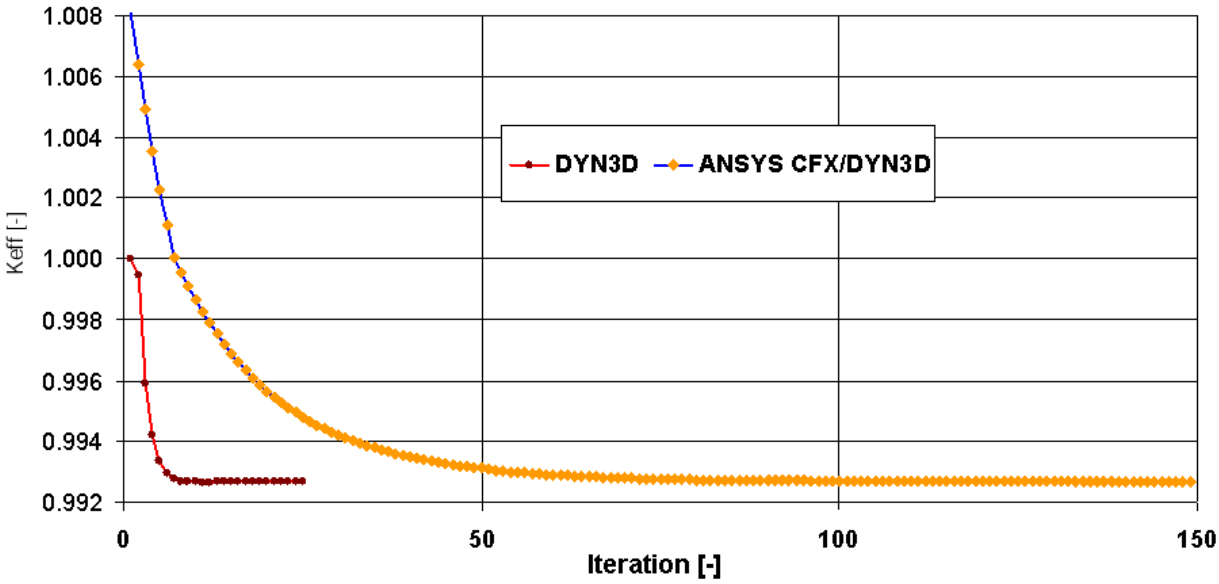

Fig. 5 Convergence of steady-state calculations

3.2 Transient Problem

For the verification of the implementation of the transient calculation option the withdrawal of the control rod from the central fuel assembly at hot zero power (HZP) was selected. The initial position of the control rod was selected with 1.50 m from lower edge. The time for full withdrawal was set to 10 s. Time-explicit coupling had been implemented so far, only. Calculations were carried out with variation of the time step size. The results of the calculations with time steps of 10 and 1 ms are shown on Fig. 6 and Fig. 7. For comparison purposes the iteration within each time step in the DYN3D stand-alone code was deactivated.

The power starts to rise remarkably after 3 s. A power peak occurs which is compensated by the Doppler feedback. Due to continuing control rod extraction the power will rise further. Here, only the first 10 s are analyzed. This includes the first power maximum and the power decrease due to fuel temperature increase.

The overall behavior of the core power is identical in all calculations. Small differences are to be seen in the maximum value reached. This maximum reduces with decreasing time step. The difference in the maximum core power is about 3 MW. This difference is acceptable considering the following: The introduced positive reactivity during the transient is slightly higher than 1 $. In the reactivity range around 1 $ the power behavior is very sensitive to changes in the feedback parameters. Therefore, smallest differences between the different transient flow solvers can have significant effect on the time-dependent feedback.

