Extension of the Simulation Capabilities of the 1D System Code ATHLET by Coupling with the 3D CFD Software Package ANSYS CFX

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ABSTRACT

The thermal-hydraulic system code ATHLET (Analysis of THermal-hydraulics of LEaks and Transients) is developed at Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) for the analysis of anticipated and abnormal plant transients, small and intermediate leaks as well as large breaks in light water reactors. The aim of the code development is to cover the whole spectrum of design basis and beyond design basis accidents (without core degradation) for PWRs and BWRs. In order to extend the simulation capabilities of the 1D system code ATHLET, different approaches are applied at GRS to enable multidimensional thermal-hydraulic representation of relevant primary circuit geometries. One of the current major strategies at the technical safety organization is the coupling of ATHLET with the commercial 3D Computational Fluid Dynamics (CFD) software package ANSYS CFX. This code is a general purpose CFD software program that combines an advanced solver with powerful pre- and post-processing capabilities. It is an efficient tool for simulating the behavior of systems involving fluid flow, heat transfer, and other related physical processes. In the frame of the German CFD Network on Nuclear Reactor Safety, GRS and ANSYS Germany developed a general computer interface for the coupling of both codes. This paper focuses on the methodology and the challenges related to the coupling process. A great number of simulations including test cases with closed loop configurations have been carried out to evaluate and improve the performance of the coupled code system. Selected results of the 1D-3D thermal-hydraulic calculations are presented and analyzed. Preliminary comparative calculations with CFX-ATHLET and ATHLET stand alone showed very good agreement. Nevertheless, an extensive validation of the developed coupled code is planned. Finally, the optimization potential of the coupling methodology is discussed.

KEYWORDS

CFD, system code, coupled simulations

1. INTRODUCTION

Thermal hydraulic system codes have been extensively developed by the nuclear industry, research institutes and technical safety organizations with the goal to improve the design and safety of nuclear installations. A large number of these simulation tools are based on the lumped parameter theory. Lumped parameter programs use networks consisting of 1D cells, where mass, momentum and energy equations are solved for each fluid phase and balanced over each node of the network. System codes are extensively validated against experiments and provide reliable results at low computational cost. However, since relevant reactor fluid flow and heat transfer phenomena are 3D in nature, 1D system codes have limitations on their application for specific nuclear reactor safety (NRS) problems with pronounced 3D phenomena like boron dilution, pressurized thermal shock and main steam line break. In order to overcome these deficiencies, different approaches are implemented and utilized by the system codes' developers. Some of these are based on the "quasi 2D representation" using multiple 1D thermal-hydraulic channels, which are connected by cross-connection objects, thus accounting for cross flows between these channels. Another approach for detailed 3D simulations is the generation of tables with system codes, containing time dependent thermal hydraulic parameters which are then provided to the CFD program as boundary conditions. Unfortunately, both approaches have significant limitations. Natural 3D phenomena like thermal mixing in the downcomer of the PWR can not be simulated properly by utilizing 1D cross-connection objects. With the second approach these restrictions are not present but the feedback of the simulated CFD flow domain (e.g. downcomer) to the whole simulated system (primary loops, secondary sides) is lost.

To avoid such constraints, innovative strategies are needed. A recent trend in the nuclear reactor safety research is the direct coupling of classical system codes with modern CFD simulation tools. In the present work the coupling interface between the best estimate system code ATHLET and the commercial CFD software package ANSYS CFX is described. Furthermore, results from test cases with open thermal-hydraulic systems and closed loop configurations are discussed along with the challenges related to the coupling process.

2. CFX-ATHLET COUPLING STRATEGY

The CFX-ATHLET coupling strategy was developed in close collaboration between GRS and ANSYS Germany [1]. It is based on an explicit coupling scheme. ANSYS CFX is the master code and ATHLET the slave. The next paragraphs shortly describe the main modifications which were made in both programs.

2.1. ATHLET Modifications

In order to prepare the system code for the coupling with ANSYS CFX, several major modifications were performed by ATHLET developers [2]. ATHLET was modified in a way that it could be executed as a subroutine by another code. A key parameter was introduced, that allowed control of the program execution. It is used by ANSYS CFX to call ATHLET for different run sequences: program initialization and reading of input data, steady state and transeint calculations, program finalization, etc. Two coupling options are available within ATHLET for data transfer, which allow the user to specify different boundary conditions at the different coupling interfaces:

- Coupling Option 1: ANSYS CFX calculates pressure and temperature fields, and transfers area averaged values to ATHLET. The system code interprets these as solution variables of a control volume at the edge of its network, so that all control volume variables could be routinely calculated. With the momentum equation ATHLET determines the mass and energy flows at the interface between ATHLET and ANSYS CFX domain.

- Coupling Option 2: Using the fluid state in the last control volume of the ATHLET pipe, ANSYS CFX calculates the mass and energy flows at the interface between ATHLET and ANSYS CFX domain. These are used by ATHLET as source terms for the mass and energy balance in the connected control volume.

2.2. ANSYS CFX Modifications

The CFX-ATHLET coupling technology is based on a more general framework which has already been established in ANSYS CFX for coupling purposes with other 1D system codes. For the CFX-ATHLET project, major modifications in ANSYS CFX were related to the extension of the ANSYS CFX command language (CCL) definitions and the utilization of the shared library which contains the interface and ATHLET code. New parameters like “System Code Symm” were introduced allowing the use of a reduced ANSYS CFX geometry model with symmetry boundary conditions while a full 1D geometry model is used in ATHLET. Another important modification in the CCL block is related to the calling sequence of the junction box routine which executes ATHLET.

