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CFD-NEUTRONIC COUPLED CALCULATION OF A QUARTER OF A SIMPLIFIED PWR FUEL ASSEMBLY USING ANSYS CFX 12.1 AND PARCS

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Abstract

CSAP (Coupled Solver ANSYS CFX/PARCS), a new computational code system based on coupling the 3D neutron diffusion code PARCS v2.7 and the Computational Fluid Dynamics (CFD) commercial code Ansys CFX 12.1 has been developed as a tool for detailed nuclear reactor core calculations. This paper presents the methodology to couple the CFD code with the neutronic code and also results of steady state and transient calculations of a quarter of PWR fuel assembly. The same calculations have been performed with RELAP5/PARCS coupled code in order to compare the results obtained with ANSYS CFX/PARCS and to assess the consistency and correctness of the calculation procedure.

Introduction

In order to license a nuclear power plant (NPP) a broad range of analyses can be carried out by using 1D thermal-hydraulic Best Estimate (BE) codes able to simulate the entire plant in transient and accidental conditions. By using them, it is possible to simulate a wide variety of scenarios not only involving accident conditions, such as, for instance, Loss of Coolant Accidents (LOCAs), but also transients of interest for normal operation, like the insertion or extraction of control rods. These transients can be analyzed with the available coupled thermal-hydraulic-neutronic code systems which are capable of simulating the thermalhydraulic and neutronic behaviour of a nuclear reactor with a high grade of reliability.
Nevertheless, the detailed study of asymmetries in the power and mass flow distributions inside the fuel assemblies, even using the coarse 3D flow capabilities available in some of the BE codes, is somehow beyond the scope of these coupled code systems.
A high degree of intra-fuel assembly flow spatial resolution can be achieved with Computational Fluid Dynamic (CFD) codes, They are able to reproduce detailed 3D flow phenomena at the level of single fuel rods, and can also consider turbulence and its effect on the dynamics of the flow that determine local heat transfer phenomena of importance in the evaluation of fuel integrity. CFD codes yield very detailed velocity and temperature fields in the moderator, which can be then coupled to refined neutronic and fuel material descriptions in order to obtain an unprecedented degree of fidelity in the analysis of nuclear fuel behaviour.
This paper describes a coupling procedure between a *generic* CFD code and a neutron diffusion code and its application to ANSYS CFX 12.1, a commercial CFD code and to the 3D transient

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neutron diffusion program PARCS. The resulting coupled code system, called Coupled Solver ANSYS-CFX/PARCS (CSAP), has been verified with a steady state test considering a quarter of a fuel assembly subchannel. The results have been compared with those obtained using the coupled code system RELAP5/PARCS to evaluate the consistency and correctness of the procedure.

1. Description of the coupled procedure and the data exchange process (CSAP)

This chapter describes the problem to be solved by the coupled tools and the way in which the equations of the general CFD software ANSYS CFX 12.1 and the neutron diffusion code are solved using common variables. Furthermore the data exchange and the synchronization processes are explained in detail. As result of the process, both programs working jointly can synchronize and use as input data the output data of the other code and viceversa

A state-of-the-art CFD code is able to predict with a high degree of accuracy the thermal-hydraulic behavior (steady-state and transient) of a solid-liquid system like that represented by a fuel assembly of a nuclear reactor when single-phase flow dynamics is considered. Ferrando et al. [1] and Conner et al. [2] have assessed CFD codes, at different resolution level, for nuclear safety applications. In previous work, the power shape considered in the nuclear fuel has been assumed to have a constant shape, or be determined by a given time dependent function, not influenced by the neutronic behavior of the fuel.

A neutronics code needs the values of fundamental thermal-hydraulic variables such as moderator temperature and density, and temperatures of the solid structures in order to determine the neutron flux distribution and the power produced in the fuel in a *dynamic* manner. As mentioned previously PARCS is currently coupled to the 1D thermal-hydraulic code RELAP5 or the 3D code TRACE. The information transfer between those codes is basically similar to what is needed when a CFD code is employed instead of the coarser thermal-hydraulic codes RELAP5 and TRACE. The correspondence between the thermal-hydraulic and neutronic meshes is relatively straightforward in the case of the coarser codes. Since the dimensions of the neutronic nodes and of the thermal-hydraulic computational volumes are similar, the values of the variables can be transferred between the codes relatively unchanged. In the case of using a CFD code for the flow and heat transfer simulation, however, neutronic and thermal hydraulic meshes have very different dimensions. Figure 1.1 shows an overview of the parameters needed by the two codes to perform a coupled simulation.

The coupling the CFD code ANSYS CFX to the neutron diffusion code PARCS makes it feasible to obtain results with a higher resolution regarding the local thermal hydraulic behavior of the fuel. The power produced in the nuclear fuel is dynamically calculated by the solution of the neutron diffusion equation by PARCS depending on the *local* and *instantaneous* conditions calculated by the CFD code appropriately adjusted for the neutronic nodal mesh size. PARCS provides the power distribution in each fuel rod, and this information is used by ANSYS-CFX as heat sources in the solid elements that simulate the individual fuel rods of the fuel assembly. A conjugate-heat transfer solution developed by the authors with detailed radial and axial nodalization of individual fuel rods is then coupled to the general fluid flow ANSYS-CFX solution in the flow regions surrounding the fuel rods, and the new flow field is calculated. This is done for each time step in a transient or iteration step in a steady state solution convergence criteria and time step sizes are selected according to the characteristics of the neutronic and CFD solution at each time or iteration step, so that the more restrictive ones from the point of view of accuracy and stability are selected for both codes. In our experience, the CFD solution is usually the one controlling the calculation process.

