## Simulation of a Main Steamline Break scenario using the 3D neutron kinetic core model DYN3D coupled with the CFD software TRIO\_U

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**Abstract** - The reactor dynamics code DYN3D, developed at Helmholtz-Zentrum Dresden-Rossendorf (HZDR), was coupled with the Computational Fluid Dynamics (CFD) solver TRIO\_U, developed at CEA France, in order to replace DYN3D's one-dimensional hydraulic part with a full three-dimensional description of the coolant flow in the reactor core at higher spatial resolution. The article describes the coupling method and shows results of its application to the simulation of a Main Steamline Break (MSLB) accident of a Pressurised Water Reactor (PWR).

## I. INTRODUCTION

Reactivity and thermal power generation in the core of Light Water Reactors (LWRs) are very sensitive to changes in the feedback parameters moderator density and fuel temperature [1]. The latter is tightly connected to the moderator temperature and to the heat transfer between fuel and coolant, and thus strongly depends on the coolant flow conditions. Experimental and CFD analyses of the coolant flow in the reactor vessel have shown that coolant mixing upstream of the core is highly incomplete [2, 3, 4, 5], which may lead to large temporal and spatial gradients of temperature and boron in the core entry plane, especially in the case of cooling or boron dilution transients with asymmetric behaviour of the primary loops.

CFD methods are able to predict the coolant mixing in the pressure vessel with higher accuracy than thermalhydraulic codes and may therefore be used to provide a reactor core simulating programme with more realistic boundary conditions. In the framework of the NURESAFE project, the three-dimensional CFD solver TRIO\_U [6] was coupled with the core simulator DYN3D [7] in order to improve the prediction of coolant mixing in the reactor downcomer and in the lower plenum. In DYN3D, fuel assemblies are represented by one-dimensional coolant channels which are aligned with the vertical reactor axis. This prevents the code from reproducing lateral mixing across assembly boundaries. TRIO\_U was used to replace the core thermal-hydraulics of DYN3D for a fully three-dimensional simulation of the coolant flow on a computational mesh of higher spatial resolution as compared to the nodal mesh of DYN3D. The coupling is used to simulate a MSLB accident of a PWR.

# II. SIMULATION CODES USED AND COU-PLING METHOD

The reactor dynamics code DYN3D is a threedimensional best-estimate tool for simulating steady states and transients of LWRs and has been developed at the HZDR, Germany, for more than 20 years. It is actively developed in order to improve the implemented and to embed new physical models and numerical methods. The neutron kinetics model solves the three-dimensional neutron diffusion equations for two or multiple energy groups, or simplified neutron transport equations. Nodal expansion methods are applied that are specific for the geometry of fuel assemblies. Rectangular as well as hexagonal assembly shapes can be treated. The reactor is subdivided into axial layers of variable height, producing prismatic computational nodes which reflect the shape of the fuel assemblies. Recently, the solver was extended to trigonal prism nodes which allow a spatially refined nodalisation of hexagonal assemblies as well as the assignment of variable fuel compositions over the assemblies' cross section.

DYN3D includes a thermal-hydraulic model for one and two-phase coolant flow, and a fuel rod model. Thermalhydraulic parameters like fuel and moderator temperatures are required for the estimation of safety criteria, such as the mechanical integrity of the fuel rods. On the other hand, together with the temperature dependent moderator density they are also needed for the determination of the feedback to neutronics. The thermal-hydraulic model solves the balance equations for mass, momentum and energy of the one or two-phase coolant flow, the heat transport equation in the fuel rod, and determines the heat transfer into the coolant. In an iterative procedure, DYN3D computes the distributions of fission power, coolant temperature and density, void fraction and boron concentration over the core, as well as safety-related parameters, such as maximum fuel and cladding temperatures, fuel enthalpy, critical heat flux and cladding oxide layer thickness.

Cross sections and other neutronic parameters are provided to the code in the form of libraries for different combinations of burnup and feedback parameters, and interpolated for each individual node and time step during a transient. Boundary conditions, like pressure drop over the core, boron concentration, coolant mass flow and coolant temperature distributions over the core inlet, are provided in the form of tables or by thermal-hydraulic codes coupled to DYN3D. Burnup distributions can be provided as input data or calculated by simulating power operation histories. Transient calculations may account for perturbations of the core inlet temperature, mass flow, boron concentration, outlet pressure, pressure drop and for control rod movement.

The code TRIO\_U is an open-source CFD simulation

software, developed at CEA France. The code is designed to treat turbulent flows, fluid/solid coupling, multiphase flows (by means of front and particle tracking) or flows in porous media. Problem types that can be handled and which are relevant for LWR simulation comprise purely turbulent hydraulic as well as thermal-hydraulic problems with and without dissolved species transport. For these problem types, TRIO\_U solves the conservation equations of mass , momentum, internal energy and dissolved species concentration. TRIO\_U makes use of the Boussinesq approximation, assuming constant values of fluid density  $\rho_{\rm ref}$  everywhere except in the body force term of the momentum equation. There, temperature and concentration dependency is represented by expansion coefficients  $\beta_T$  and  $\beta_C$ . Also, the specific heat capacity  $c_p$  is assumed to be constant.

