PROTOTYPE COUPLING OF THE CFD SOFTWARE ANSYS CFX WITH THE 3D NEUTRON KINETIC CORE MODEL DYN3D

S. Kliem and U. Rohde
Forschungszentrum Dresden-Rossendorf; Institute of Safety Research
P.O.B. 510119; D-01314 Dresden; Germany
S.Kliem@fzd.de; U.Rohde@fzd.de

J. Schütze
ANSYS Germany GmbH
Birkenweg 14a; D-64295 Darmstadt; Germany
Jochen.Schuetze@ansys.com

Th. Frank
ANSYS Germany GmbH
Staudenfeldweg 12; D-83624 Otterfing; Germany
Thomas.Frank@ansys.com

ABSTRACT

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 by 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. This test problem was a mini-core consisting of nine real-size fuel assemblies. Comparison was performed with the DYN3D stand-alone code. In the steady state, the effective multiplication factor obtained by the ANSYS CFX/DYN3D codes shows a deviation of 9.8 pcm from the DYN3D stand-alone solution. This difference can be attributed to the use of different water property packages in the two codes. The transient test case simulated the withdrawal of the control rod from the central fuel assembly at hot zero power. 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 1 MW at a power level of 50 MW. Beside the different water property packages, these differences are caused by the use of different flow solvers.

Key Words: Computational Fluid Dynamics, 3D neutron kinetics, Code coupling

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 feedback 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

PHYSOR 2010 – Advances in Reactor Physics to Power the Nuclear Renaissance
Pittsburgh, Pennsylvania, USA, May 9-14, 2010

2/10

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.
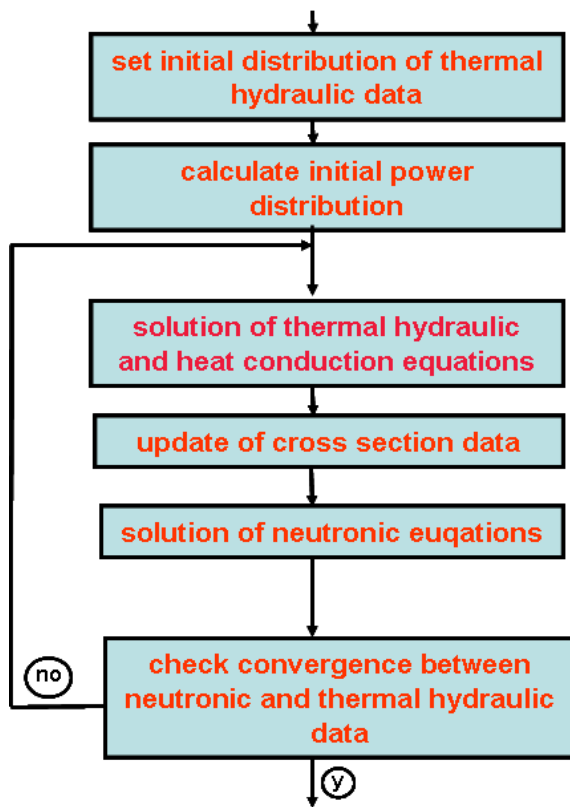

Figure 1. Standard iteration scheme in DYN3D for steady-state calculations
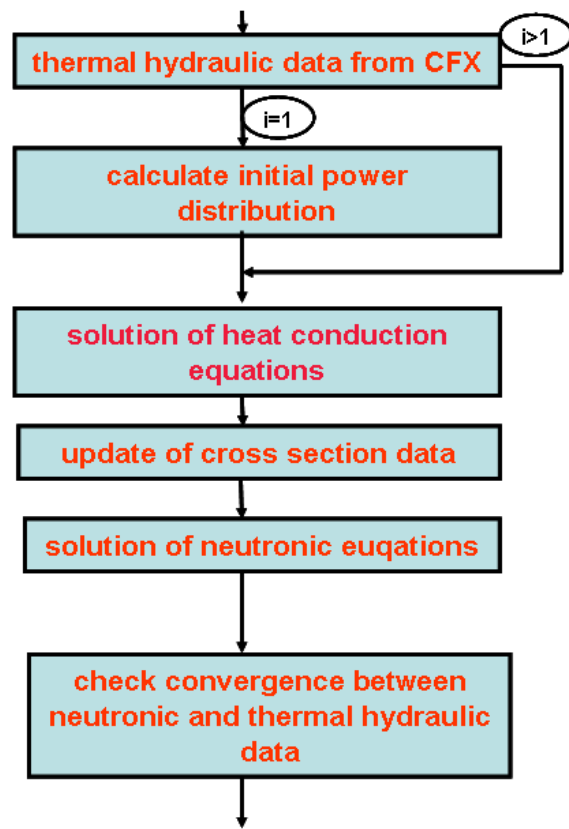
Figure 2. Iteration scheme in ANSYS CFX / DYN3D for steady-state calculations (DYN3D part)

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 interactive and CCL 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). 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 at the end of each time-step. An extension to a semi-implicit coupling with iterations between the codes within each time step is planned to be implemented.