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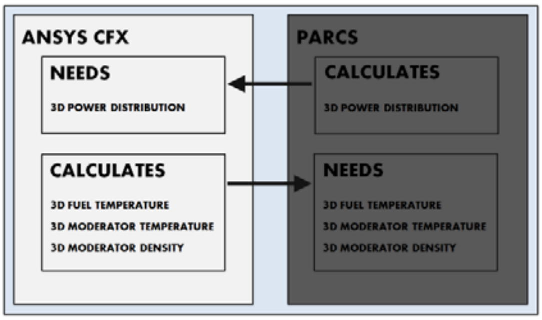

Figure 1.1. Overview of the parameters needed by the two codes to perform a basic coupled simulation

1.1 Description of the Coupled Solver ANSYS-CFX/PARCS

The development of the coupling scheme was performed in two phases, since the two codes use different nodalizations and there is a need of a separated averaging and interpolating procedures. Figure 1.2 describes the complete data exchange flow:

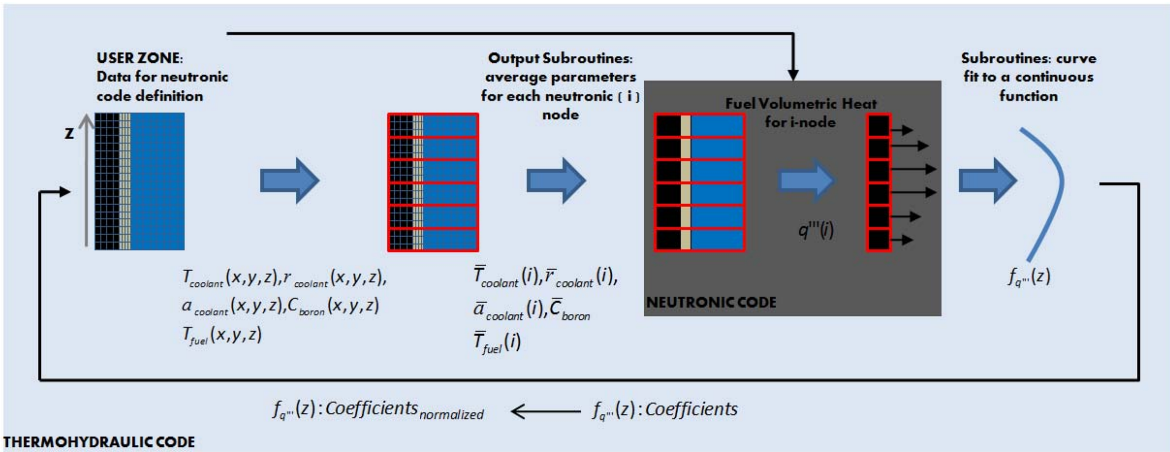

Figure 1.2. Data exchange flow

- **Phase A**: development of a set of subroutines for the calculation of the averaged values needed by the neutronic calculation.
- **Phase B**: development of the data exchange and synchronization subroutines; interpolation of neutronic data needed by the CFD calculation.

The dynamic library CSAP contains a group of 8 subroutines; they were developed in Fortran/C Mixed-Language Programming. The subroutines called directly from ANSYS CFX have been programmed in FORTRAN while the subroutine to synchronize and exchange data with PARCS by the mean of the PVM calls in C. The compilation has been realized under Linux using "Intel Fortran" and "gcc" compilers and has been linked to headers and shared PVM libraries. The correct working of the CSAP library has been tested on both Debian 5.0 and Mandriva 2010.2.
PVM is an integrated set of software tools and libraries that emulates a general-purpose, flexible, heterogeneous concurrent computing framework on interconnected computers of varied architecture [3]. In PVM a task is defined as a computational unit, analogous to a Unix process. The applications can be parallelized using passing through messages construction.

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1.1.1 Development of Phase A

A FORTRAN subroutine library has been developed in order to manage the data flow during the ANSYS CFX calculation. The library subroutines are developed using the "USER FORTRAN" interface offered by ANSYS. The goal of these subroutines is to calculate the *volume averaged* value of heat structure temperature, moderator temperature and density in each of the sub-domains defined for data exchange. The subroutines allow the calculation without previous definition of the domains during the meshing phase. This simplifies the geometry creation, the meshing phase and requires fewer interfaces to be defined during the pre-processing. The library has been developed to work in both in serial and parallel mode, steady state and transient calculations. They are mixed "*Junction Box*" or "*User CEL*" routines.

1.1.2 Development of Phase B

A external program in C has been written called by the subroutines launched by the CFD solver when the global quantities have been already calculated and are ready to be transmitted to the neutronic process. This program not only synchronizes the two processes (CFD and neutronics) but also submits the newly calculated data in the special format needed by each process.
The data transmitted to PARCS are those related to the previous time step. They are sent at the actual time step before starting the new calculation. The neutronic feedback is then used in the actual time step calculation. No time step shift for data transfer is needed.

1.2 Details of the tasks fulfilled by the CSAP subroutines

In figure 1.3, a scheme of the communication between processes is shown.

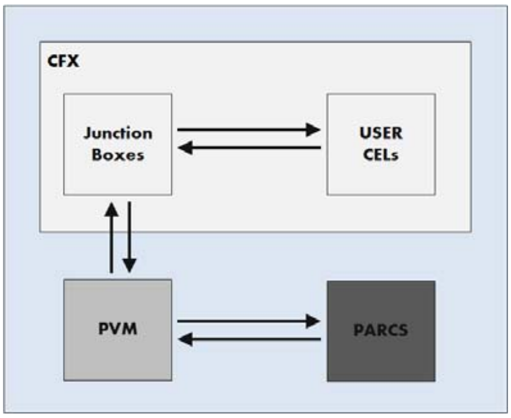

Figure 1.3. Schematic representation of the communication between processes

The developed subroutines are contained in the dynamic library *libcsap.so*. The tasks carried out by each of them are summarized next. In figure 1.4 a flow diagram representing the coupling scheme is shown. The coupling scheme is purely *explicit*. The thermal-hydraulic data calculated by ANSYS CFX and elaborated by CSAP are used for the calculation of the power distribution in PARCS at iteration *n*. This calculated heat distribution is then used in the thermal-hydraulic calculation at iteration *n+1*.