2.3. Coupling Procedure

The coupling procedure of CFX-ATHLET is based on an explicit coupling scheme, where ANSYS CFX is the master code and ATHLET the slave. The first time step is done by the CFD program, and after the execution of the junction box routine the solution variables are given to ATHLET. With the new boundary conditions the system code calculates the same time interval and returns its results to ANSYS CFX, which continues with the next step (Fig.1).

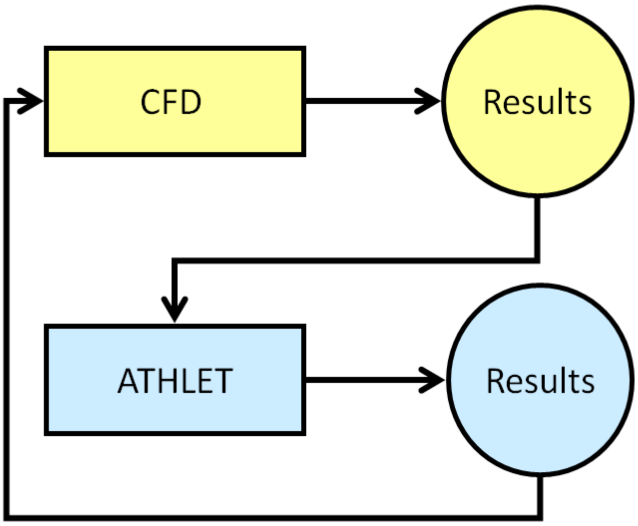


Fig. 1 CFX-ATHLET Coupling Procedure.

The advanced time integration module FEBE is a standard feature in ATHLET and can execute several smaller time steps if necessary, until the time specified by ANSYS CFX is reached. This option significantly increases the simulation stability, because the ATHLET time step size is not prescribed by the CFD code. In some coupled test cases it was observed that the system code performs even smaller time steps than ANSYS CFX. The coupling interface and ATHLET are linked in a shared library which is executed by ANSYS CFX after every time step.

2.4. Boundary Conditions

For the first coupled simulations, *Inlet* – *Outlet* boundary conditions in ANSYS CFX were used. In ANSYSY CFX, an *Inlet* boundary condition is used where the flow is predominantly directed into the ANSYS CFX domain and *Outlet* - for flows directed outside the ANSYS CFX domain. ATHLET obtains pressure and temperature from the CFD tool and after finishing the time step provides mass flow and enthalpy to ANSYS CFX *Inlet*. The calculation of these parameters is inverted when the coupling interface is at the *Outlet*. Multiple coupled calculations were successfully performed with the *Inlet* – *Outlet* boundary conditions showing good results. However, the simulation of flow reversal is not possible, because only positive mass flows can be specified at the ANSYS CFX *Inlet* and only negative mass flows at the ANSYS CFX *Outlet*. In reality, reverse flows occur during transients which are relevant for the nuclear reactor safety (trip of one main circulation pump, etc), and therefore, such conditions need to be addressed by the coupled system. For this reason the interface code was modified to allow the use of *Opening* – *Opening* boundary conditions in ANSYS CFX. ANSYS CFX *Opening* is used at a boundary where the flow direction can change (into or out of the CFD domain). With the new strategy, ATHLET provides fluid velocity instead of mass flow rate at the ANSYS CFX inlet *Opening*. In the first calculations constant temperatures and densities were used, however a full thermal coupling was introduced later. Figure 2 shows the exchanging parameters for both boundary configurations.

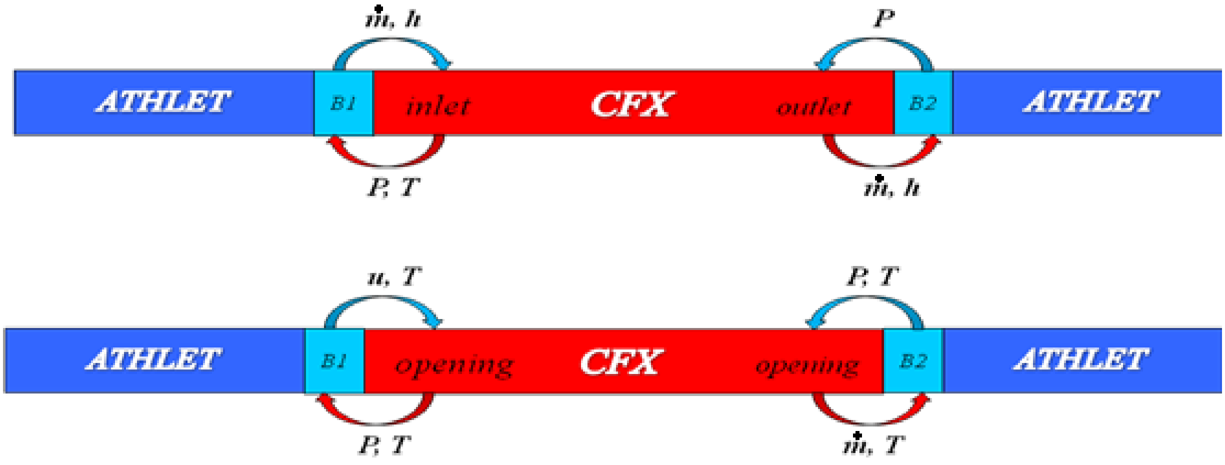


Fig. 2 Exchange Parameters for Both Boundary Configurations.