Neither the iteration scheme nor the convergence criteria were changed in the 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 nine real size PWR fuel assemblies (Fig. 3). The fuel assemblies have a cross section of 0.21 m*0.21 m and a height of 3.60 m. The flow rate in this mini-core was set to 739 kg/s, the inlet temperature is 286 °C.

Figure 3. Scheme and DYN3D mesh of the mini-core
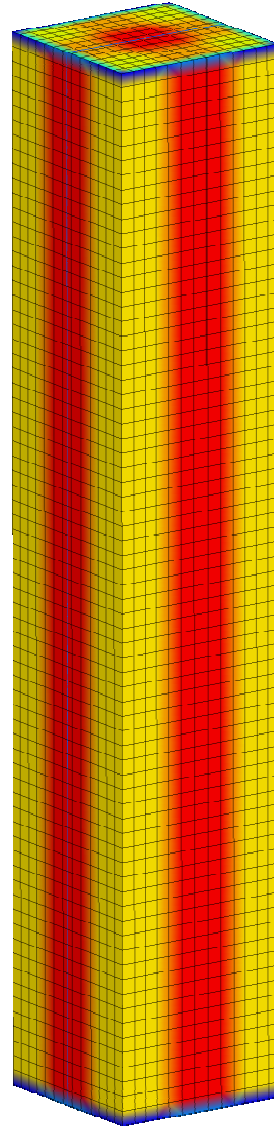
Figure 4. ANSYS CFX calculation grid of the mini-core

PHYSOR 2010 – Advances in Reactor Physics to Power the Nuclear Renaissance
Pittsburgh, Pennsylvania, USA, May 9-14, 2010

5/10

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 14.308 nodes. The fluid flow solver in ANSYS CFX was set up so as to only allow purely 1D flow in parallel channels in order to ensure the comparability with the DYN3D stand alone results.

3.1. Steady-State Problem

For the verification of the steady-state calculation procedure, the power of the mini-core was set to 50 MW. This ensures an average heat-up of about 13 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 9.8 pcm, only.
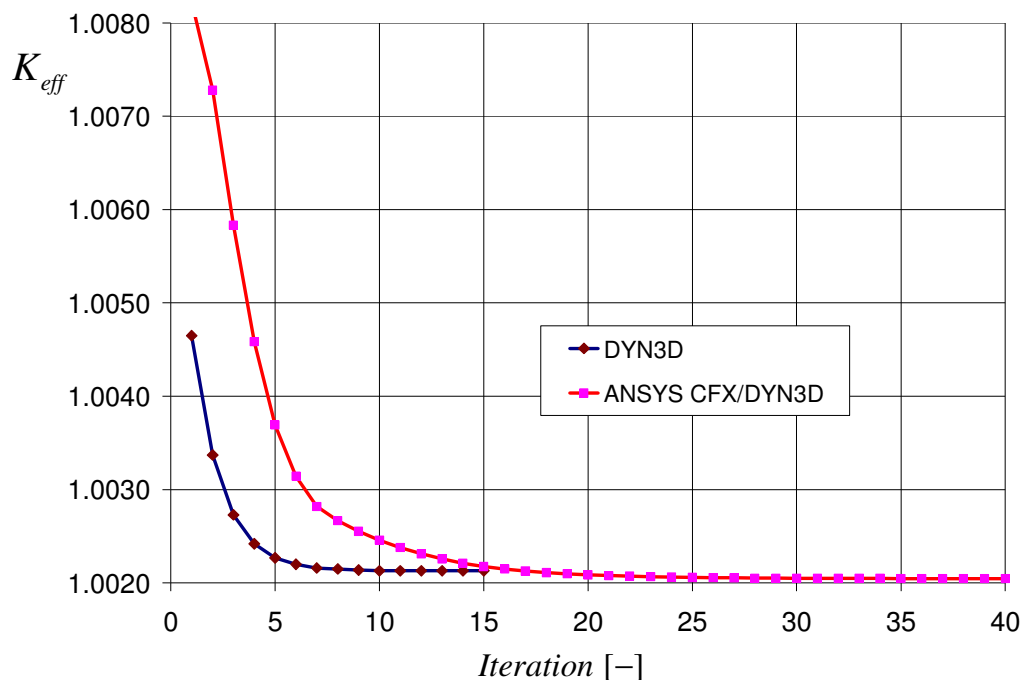