Before the simulation starts, a *Junction Box* routine is called during the "*User Input*" stage of the simulation before starting the solution stage. In a parallel run, this call is made only on the master process. This step creates and initializes files for temporary storage of the information of the processes on each partition.

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During the solution stage the calculation of the data to be transmitted between the codes is done after the end of the iteration *n* and before iteration *n+1*. This is needed because the data should be collected from ***all*** partitions. At this point the data calculated at iteration *n* are sent to PARCS through PVM and are used to calculate the power distribution that is transferred to ANSYS CFX to be used at iteration *n+1*. Before applying the power distribution as an energy source term an interpolation procedure is needed. The interpolation coefficients are calculated for the data of the power distribution delivered by PARCS through PVM using a *least squares polynomial fitting* procedure. In this way a *continuous* function for the energy source distribution is obtained and the appropriate value can be calculated and applied to each CFD mesh point. In this manner the coarser nodal mesh of PARCS can be consistently mapped to the much more detailed one used by ANSYS-CFX.

When the CFD solver reaches the convergence criteria set during the pre-processing phase, or the stop command is sent by the user, the CSAP library indicates the correct end of the thermal-hydraulic calculation to PARCS, so that also the neutronic calculation can terminate cleanly the calculation process.

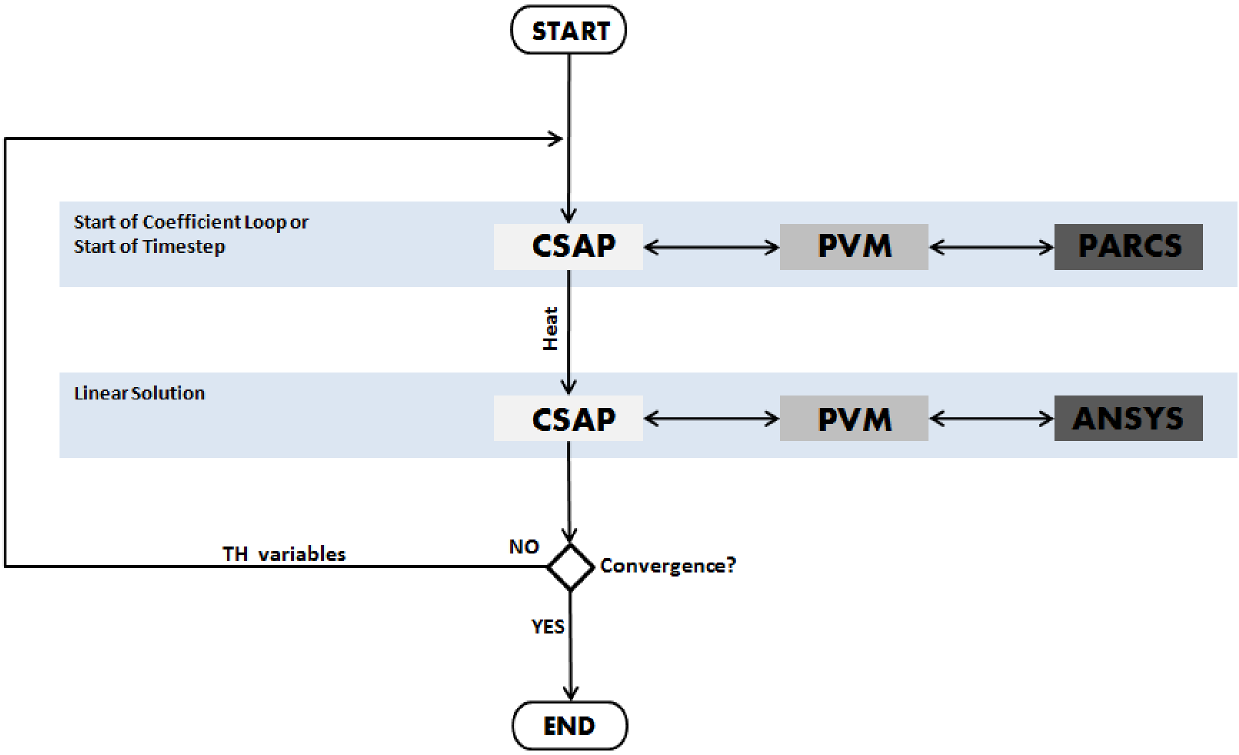

Figure 1.4. Explicit coupling scheme flow diagram

2. Description of the models used for validation

This chapter describes the problem to be solved by the coupled tools and the way in which the geometrical model has been implemented in the CFD and neutronic code.
A quarter of the nuclear reactor fuel assembly will be examined; a simplified sketch of the model cross section is shown in figure 2.1. The entire fuel assembly is composed by 16x16 positions while a quarter by 8 x 8: 59 fuel rods and 5 control rods. The fuel rod cladding outer diameter is 10.75 mm. The fuel pellet has a diameter of 9.11 mm and the gap has a thickness of 0.095 mm. The external diameter of the control rod is 13.8 mm. Four different domains have been identified: one fluid, for the moderator, and three different solid domains for fuel, clad and gap.