The part of DYN3D which solves the one-dimensional equations of momentum, boron and heat convection in a fuel assembly-wise manner is to be replaced by the fully threedimensional simulation capabilities of TRIO\_U. However, for the sake of acceptable computation times no attempt is made to model the coolant flow down to the fuel pin level. Instead, a porous body approach is used for modelling the reactor core. DYN3D computes the heat conduction in the fuel and the cladding, as well as the heat transfer into the coolant based on the coolant velocity which it receives from TRIO\_U. For this purpose, DYN3D makes use of well-established correlations for the heat transfer at rod bundles that are implemented in its thermal-hydraulic module and which account for different heat transfer regimes occurring at heated surfaces. The actual data interface between the codes is the volumetric heat source  $\dot{q}^{\prime\prime\prime}$  calculated by DYN3D and sent to TRIO\_U. In the opposite direction, boron concentration, coolant velocity  $v_z$ , temperature T and pressure p are sent to DYN3D. The quantities received from TRIO\_U are needed to correctly calculate the neutronic feedback on nuclear power as well as the heat transfer into the coolant.

On the coding level, the coupling of DYN3D and TRIO\_U makes use of the SALOMÉ platform (http://www.salome-platform.org). It is an opensource software for pre and post processing numerical simulations as well as a programming framework for the integration and coupling of third-party simulation codes based on open standards. For the purpose of code coupling it provides programming classes and methods for data storage, data interpolation and the generation of computational meshes. For performance reasons, the coupling executable does not make use of SALOMÉ's graphical user interface, but is configured by means of a text file in the ini format and run from the command line. Nevertheless, result files are written in SALOMÉ's native MED format and can be immediately evaluated by its post-processing tools. Instructions for building and using the coupling application are given in [8].

In order to communicate with each other, the simulation codes to be coupled must implement a common programming interface. For this, SALOMÉ defines ICOCO which stands for Interface for Code Coupling. [9]. It is a purely abstract C++ programming interface to be implemented in the codes. Every code is represented by a programming object whose methods allow a supervising programme to initialise and terminate the

code, to increment the problem time, to invoke the solution of a time step, to extract solution fields from the code and to send fields to the code. Fig. 1 sketches the coupling between DYN3D and TRIO\_U and shows the exchanged quantities.



Fig. 1. Coupling scheme and quantities transferred between DYN3D and TRIO\_U

#### **III. MSLB SIMULATION RESULTS**

The transient response of a light water reactor to a secondary-side steam line break was simulated using the newly developed coupling between TRIO\_U and DYN3D. The computational domain of the problem comprises the reactor vessel with its four inlet nozzles of the corresponding primary coolant loops, the downcomer, the lower plenum up to the core inlet plane, and the reactor core up to the core outlet plane. The time-dependent boundary conditions at the nozzle inlet (coolant mass flow, temperature, boron concentration) are provided as tabulated input data and were generated by prior system-code calculations.

In Fig. 2a and b, the computational geometries of the pressure vessel and of the reactor core are shown as surface meshes, while Fig. 2c is a sectional view of the entire computational mesh in the vertical plane of the loop 1 and 3 inlet nozzles. Two separate, unstructured meshes composed of tetrahedral cells are used to model the reactor in the CFD calculation done by TRIO\_U. DYN3D calculates on a low-resolution nodal mesh which is shown in Fig. 2d. It divides the reactor core into 32 layers between inlet and outlet, while every fuel assembly is represented by one node horizontally, giving a total of  $32 \times 193 = 6176$  nodes. The refined core mesh for the CFD calculation, Fig. 2b, is obtained by subdividing the DYN3D nodes into a total of 1778688 tetrahedral cells.

The reference reactor is a 4-loop PWR of Westinghouse design whose core configuration and materials composition is given in [10]. At the beginning of the transient, the core is at end-of-cycle and hot-zero power, with zero boron concentration in the primary coolant and zero decay heat power. The transient is initiated by a double-ended main steam line break at the outlet nozzle of the steam generator in loop 1. This leads to a sudden evaporation of secondary coolant and thus to a strong temperature drop of the secondary coolant. As the temperature difference between the primary and the secondary sides of the steam generator increases, more heat is removed from the primary coolant which causes the primary

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Fig. 2. Mesh geometries for the coupled DYN3D-TRIO\_U simulation; a) pressure vessel model in TRIO\_U (partial surface mesh), b) reactor core model in TRIO\_U, c) vertical section of the TRIO\_U mesh in the plane of loop 1 and loop 3 inlet nozzles, d) reactor core nodal mesh for DYN3D

loop temperature to also drop. As a consequence, the reactor core suffers an overcooling, which causes it to become critical and to produce a power excursion. To increase the power generation during the transient and to achieve an additional asymmetry in the core a fuel assembly with a stuck control rod was assumed. The assembly position was chosen to be in the same sector of the core which is also expected to be most affected by the overcooling originating from loop 1. During the transient, all primary loop pumps continue to work at the same constant volumetric flow rate. Fig. 3 shows the primary coolant temperatures at the pressure vessel inlet nozzles during the transient.