3. COMPARISON OF THE WATER AND STEAM PROPERTIES PACKAGES OF ATHLET AND ANSYS CFX

The comparison of the water and steam properties packages of ATHLET and ANSYS CFX was an important step which had to be performed before the coupled simulations. Identical or at least very similar thermal hydraulic parameters for a specified thermal hydraulic state is a prerequisite for a good convergence of the CFD code and simulation stability and hence for reliable results. For the coupled simulations, IAPWS IF97 water data was selected in ANSYS CFX code [3]. ATHLET utilizes IAPWS 80/95 package which is based on the state variables pressure, liquid and vapor temperatures [4]. Fortunately, both packages are based on the same standard thermal hydraulic data tables. Nevertheless, a small parameter table with several states was prepared and used to evaluate the differences, which could appear from the different interpolation techniques in both programs. For a given pressure and enthalpy, the corresponding temperature and density were calculated with ATHLET and ANSYS CFX. The comparison of the values showed very good agreement with differences not larger than 0.098% (Table 1). It should be mentioned that the pressure and enthalpy were varied in a very small range, relevant for the performed coupled calculations. More comparative calculations in a wider pressure-enthalpy or pressure-temperature range are needed. Moreover, a comparison of further thermal hydraulic properties is planned.

Table 1. Water Properties Calculated with ANSYS CFX and ATHLET

PRESSURE [bar]	**ENTHALPY [J/kg]**	**TEMPERATURE [^{0}C]**			**DENSITY [kg/m^3]**		
		CFX	ATHLET	Difference [%]	CFX	ATHLET	Difference [%]
98.100	855000	199.810	199.840	-0.0150	871.020	871.090	0.0080
98.200	855000	199.810	199.838	-0.0140	871.039	871.098	0.0067
98.300	855000	199.800	199.837	-0.0185	871.049	871.107	0.0066
98.399	855000	199.779	199.836	-0.0281	871.090	871.115	0.0029
98.100	856920	200.240	200.272	-0.0160	870.530	870.598	0.0078
98.250	859930	200.910	200.946	-0.0179	869.770	869.838	0.0078
98.350	861920	201.339	201.392	-0.0259	869.280	869.335	0.0063
98.396	864090	201.800	201.878	-0.0387	868.750	868.780	0.0035
150.060	950630	220.700	220.926	-0.1024	850.099	850.442	0.0402
150.060	1276400	288.470	288.753	-0.0981	748.239	748.414	0.0233

4. PIPE MODELING IN ATHLET AND ANSYS CFX

For the coupled simulations straight pipes were modeled using ATHLET and ANSYS CFX. In the input deck of the system code an ordinary 5.0 m long circular pipe with 0.2 m diameter and without internal connections was defined. The ATHLET pipe was discretized with 30 nodes. In the calculations dimensionless Darcy-Weisbach friction factors between 0.1 and

0.2 were used. For the CFD simulations a CAD model of the same pipe was created using ANSYS Design Modeler. In order to save computation time, only one fourth of the pipe was modeled and symmetry boundary conditions were specified at the symmetry planes. The geometry was then exported to ICEM CFD and a structured mesh was generated. It consisted of approx. 134 000 elements. The largest element has a length of 22 mm (Fig.3). The quality of the mesh was good, with all element angles greater than 45^0.

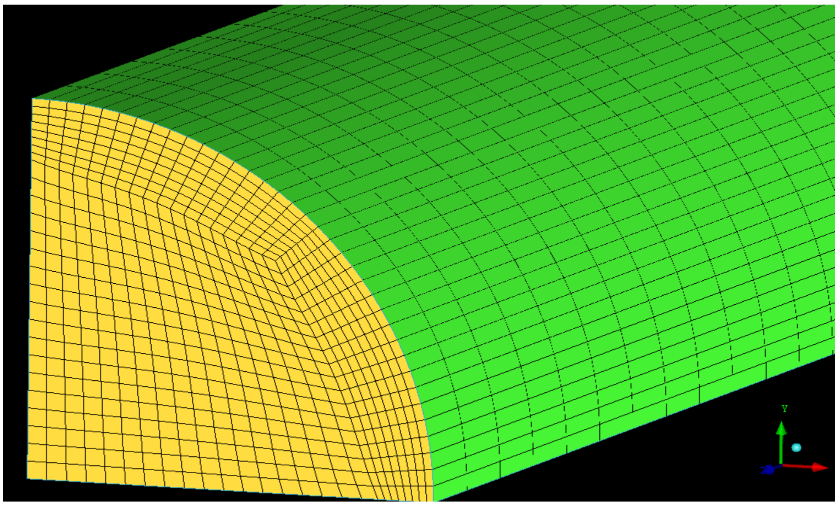


Fig. 3 Structured Mesh of a One Fourth Pipe Model.