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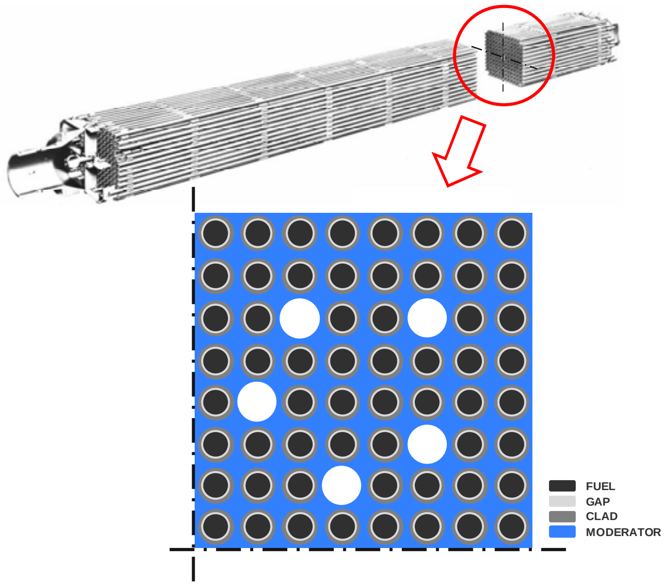

Figure 2.1. A PWR fuel assembly and a scheme of the channel cross section

The boundary conditions are summarized in Table 2.1.

Table 2.1: Boundary conditions for the steady state calculation

Moderator Inlet Temperature	567.7 K
Moderator Mass Flow Rate	22.277 kg/s
Reference Pressure	15.51 MPa
Average power of FA at full power	17.005 MW

2.1 Description of the ANSYS CFX model

Several CFD meshes were tested in order to set up the computational domain. After a mesh sensitivity analysis the shortest computational time and also independency of the results from the calculation mesh the model with by ca. 1350000 nodes representing one quarter of a nuclear reactor simplified fuel assembly using symmetric boundary conditions for the axial cut planes. This geometrical model is used to maintain the computational resources to a relatively low level but to test the coupling methodology with geometry close to reality.
The model consists of four different domains: one fluid and three solid domains (see figure 2.2). All of them are connected together by interfaces with the heat transfer option “Conservative Heat Flux”. Heat is only generated in the fuel domain but is transferred to the fluid through heat conduction in the gap and in the clad regions. The gap is modeled based on the gap conductance model. Heat transfer in the gap is in reality taking place based on different mechanisms: heat conduction, solid contact if the fuel pellet is cracked and restructured and radiation. Usually convection is neglected due to the conditions of the gas mixture contained in the fuel rod. For this reasons since approximation is required, the material contained in the gap has been defined in a solid state with characteristics of conductivity and density based on those included in the manual of RELAP5 to ensure the comparison between the results. In ANSYS CFX the material database has been extended in order to handle the materials used by RELAP5 and to ensure the compatibility between the

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results. The boundary conditions used for the CFD simulation are those reported in Table 2.1. A RANS turbulence model, based on the SST, for the liquid phase is used.

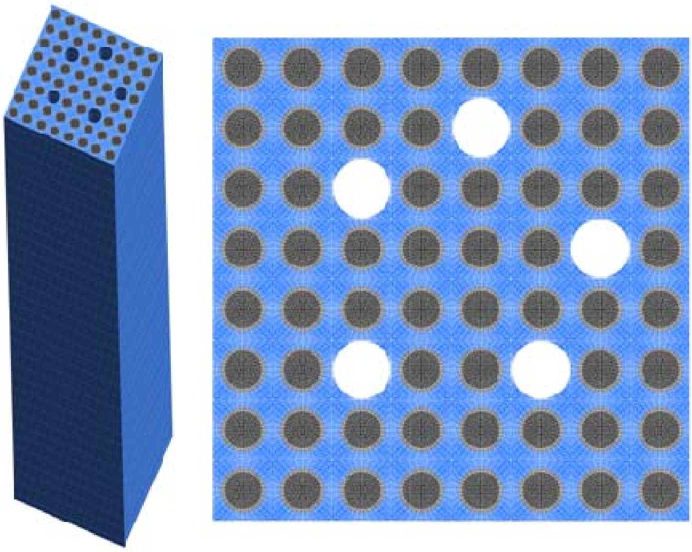

Figure 2.2. Overview of the quarter of fuel assembly model

The elementary mesh element used to build up the fuel assembly model is based on the scheme used to mesh a subchannel and it is shown in figure 2.3.

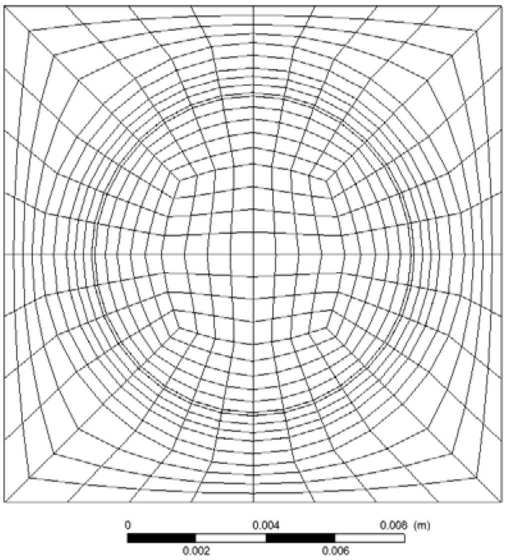

Figure 2.3. The cross section mesh used to build up the computational domain of the quarter of fuel assembly (detail of subchannel)

2.2 Description of the PARCS model

A 3D neutronic model of a generic PWR fuel assembly with the characteristics explained above has been created using PARCS 2.7. The cross sections and neutronic parameters for the fuel assembly have been calculated with the SIMTAB methodology based on the joint use of CASMO/SIMULATE and developed at the Polytechnic University of Valencia together with

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Iberdrola [4] [5] [6]. It can handle a wide spectrum of transient conditions since it has been generated for a broad range of temperature and pressure conditions.
The method used for the calculation of the Doppler temperature in the fuel is based on the LINC option. The fuel average heat structure temperature is calculated on the basis on the fuel centerline and outer surface temperature calculated by a thermal hydraulic code. The numeric scheme used for calculation is Hybrid.
The geometrical description of the fuel assembly model contains 34 nodes in the vertical direction (first node 14 cm, nodes 2 to 33 10.625 cm and last node 20 cm) and 1 in the radial direction both 23 cm long.
The boundary conditions are set, as done for full core LWR analysis, as reflective in the *x* and *y* directions (neutrons are reflected back into the core). The *z* boundary conditions for the upper and lower surface of the model are set as zero flux. Each node is assigned to a different planar region. It means that the neutronic parameters in each region are calculated independently to the others.