Figure 5. Convergence of steady-state calculations

The coolant temperatures between the two calculations match very well (not shown). A small difference is found in the axial density distribution (Fig. 6 shows the axial density distribution in three different channels; differences are most visible in the upper part of Channel 1, only). The reason for the differences

was found in different material property packages. CFX uses the current standard for water properties IAPWS-IF97 while DYN3D uses the former standard IFC-67. Variation calculations have shown that the difference in K_{eff} fully vanishes if identical properties are used. The same result was reached by lowering the inlet temperature in the CFX/DYN3D coupled calculation by as little as 0.155 K. It should be noted that this difference in temperature is within the accuracy of both water properties formulations, which is 0.25 K.
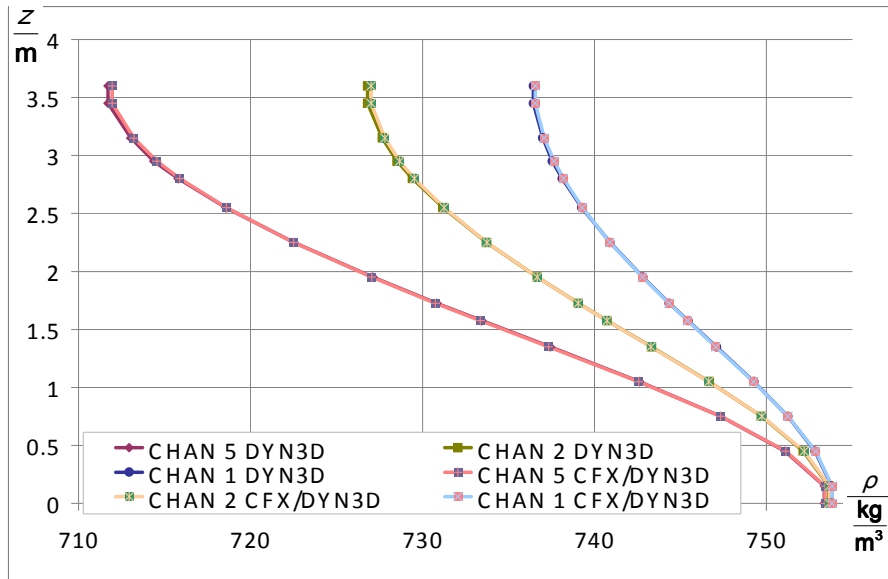

Figure 6. Axial coolant density distribution in three channels of the mini-core

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 20 s. Since a 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. 7 and Fig. 8. For comparison purposes the iteration within each time step in the DYN3D stand-alone code was deactivated.

The power starts to rise remarkably after 7 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.

PHYSOR 2010 – Advances in Reactor Physics to Power the Nuclear Renaissance
Pittsburgh, Pennsylvania, USA, May 9-14, 2010

7/10

The overall behavior of the core power is identical in all four calculations. Differences are to be seen in the maximum value reached. This maximum reduces with decreasing time step size in both codes. Both codes converge to different maximum values. This was proven by further reduction of the time step. The difference in the maximum core power is about 1 MW. This difference is acceptable considering the following: The introduced positive reactivity during the transient is slightly below 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. One such difference is already known to lie in different water material property packages.