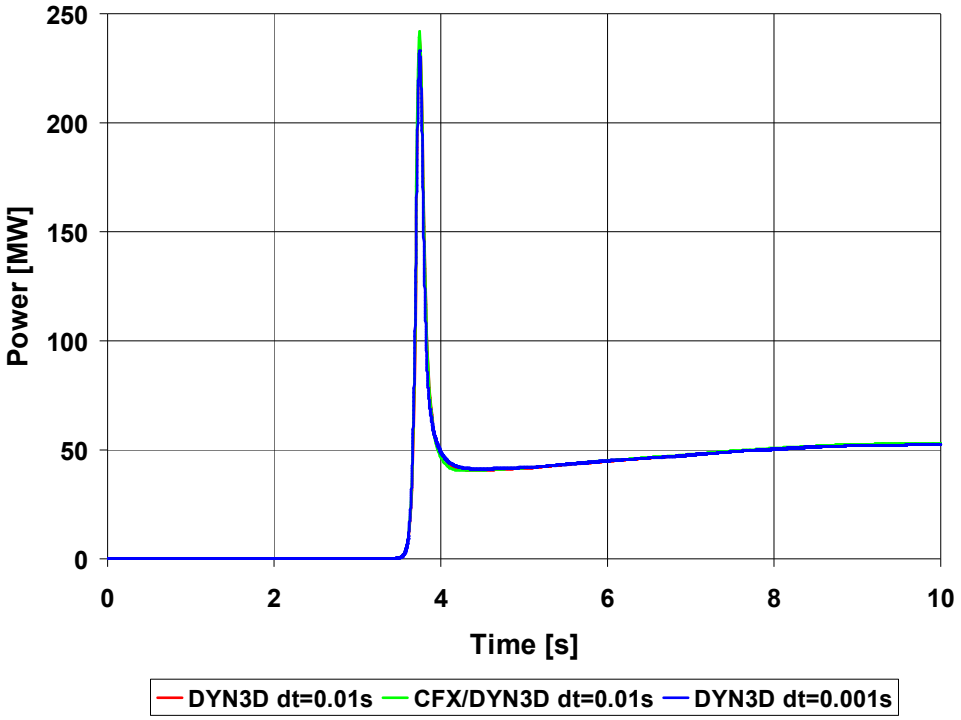

Fig. 6 Core power behavior in the DYN3D and CFX/DYN3D calculations

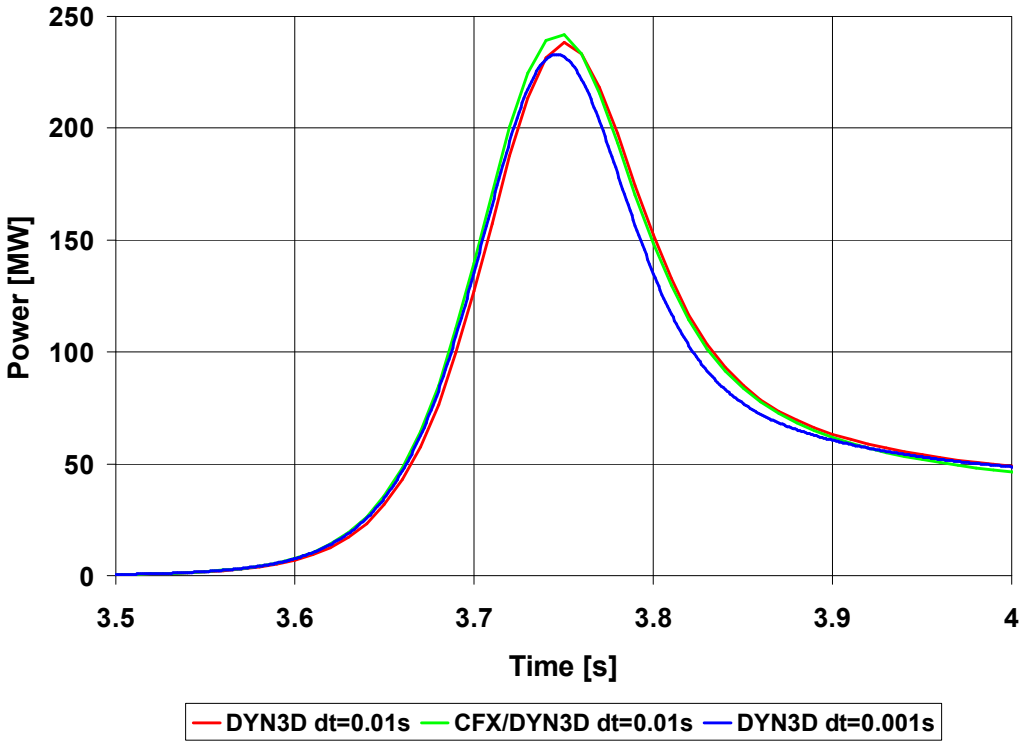

Fig. 7 Core power behavior in the DYN3D and CFX/DYN3D calculations (zoom)

4. Full core test case

The full core test case is a VVER-1000 core with 163 hexagonal fuel elements with a total power of 3000 MW. It is fed with a coolant mass flow of 18000 kg/s. Temperature and pressure of the coolant at the entry are 285 °C and 15.72 MPa, respectively. The boron concentration amounts to 952 ppm. An unstructured, tetrahedral mesh was used for the flow simulation, which consisted of 1,256,818 nodes (Fig. 8). The temperature and heat source distributions are shown in Figs. 9 and 10. It should be noted that the steep temperature changes between neighbouring fuel elements found in the simulation are due to the fact that a core configuration at the begin of a fuel cycle is used with relatively big differences in the power of the single fuel assemblies.