5. TEST SIMULATIONS WITH THE COUPLED CODE SYSTEM CFX-ATHLET

The very first simulations with CFX-ATHLET were based on the coupling option 1, described in section 2.1. The analyses showed good results. In the next paragraphs more complicated test configurations are described. In all simulations the SST turbulence model was used and the time step was set to 0.05 s. In the cases with closed loop configurations it had to be reduced to 0.01 s.

5.1. Open Thermal Hydraulic System

As a next step an open thermal hydraulic system with two coupling interfaces was modeled. The main objective of this case was to demonstrate the ability of the coupled system CFX-ATHLET to cope with flow reversal. Figure 4 shows the test configuration consisting of two ATHLET and one ANSYS CFX pipe. Each pipe is 5.0 m long and has a diameter of 0.2 m. At the inlet of ATHLET pipe 1 a FILL boundary condition was defined which enables the specification of time dependent mass flow rate and enthalpy. At the outlet of ATHLET pipe 2 a time dependent volume (TDV) was connected in which constant pressure of 9.8 MPa and temperature at 200 ^{0}C were specified. During the simulation the FILL mass flow rate was gradually increased from 0 kg/s to 200 kg/s, kept constant for 3 seconds at this level and then decreased to -200 kg/s with the same gradient (Fig. 5). At 13 s simulation time flow direction reverses. Figure 6 shows the pressure in Branch 1 (B1, Fig. 4), which follows the mass flow progression. Three discontinuities are observed at 5 s, 8 s and 18 s. These are due to the abrupt changes in the boundary mass flow curve. From 0 s to 5 s the fluid is accelerated and the total pressure loss is the sum of the acceleration pressure loss and the fluid friction loss. From 5 s to 8 s the mass flow is kept constant and the acceleration pressure loss is zero, hence the pressure has to decrease at 5 s and stabilize at a certain level. The same explanation applies for the spike at 18 s, but because of the fluid deceleration between 8 s and 18 s, the system pressure stabilizes at a slightly higher value after 18 s. This was the first calculation which demonstrated the ability of the new coupled system to deal with more than one coupling interface and flow reversal at the same time. Pressure or velocity oscillations were not observed. Moreover, during the whole simulation, the CFX solution was converged to a tight convergence criteria of Residual MAX $<10^{-4}$ which was generally reached within less than 5 iterations per time step.

Fig. 4 Open Thermal Hydraulic System.

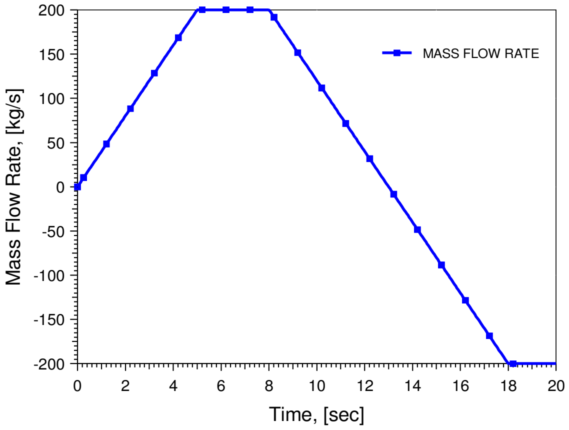


Fig. 5 FILL Mass Flow Rate.

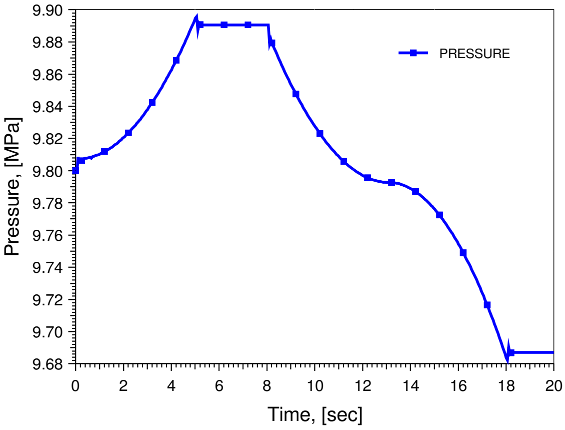


Fig. 6 Pressure in Branch B1.

5.2. Open Thermal Hydraulic System with Thermal Coupling Test

According to the coupling procedure, ATHLET and ANSYS CFX exchange temperatures at their interfaces. In normal flow conditions (fluid propagates from left to the right, i.e. inlet to outlet, Fig. 4) ANSYS CFX obtains the value from ATHLET, while in reverse flow conditions this is vice versa. At the outlet *Opening* ANSYS CFX provides temperature which is converted to enthalpy at the coupling interface. The enthalpy, the mass flow rate and the velocity are used to calculate the energy flow, which is then transferred to the first control volume of ATHLET pipe 2. In order to test this coupling sequence, a mass flow curve similar to the one used in the previous test case was defined. A temperature of 200 ^{0}C was specified in all three pipes, see Fig. 4. The FILL temperature was then decreased with time according to Fig. 7. Shortly before 4 s simulation time the cold water reaches the ANSYS CFX domain, propagating towards ATHLET pipe 2 (Fig. 8, Fig. 9). The fluid velocity is in the range of 7 m/s. After several seconds all three pipes are filled with cold water at a temperature of 160 ^{0}C. Flow reversal occurs 16 s after the start of the simulation. From that point in time, 200 ^{0}C hot water coming from the TDV starts entering the ATHLET pipe 2, then the ANSYS CFX pipe and finally reaches ATHLET pipe 1, see Fig. 8. The advantage of the 3D CFX-ATHLET simulation over standard 1D calculation is shown in Figures 9 and 10, which illustrate the three dimensional temperature distributions inside the ANSYS CFX pipe at 4 s and 19 s respectively. The left picture shows clearly the cold water entering the ANSYS CFX domain coming from the ANSYS CFX inlet *Opening* while Fig. 10 depicts 200 ^{0}C hot water from the TDV entering from the ANSYS CFX outlet *Opening* in reverse flow conditions.