Further investigation on the transport of a temperature perturbation through the reactor core confirmed that the DYN3D flow solver shows some additional difference in comparison to the ANSYS CFX flow solver, whose results can be taken as the reference.
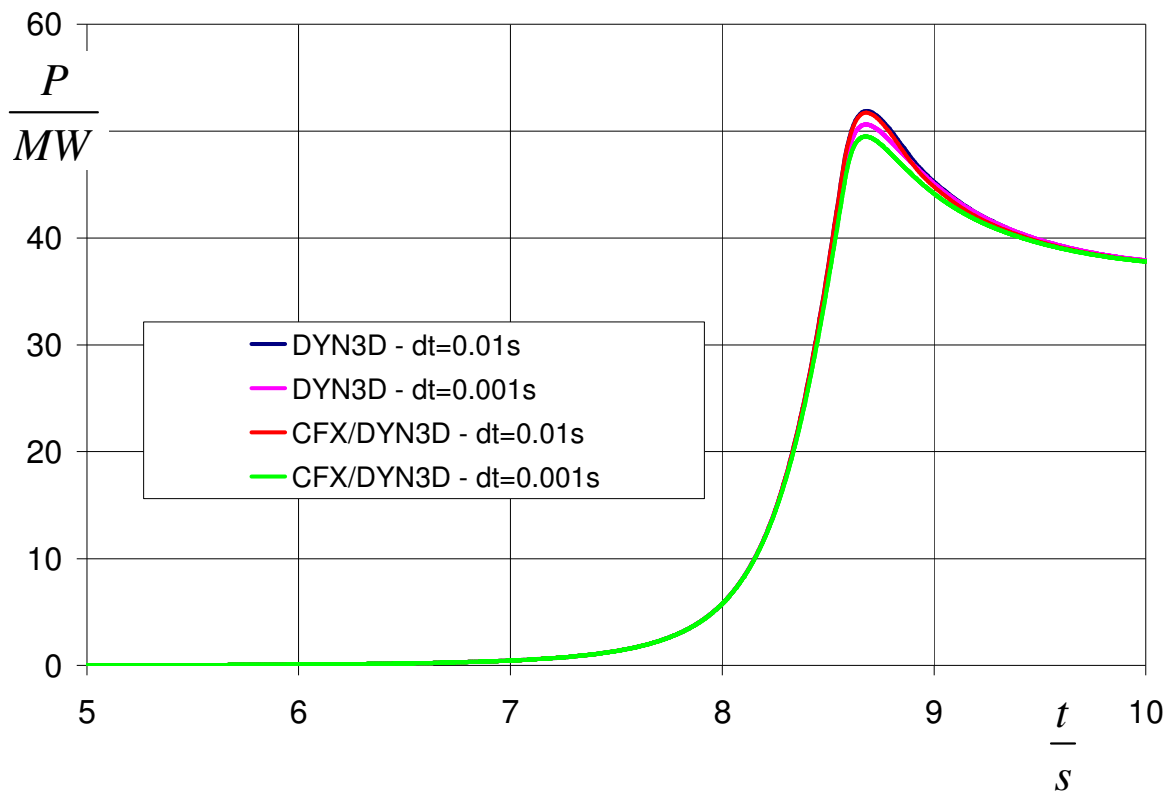

Figure 7. Core power behavior in the DYN3D and CFX/DYN3D calculations
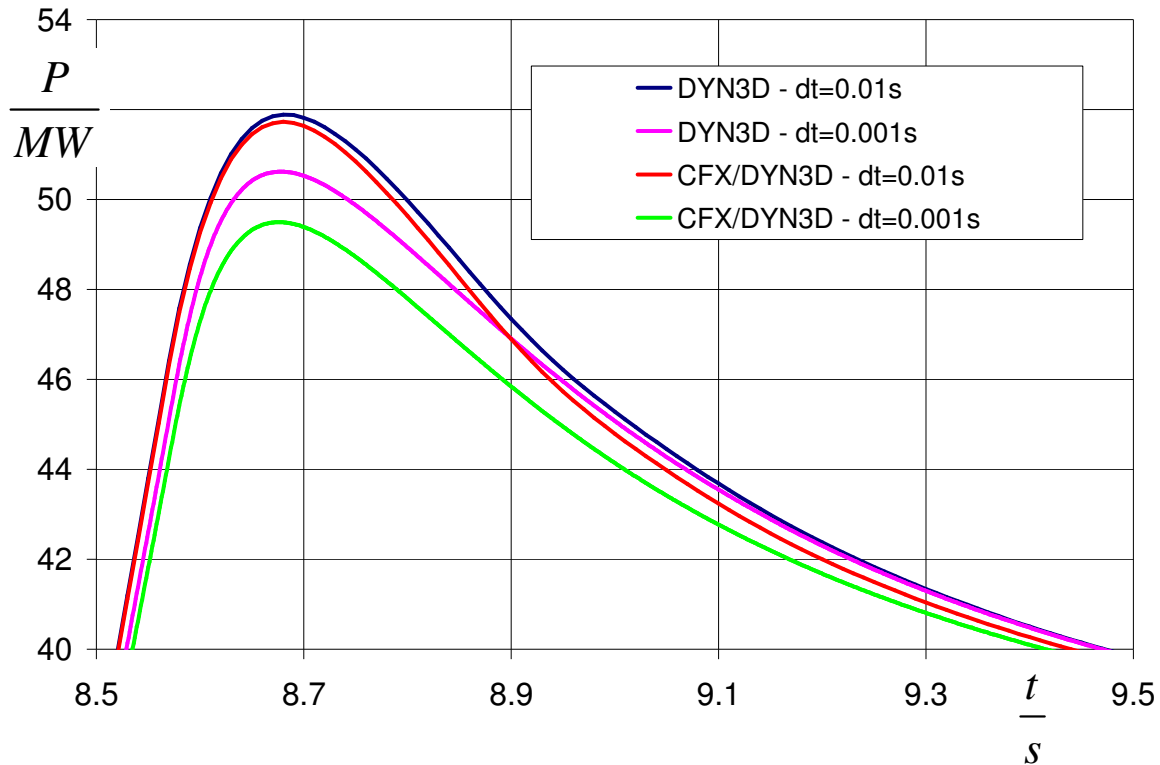
Figure 8. Core power behavior (zoom)