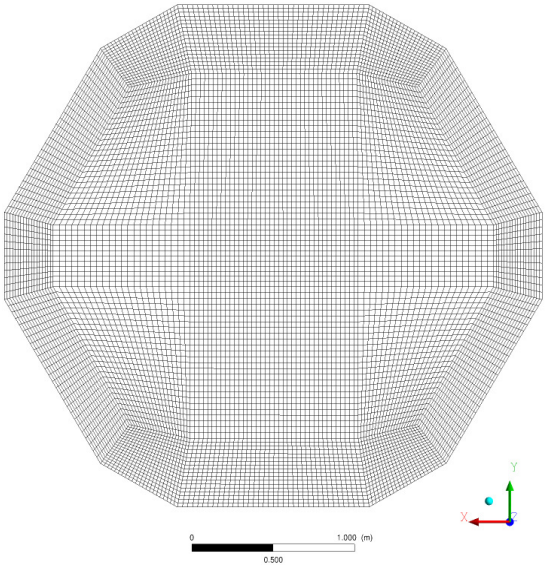

Fig. 8 Computational grid (top view) of a VVER-1000 core

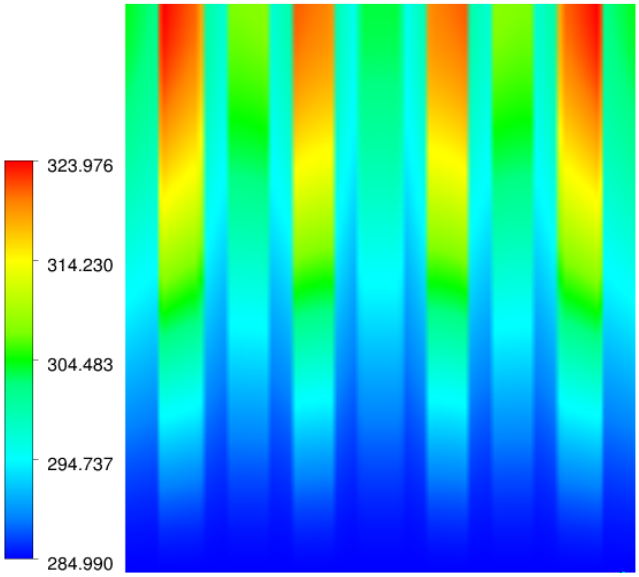

Fig. 9 Temperature (°C) distribution in the z-y plane

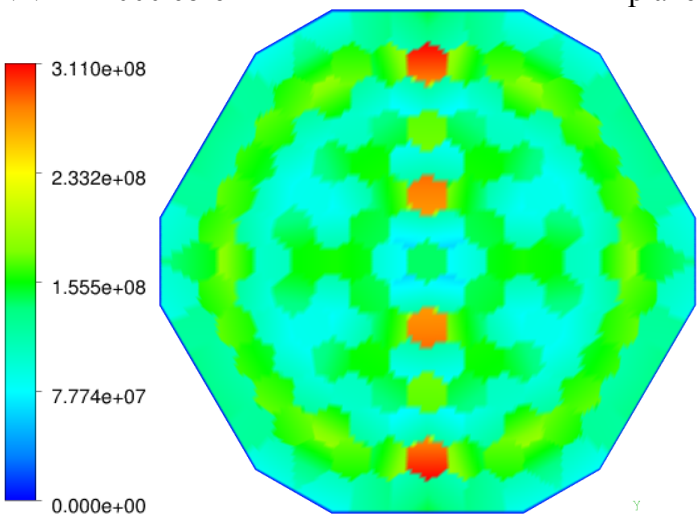

Fig. 10 Heat source (W/m^3) distribution at z=1.38 m above bottom

A small lateral coolant flow from the circumference of the core centre can be observed. It is driven by the acceleration of the liquid in the centre due to the stronger heating. This flow increases

the exchange of heat in the lateral direction by advection and leads to a 'smearing' of the step-like temperature profile that is usually being found in a pure DYN3D calculation with its 1D thermal hydraulic model.

5. Conclusions and future work

The coupling of the CFD code ANSYS CFX with the neutron-kinetic core model DYN3D was successfully accomplished. The new coupled code system ANSYS CFX/DYN3D allows for more realistic analyses of coupled thermal hydraulics – neutron kinetics problems. Steady-state and transient verification calculations for a small-size test problem confirmed the correctness of the implementation of the coupling.

After this verification a steady-state full power calculation for a full VVER-1000 reactor was carried out in order to show the applicability of the new code system to real problems.

Further verification and validation is needed before its application to accident scenarios. In the near future the semi-implicit time domain coupling should be introduced in the coupling. The extension of the coupling to two-phase flow conditions is a further precondition to carry out realistic accident analyses. In this field additional methodical work has still to be done, e.g. on the splitting of the volumetric heat source between liquid heat-up and vaporization and on two-phase flow treatment in the porous body approach. Further work will also be done on the automated mesh generation for the coupled code.

One of the first applications could be the analysis of a boron dilution accident including the 3D coolant mixing in the downcomer and lower plenum.

Acknowledgement

The projects this paper is based on were funded by German Federal Ministry of Economics and Technology (Contract numbers 150 1328 and 150 1358).

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