2.3 Description of the RELAP5 model

In RELAP5 the 1D thermal-hydraulic model of a generic fuel assembly is modeled using the PIPE component connected in parallel to the HEAT STRUCTURE, the solid representing the fuel rods. The PIPE is formed by 34 nodes but only the nodes 2 to 33 represent the actual active length of the fuel assembly, that it the heated fuel rod length. The heat exchange area between PIPE (only all along the active length) and HEAT STRUCTURE is set to be the total external surface of all the fuel rods contained in the fuel assembly. No fuel spacers have been considered, and only friction pressure losses along the fuel rods contribute to the pressure drop in the fuel assembly.
The boundary conditions applied are summarized in Table 2.1. In this way, it is possible to use a relatively simple modeling strategy to represent in an effective way even complicated geometries.

3. Results of simulation

The procedure described above to couple the CFD code ANSYS CFX and the neutronic code PARCS has been validated by comparing the results with those produced by the coupled results obtained using RELAP5/PARCS.
Both steady state and transient simulations have been performed and the results will be explained in the next sections.
Partitioning strategy plays an important role not only to minimize the communication time while maintaining the load balance. In this special case, it is playing an important role to obtain acceptable results by the means of user develop subroutines.
For a given calculation domain, depending on the partitions number, it could happens that each single subdomain (e.g a single rod, clad o gap) could be shared between partitions (see figure 3.1). In fact, local deviations between the subroutines and post calculated results in the near partitions border regions have been noticed. This created problems obtaining the average values to be exchanged to PARCS due to the fact that ANSYS CFX uses a node based partitioning method. The problem has been overcome using the fully automatic MeTIS partitioner with the default options. For the liquid domain this does not represent a problem since the gradients of the analyzed scalar quantities are limited compared to those in the fuel structures.
An analysis of the wall clock time for a transient calculation has been performed in function of the number of the processors used for calculation and the result is shown in figure 3.2.

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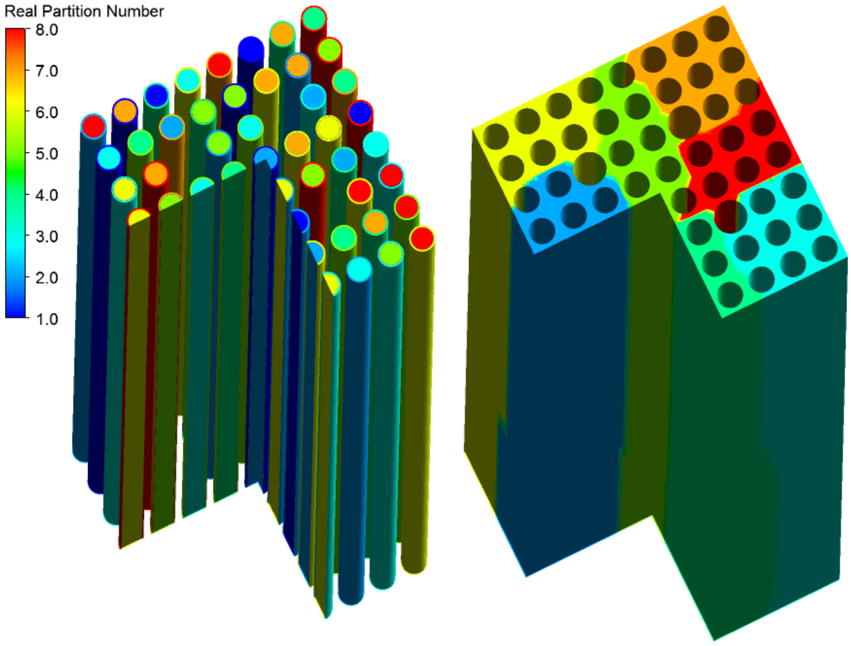

Figure 3.1. Partitioning in the fuel structures (left) and in the moderator (right) domain

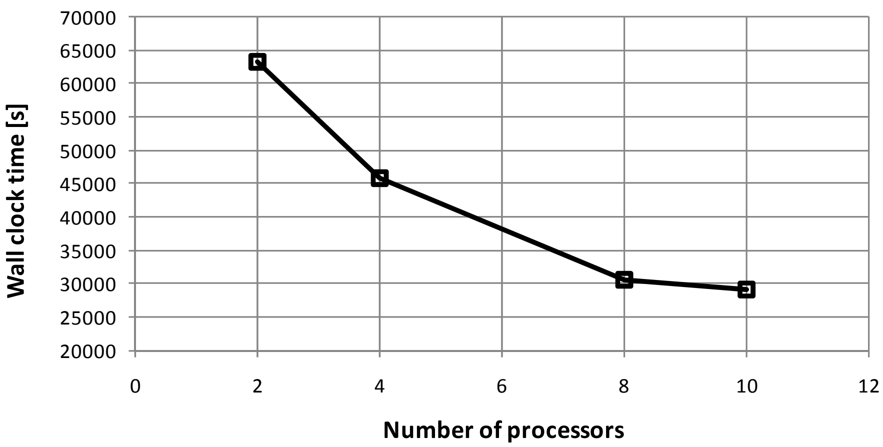

Figure 3.2. Wall clock time of a 25 s transient simulation - Inlet moderator temperature step (-50 K), time step 0.2 s.

3.1 Results of the steady state coupled simulation

A steady state ANSYS CFX/PARCS coupled calculation has been performed. The power distribution (assumed all rods have the same power) (figure 3.3 left) along the flow axis and the radial heat structure temperature profile at z = 164.69 cm (figure 3.3 right) obtained with RELAP5/PARCS match perfectly the ANSYS CFX/PARCS one.