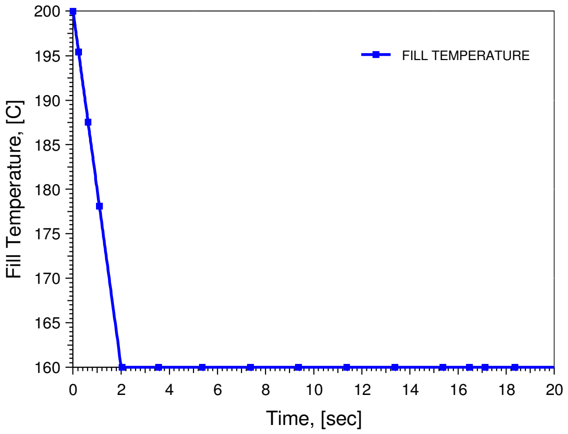


Fig. 7 FILL Temperature.

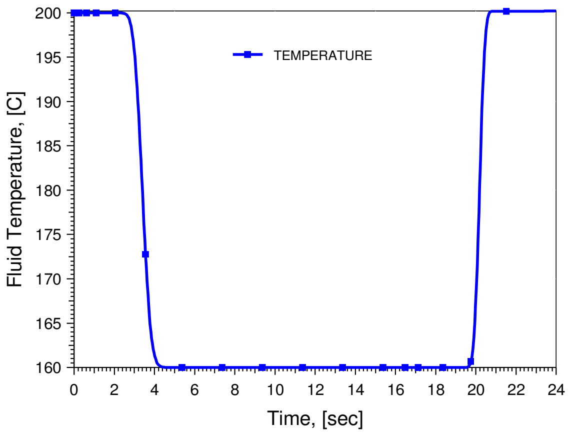
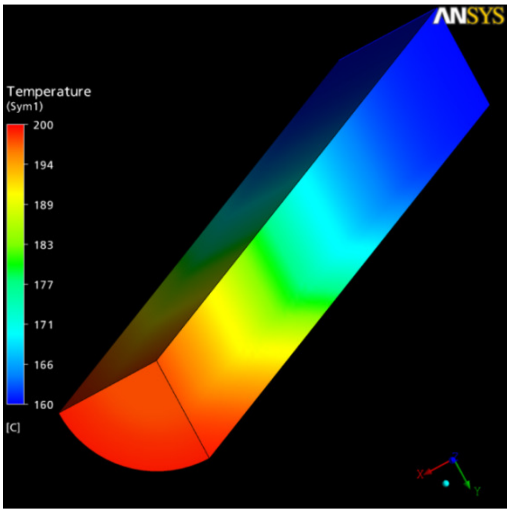


Fig. 8 Fluid Temperature in Branch B1.



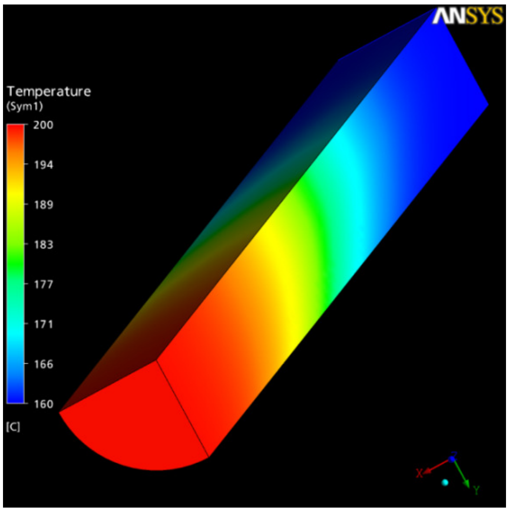


Fig. 9 Temperature Distribution at 4 s. Fig. 10 Temperature Distribution at 19 s.

5.3. Comparison between CFX-ATHLET and ATHLET Stand Alone for a Closed Loop Configuration with Simplified Pressure Control

The simulation of a closed loop is a greater challenge for the coupled thermal-hydraulic system. Stable steady state calculation and reliable results could be achieved only when mass and energy are strictly conserved within both programs and in the coupling interface. Since this was not the case in the first closed loop calculations, mass conservation issues were resolved with the attachment of TDV to the closed system. It adds or subtracts fluid mass from the loop. In the real PWR plant, the pressurizer compensates for fluid volume changes in the primary system. In order to test the capabilities of CFX-ATHLET to simulate closed loop configurations, two 20 m long ATHLET pipes with diameter of 0.2 m and the already described CFX pipe were coupled in a closed loop configuration, see Fig. 11. Furthermore, a simplified pressure control is realized with a third ATHLET pipe which connects to the loop a TDV with 9.8 MPa constant pressure and 200 ^{0}C temperature. In the middle of pipe 1 a pump is modeled. The steady state calculation is performed for stagnant flow conditions. At the beginning of the transient calculation the pump power is gradually increased and after 1 s stabilized at a certain level, creating a pressure difference of 0,347 MPa. Figure 12 shows the mass flow rates calculated by the coupled system and ATHLET stand alone, which correspond to this pressure difference, pipe cross-section area and fluid density. After 5 s of operation at that level, the pump power is gradually decreased and then the pump is operated in reverse mode. This generates negative pressure differences and flow reversal could be observed after 7 s simulation time. The pressure behavior is shown in Fig. 13 and it follows the boundary conditions imposed by the pump.