4. 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.

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.

ACKNOWLEDGMENTS

REFERENCES

1. U. Grundmann, U. Rohde, S. Mittag, "DYN3D – Three Dimensional Core Model for Steady-State and Transient Analysis of Thermal Reactors" *Proc. of the 2000 ANS International Topical Meeting on Advances in Reactor Physics and Mathematics and Computation into the Next Millennium (PHYSOR 2000)*, Pittsburgh, USA, CDROM, (2000)
2. C. Beckert, U. Grundmann, "Development and verification of a nodal approach for solving the multigroup SP3 equations", *Annals of Nuclear Energy*, **35/1**, pp. 75-86 (2008)
3. Y. Kozmenkov, S. Kliem, U. Grundmann, U. Rohde, F.-P. Weiss, "Calculation of the VVER-1000 coolant transient benchmark using the coupled code systems DYN3D/RELAP5 and DYN3D/ATHLET", *Nucl. Eng. Design*, **237**, pp. 1938-1951 (2007)
4. S. Kliem, Th. Höhne, U. Rohde, F.-P. Weiss, "Experiments on slug mixing under natural circulation conditions at the ROCOM test facility using high resolution measurement technique and numerical modeling", *Proceedings of the OECD/NEA & IAEA Workshop: "Experiments and CFD Codes Application to Nuclear Reactor Safety"*, Grenoble, France, CDROM, paper MIX-03, (2008)
5. Th. Höhne, S. Kliem, U. Bieder, "Modeling of a buoyancy-driven flow experiment at the ROCOM test facility using the CFD-codes CFX-5 and TRIO_U", *Nucl. Eng. Design*, **236**, pp. 1309-1325 (2006)
6. Th. Höhne, S. Kliem, U. Rohde, F.-P. Weiss, "Buoyancy driven coolant mixing studies of natural circulation flows at the ROCOM test facility using ANSYS CFX", *Nucl. Eng. Design*, **238**, pp. 1987-1995, (2008)
7. Th. Höhne, S. Kliem, R. Vaibar, "Experimental and numerical modeling of transition matrix from momentum to buoyancy-driven flow in a pressurized water reactor", *J. of Engineering for Gas Turbines and Power*, **131**, pp. 012906-1 – 012906-10 (2009)
8. D. Lucas, I. Tiselj, Y. Hassan, F. Moretti, "Computational Fluid Dynamics (CFD) for gas-liquid flows", *Science and Technology of Nuclear Installations*, **vol. 2009**, Article ID 725247(2009)
9. ANSYS Inc., *ANSYS 12.0 User's Guide,* Canonsburg, PA, USA (2009)
10. A. Papukchiev, "Coupling of ANSYS CFX and ATHLET: Progress Report", Presentation at the 16th meeting of German CFD Network, 07-08, October, 2009, Garching, Germany (2009)
11. S. Kliem, Y. Kozmenkov, T. Höhne, U. Rohde, "Analyses of the V1000CT-1 benchmark with the DYN3D/ATHLET and DYN3D/RELAP coupled code systems including a coolant mixing model validated against CFD calculations", *Progress in Nucl. Energy*, **48**, pp.830-848, (2006)
12. Th. Frank, C. Lifante, C.L. Waata, J. Schuetze, Final Report in the German GRS-BMWi Project No. 150-1328 "Development of CFD Software for Simulation of Multidimensional Flows in Reactor Cooling Systems", ANSYS Germany GmbH, Otterfing, Germany, ANSYS Technical Report ANSYS/TR-09-02, (2010) (in preparation, in German language)