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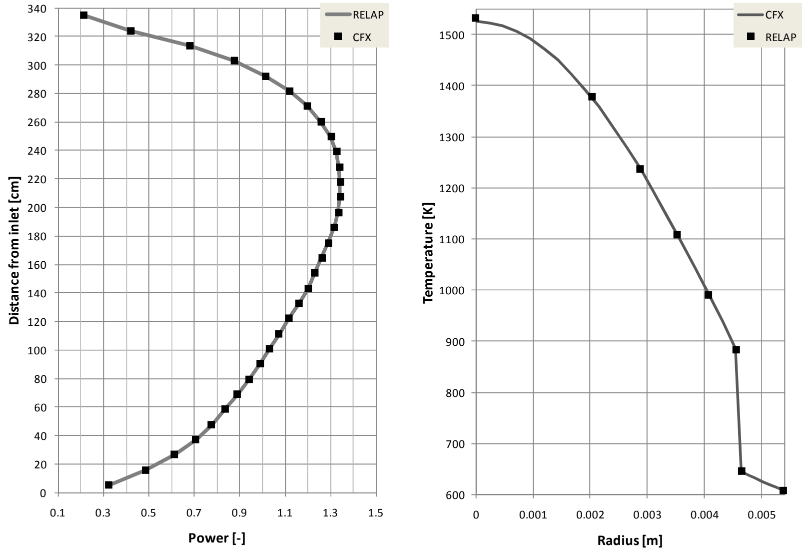

Figure 3.3. Comparison of the steady state power distributions (left) and heat structure radial temperature profile at z = 164.69 cm(right)

Also the average fuel centerline temperature (figure 3.4 left) and the average fuel outer surface along the flow axis (figure 3.4 right) obtained with RELAP5/PARCS match perfectly the ANSYS CFX/PARCS one.

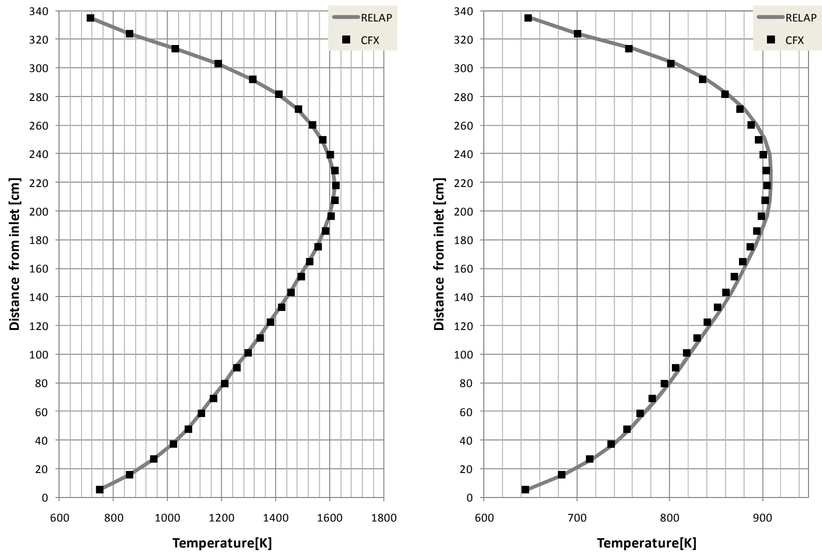

Figure 3.4. Comparison of the steady state fuel centerline temperature (left) and fuel outer surface temperature (right)

The average the moderator temperature, moderator density and velocity along the flow axis are shown in the diagrams of figure 3.5. The values of the ANSYS CFX-PARCS coupled calculation are volume averages for those computational volumes that are contained in one of the much coarser computational volumes of RELAP5. The results show a near perfect agreement between both coupled solutions, thus validating the coupling procedure developed in CSAP. It is important to note that these results do not show all the capabilities of the ANSYS CFX-PARCS coupled code system,

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since detailed local values for flow and fuel rod variables have not been plotted, and the problem chosen does not contain intra fuel assembly asymmetries: all fuel rods have the same power. The choice of problem was dictated by the capabilities available in RELAP5-PARCS, so that both simulations could be rigorously compared.
The k-effective calculated by the RELAP5/PARCS simulation is 1.054313 and that calculated by ANSYS CFX/PARCS is 1.054482. The reactivity difference is about 1.6029 pcm and can be considered acceptable.