As a very preliminary verification step of the CFX-ATHLET results, the same calculation was performed with ATHLET stand alone. This approach is feasible, since the fluid flow in this particular case is not dominated by 3D effects and therefore could be reproduced by the 1D system code in a very reliable way. The comparative analyses showed excellent agreement between both calculations (Fig.12, Fig. 13). The coupled simulation was stable, the pressure matched exactly the pressure predicted by ATHLET. One should keep in mind that closed loop is a challenge for every coupled thermal hydraulic code system because oscillations with increasing amplitude or even pressure wave propagation through both domains could occur.

Figure 14 shows 2D velocity profiles from the outlet *Opening* of the ANSYS CFX pipe at 0 s, 5 s, 7 s and 12 s problem time. At the beginning of the simulation the velocity is 0 m/s (0 s, top left figure) and then in the next few seconds its value increases to approx. 7 m/s (5 s, top right). This picture shows the fully developed velocity profile in the ANSYS CFX pipe. At 7 s problem time fluid velocity decreases to 0 m/s (7 s, bottom left) and from that moment the flow direction reverses. The last figure (12 s, bottom right) exposes velocity profile at about -7.0 m/s (reverse flow).

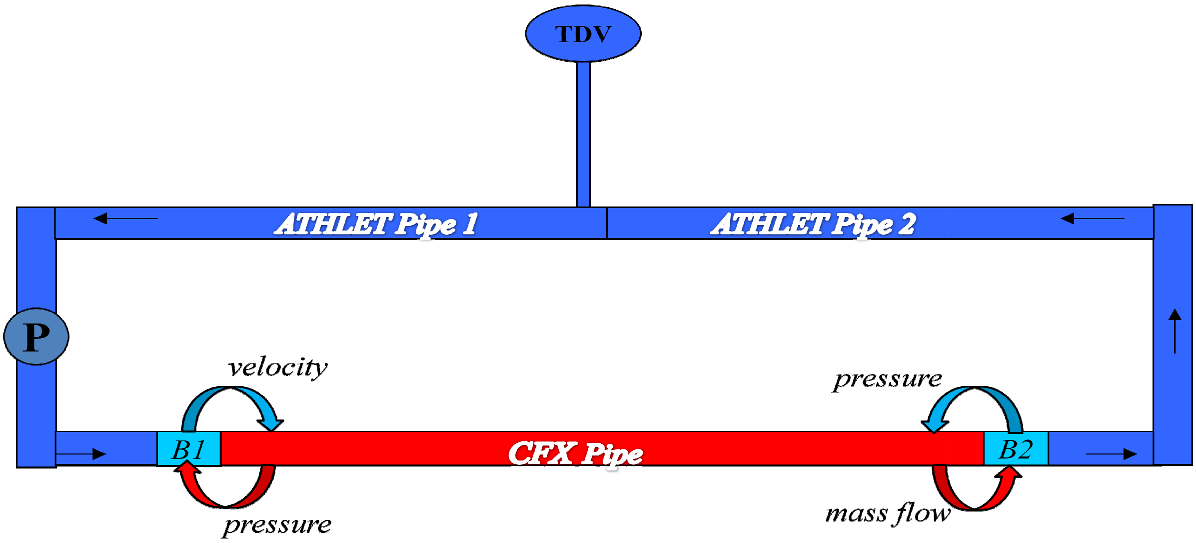


Fig. 11 Closed Loop Configuration.

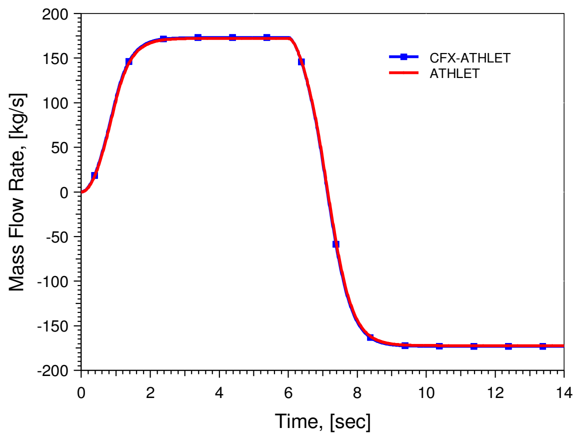


Fig. 12 Mass Flow Rate.

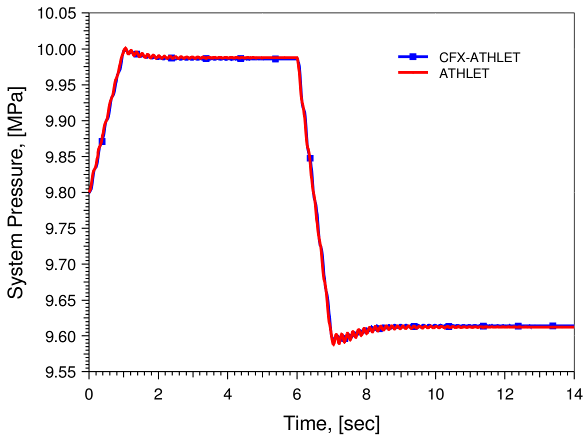


Fig. 13 Pressure.

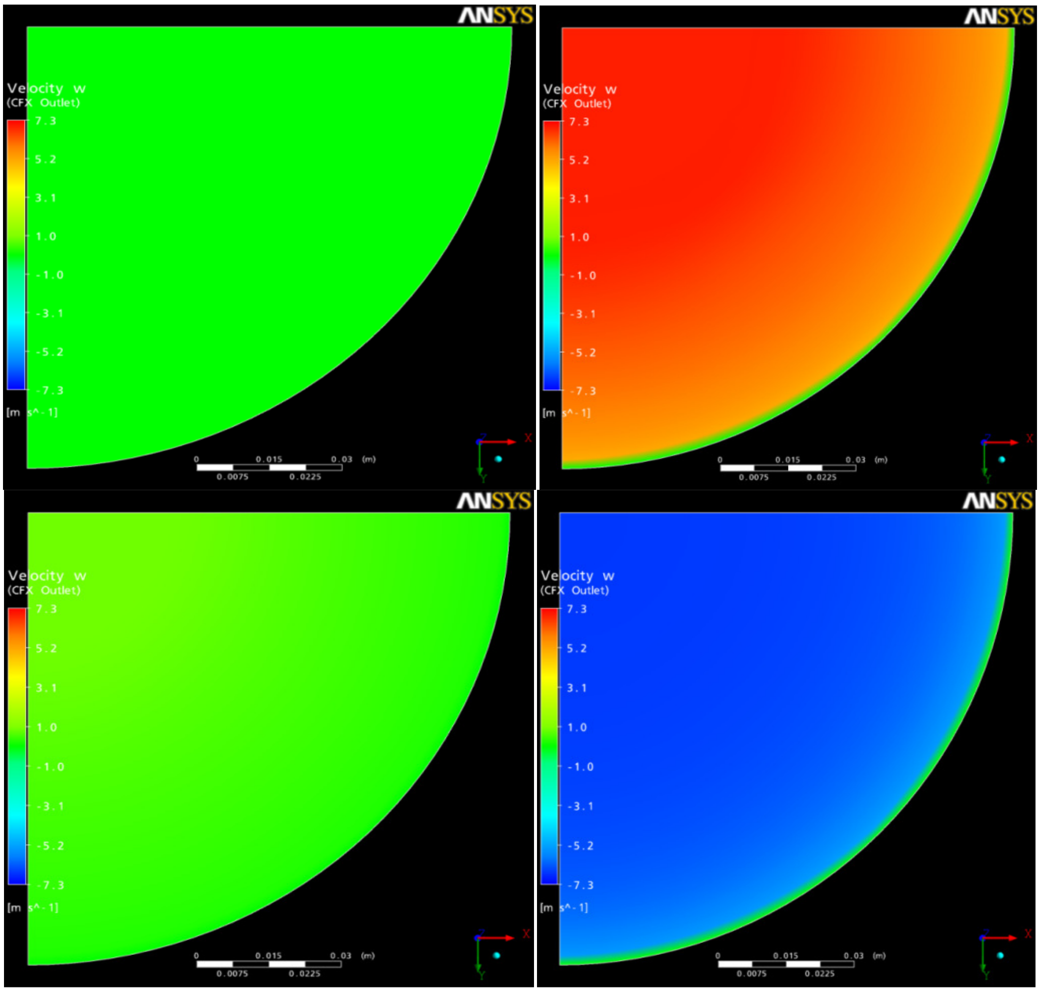


Fig. 14 2D Velocity Profiles at CFX Outlet Opening at 0, 5, 7 and 12 s.

6. IMPROVEMENT OF THE SIMULATION STABILITY

With the coupled CFX-ATHLET software system consistent simulation results were obtained, however several calculations showed considerable stability issues. Two major factors are responsible for this: mass conservation inconsistencies and the explicit coupling scheme. The first issue appears mainly in closed loop systems. In order to conserve mass and momentum, the fluid mass transferred from the last control volume of ATHLET pipe 1 to the inlet *Opening* of the ANSYS CFX domain should be the same as the one provided by the ANSYS CFX outlet *Opening* into the first control volume of ATHLET pipe 2 (if no heating, cooling, etc occurs in ANSYS CFX domain). Unfortunately, this is not the case and the mass flows differ slightly, due to the fact that ANSYS CFX obtains velocity from ATHLET at its inlet *Opening* and not mass flow rate. Analyses showed that in a closed loop simulation without pressurizer or TDV small amount of fluid mass is lost during the calculation resulting in pressure decrease over time. This also leads to additional issues related to the convergence of the CFD code. The reason for the observed differences in mass flow rates was finally found to be adressed to discretization related differences in ATHLET assumed cross-sectional pipe area and the ANSYS CFX calculated pipe cross-sectional area resulting from integration over inlet/outlet boundary conditions. To overcome these mass conservation problems a consistent mass flow – velocity conversion was developed and implemented in the interface code. This led to a very good conservation of the fluid mass in the whole system and thus stable pressure over the simulation time even for closed loop configurations without TDV.