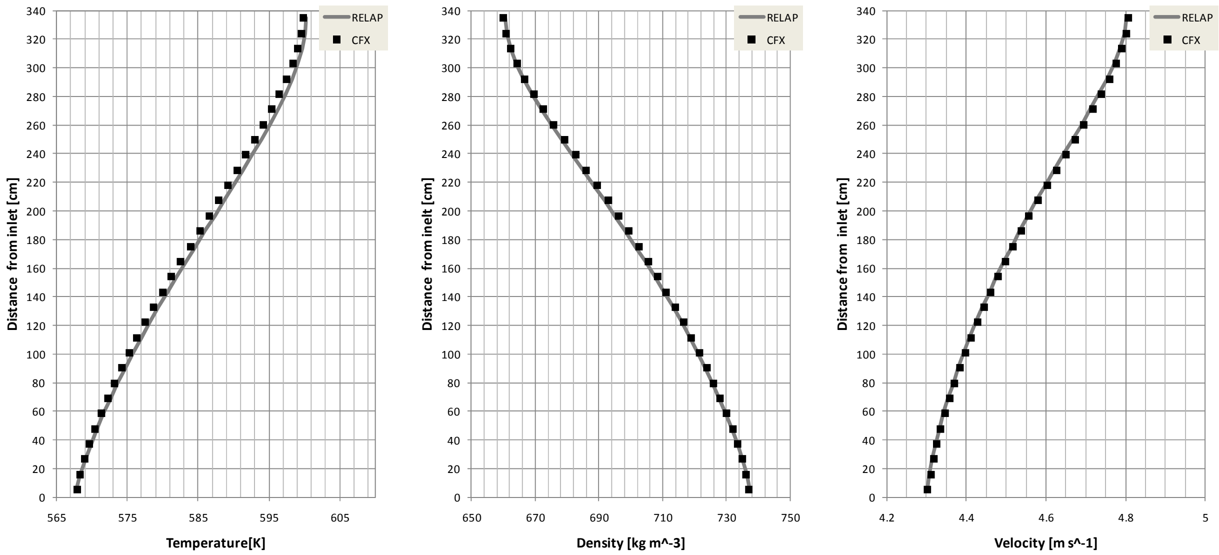

Figure 3.5. Comparison of the steady state average moderator temperature (center), moderator density (center) and moderator velocity (right) obtained with RELAP5/PARCS and ANSYS CFX/PARCS coupled calculation

3.2 Results of transient coupled simulation

Two different transient simulations have been realized and the results are shown in figure 3.6 and 3.7.

3.2.1 Results of "sinus" transient simulation

Figure 3.6 shows the results of a time dependent moderator inlet temperature changing following a sinus function with an amplitude of 20 K and a period of 20 s.
This transient could be representative of operational transient that could take place during a nuclear reactor normal operation. The temperature change is quite limited and the phenomena are taking place with a relatively slow time constant.
The results obtained with ANSYS CFX/PARCS and with RELAP5/PARCS are compared at three different axial locations: node 2 node 16 and node 31 of the RELAP5 HEAT STRUCTURE nodalization. The average transient heat structure temperature (figure 3.6 upper) and the average transient moderator temperature (figure 3.6 lower) obtained with RELAP5/PARCS match perfectly the ANSYS CFX/PARCS one.

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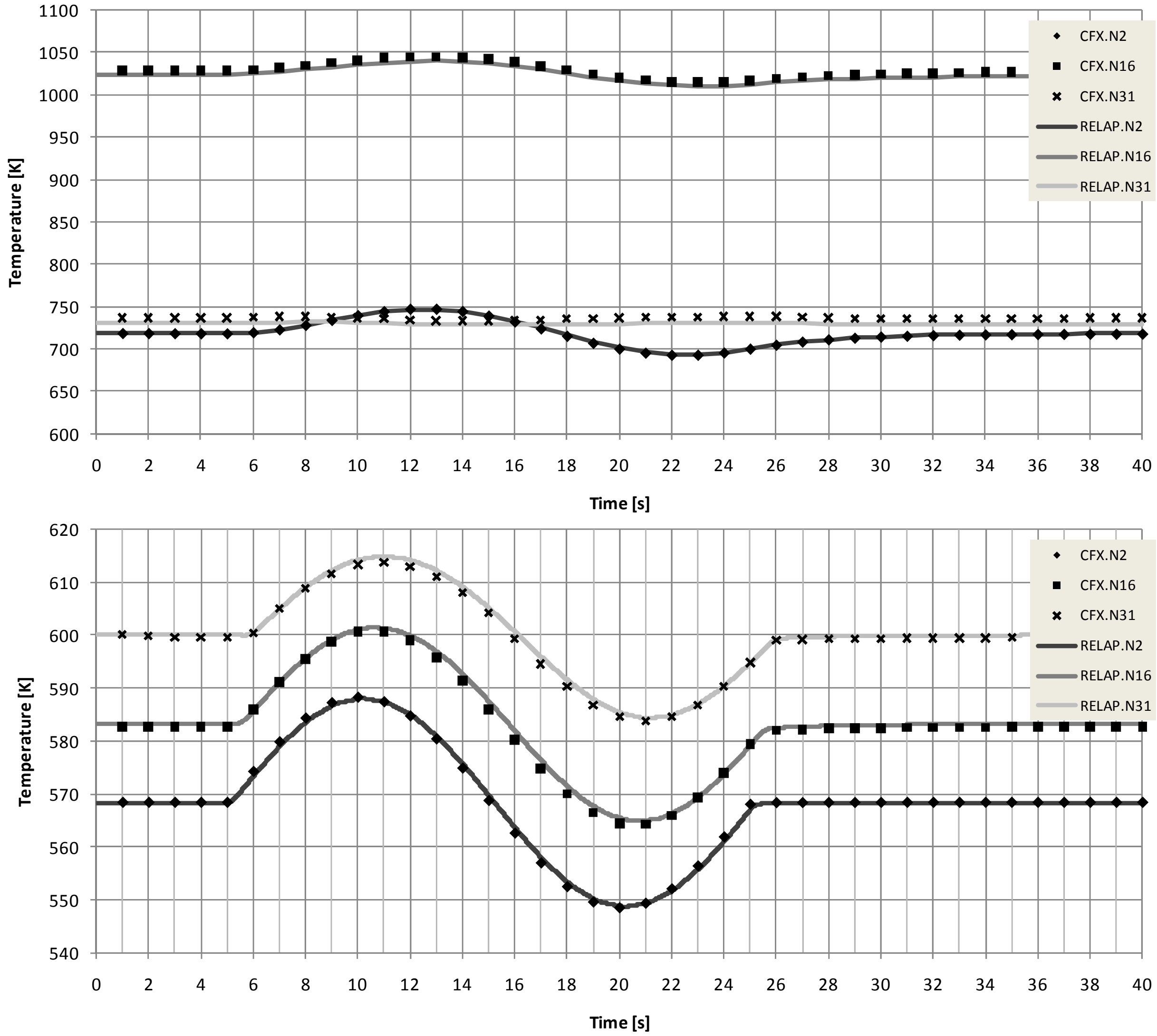

Figure 3.6. Comparison of the transient average heat structure temperature (upper) and moderator temperature (lower) at three different axial locations obtained with RELAP5/PARCS and ANSYS CFX/PARCS coupled calculation - Inlet moderator temperature

3.2.2 Results of the "step" transient simulation

Figure 3.7 shows the results of a time dependent moderator inlet temperature changing following a step function. The inlet water temperature suddenly decreases of 50 K.
This transient could be representative of an accidental condition where safety related mechanisms are taking place and suddenly water is injected at a lower temperature to help the cooling down of the reactor. In this case the phenomena time constants are smaller than the previous simulation.
The results obtained with ANSYS CFX/PARCS and with RELAP5/PARCS are again compared at the same three different axial locations. The average transient heat structure temperature (figure 3.7 upper) and the average transient moderator temperature (figure 3.7 lower) obtained with RELAP5/PARCS match perfectly the ANSYS CFX/PARCS one.