The second major instability problem is due to the nature of the explicit coupling strategy, where thermal-hydraulic parameters are exchanged only when the time step is already finished and there is no possibility to repeat it. The exchanged values appear as small perturbations for the codes which can cause pressure and velocity oscillations. In worst cases these could eventually increase with time and lead to solution divergence. One efficient way to avoid such instabilities is the implementation of fully implicit or semi-implicit coupling strategies.

7. FUTURE WORK

The future work on the coupled system CFX-ATHLET is focused on the improvement of the existing explicit strategy and the semi-implicit one, which is currently being developed at GRS. Its main advantage is the convergence of the exchanged thermal-hydraulic parameters before the initiation of the next time step. As already discussed, this is an important aspect concerning simulation stability. Figure 15 shows a simplified block scheme of the semi-implicit coupling. The main idea behind the semi-implicit scheme is that both programs repeat the current time step with updated boundary conditions until a specified convergence criteria (pressure, velocity, etc) in the interface programs is reached. After convergence is achieved, ANSYS CFX closes the time step and initiates the next one. The main advantage of this strategy is that after several iterations between ANSYS CFX and ATHLET consistent velocity – pressure combination for the current time step is found. Potential drawback of this method is the larger computation time due to the code-to-code iterations, which could make a semi-implicit simulation more expensive. On the other hand, semi-implicit coupling could eventually allow larger time steps compared to the explicit coupling because of the better convergence resulting from the already mentioned consistent velocity – pressure combination.

Some improvements in CFX-ATHLET will be related to the generation of appropriate velocity profiles at the ANSYS CFX inlet *Opening*. At present, a flat velocity profile is generated from the mean velocity provided by ATHLET. Although good results have been achieved so far, realistic velocity profile will further improve the simulation.

Special attention will be also paid to the validation of the developed coupled system. Comparative calculations with CFX-ATHLET and ATHLET stand alone were only the first step of the verification process. Dedicated experiments for validation of coupled codes have already been performed at Paul Scherrer Institute in Switzerland [5]. Further activities in this direction are also planned within the frameworks of several European projects.

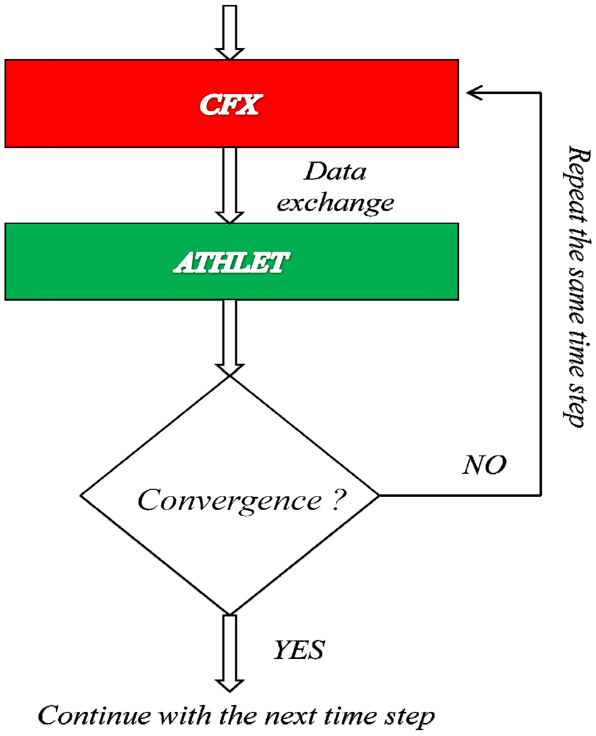


Fig. 15 Simplified Block Scheme of Semi-Implicit Coupling Strategy.

8. CONCLUSIONS

System codes like ATHLET, CATHARE, TRACE are being developed and used for more than 30 years by the nuclear reactor industry, technical safety organizations and research institutions for the simulation and analysis of anticipated and abnormal plant transients, loss of coolant accidents and other operational sequences in light water reactors. However, since system codes are based on one dimensional models, they are not always capable to predict complex flow behavior dominated by 3D phenomena like thermal mixing in the PWR downcomer, etc. In order to overcome these limitations and extend the capabilities of the GRS best estimate code ATHLET, an explicit coupling strategy was developed to couple ANSYS CFX and ATHLET. Multiple test calculations based on open thermal hydraulic systems and closed loop configurations were performed. As a preliminary verification step, comparative simulations with ATHLET stand alone were carried out. These proved the capability of the new code system CFX-ATHLET to correctly predict thermal hydraulic behavior of open and closed systems with two coupling interfaces. Furthermore, developmental effort is put in the improvement of the calculation stability by introducing a consistent mass flow – velocity conversion which helped to enhance the mass conservation within the CFX-ATHLET system. Future work is concentrated on the development of a semi-implicit coupling scheme and experimental validation of the simulation results.

ACKNOLEDGEMENTS

The presented work was performed within a project funded by the German Federal Ministry of Economics and Technology under grant No. 1501328 and RS 1184.

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