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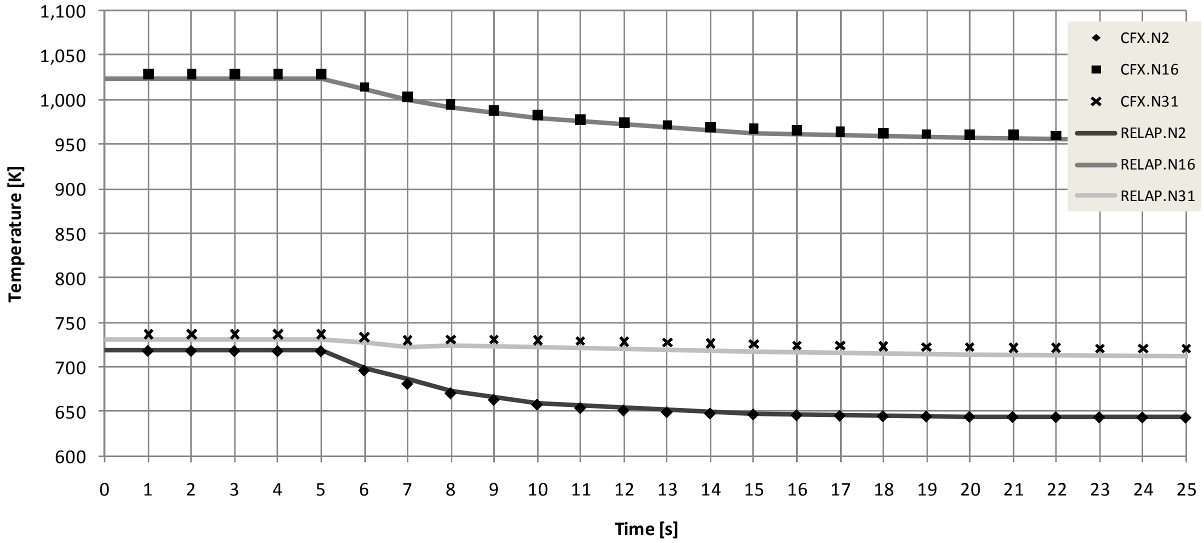

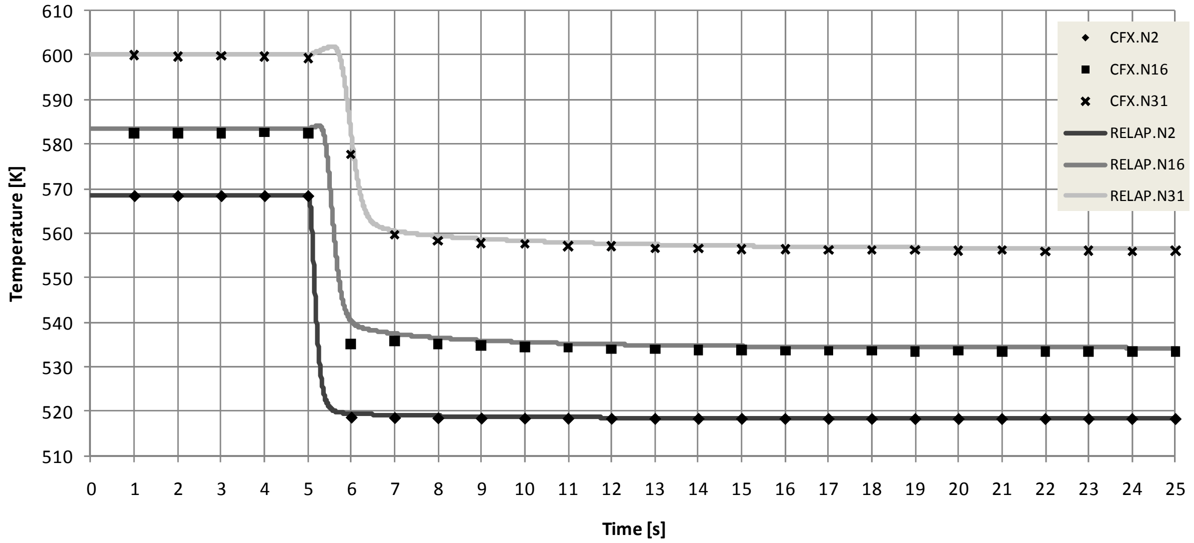

Figure 3.7. Comparison of the transient average heat structure temperature (upper) and moderator temperature (lower) at three different axial locations obtained with RELAP5/PARCS and ANSYS CFX/PARCS coupled calculation - Inlet moderator temperature step (-50K)

4. Conclusion

The generic coupling procedure between the CFD code, in the application shown ANSYS CFX, and the neutron diffusion code PARCS has been presented and tested on with a simplified fuel assembly model. The results obtained validate the procedure in both steady state and transient conditions. Further development is focused on the extension of the coupling code CSAP to make use of the 3D fuel rod power distribution reconstruction module included in PARCS and on the validation of the procedure with larger, more resource intensive models by considering one or more complete fuel assemblies in order to investigate more complex 3D flow-neutronic coupled phenomena.

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