The response of the thermal power to the overcooling transient is shown in Fig. 4. The power reaches the peak after 92 s with a delay of 16 s as compared to the minimum coolant temperature of loop 1, cf. Fig. 3. It starts to drop as the coolant temperatures grow in all primary loops. Temperature distributions over two cross sections of the core, namely at the inlet and the outlet positions, are shown in Fig. 5. Up to the first 6 seconds of the simulated transient, the overcooling is the same for all loops, cf. Fig. 3. The inlet temperature distribution reveals that the outer zone of the core is more affected by overcooling than its centre and that there is a diagonal band extending across the core with little overcooling. As time advances, temperature differences between hotter and



Fig. 3. Coolant temperature at the cold legs of the primary loops during MSLB transient

overcooled zones grow and a sector of overcooling forms around the loop 1 inlet position in the core inlet plane. Later on, as it can be seen for t = 160s, this overcooling sector vanishes again because the inlet temperatures of all loops start to approach each other after the passage of the minimum temperature. In the outlet plane, beginning at t = 14 s, a spot of elevated coolant temperature forms around the position of the assembly with the stuck control rod.



Fig. 4. Reactor power during MSLB transient, comparison of coupled Reactor Pressure Vessel (RPV)/core simulation and core-only simulation with given core inlet temperature distribution

Based on coolant mixing tests at the ROCOM facility [3, 11], an MSLB simulation was carried out which uses a time-dependent coolant temperature distribution over the core inlet plane as the upstream boundary condition. The ROCOM facility is a downscaled RPV model of a KONVOI reactor, instrumented with conductivity measurement technique, that was mainly used to investigate the coolant mixing behaviour upstream of the core zone. The tests cover a number of transient scenarios with single and multiple loop flow rate and concentration variations. The measured mixing scalar distribution of a test with single-loop disturbance was scaled onto M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017, on USB (2017)

the MSLB conditions of the present study. The following comparison case with core-only simulation uses the same total coolant flow rate, but unlike the full-RPV simulation presented before, it assumes a uniform flow rate over the core inlet during the transient. The comparison case allows for investigating the effect of a non-uniform coolant flow at the core inlet on the overall reactor power and the resulting coolant temperature. The thermal reactor powers of the two cases are plotted against each other in Fig. 4. The power maximum, occurring around the same time as in the full-RPV case, is by about 0.3 GW lower (dashed curve). On the local level, power density and coolant temperature are higher in the core-only simulation, as can be seen in Fig. 7 showing the vertical profiles in the assembly with a stuck rod around the time of the power maximum. The differences of the simulation results demonstrate that the reactor power sensitively responds to variations of the feedback parameters at the inlet boundary.



Fig. 5. Core inlet (in) and outlet (out) temperature distributions at different times

Fig. 6 shows the power density distribution in a plane cutting the core vertically along the core axis and the centre line of the affected assembly. During the transient, starting at zero, the power density reaches values beyond 200 MW m<sup>-3</sup>. Despite the high energy release in the affected assembly during the power peak at t = 92.5 s, the coolant passing through it only reaches temperatures around 285 °C, as shown in Fig. 7, which is similar to the stationary state value. The temperature jump with respect to the minimum inlet temperature of loop 1 is about 60 K. Fig. 7 also shows the power density profile in the affected assembly during the core power peak. Its step-like profile is due to the fact, that the power density distribution is





Fig. 6. Power density distribution in the vertical plane x + y = 0 at different times



Fig. 7. Profiles of coolant temperature and power density along the fuel assembly with stuck control rod at t = 92.5 s, comparison of coupled RPV/core simulation and core-only simulation with given core inlet temperature distribution

One interesting feature of the temperature profile in Fig. 7 is the slight decrease in the upper section of the assembly above z = 3 m. This can be explained only by lateral mixing with colder water from the neighbourhood of the affected assembly. The presence of horizontal mixing is an indication for the existence of three-dimensional coolant flow in the reactor core which cannot be modelled by standalone DYN3D.

# **IV. CONCLUSIONS**

The CFD code TRIO\_U has been coupled with the reactor dynamics code DYN3D in order to replace its onedimensional description of the core thermal-hydraulics with a fully three-dimensional simulation of the coolant flow and temperature fields on a refined grid. Coolant velocity, pressure, temperature and boron concentration fields are calculated by TRIO\_U and sent to DYN3D which calculates the core power density distribution. The latter is sent back to the CFD code and used there as a source term in the solution of the energy transport equation. Data storage and interpolation make use of the facilities provided by SALOMÉ, an opensource platform for simulation code integration. The object oriented libraries of the platform are closely integrated with M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017, on USB (2017)

the Open MPI parallelization library and are fully compatible with the parallelism of TRIO\_U.

The coupling of TRIO\_U and DYN3D was used to simulate the coolant mixing in the pressure vessel upstream of the core inlet plane as well as in the core itself. This coupling was applied to an MSLB case which involves an overcooling transient in a single loop of the primary circuit. The simulation confirmed the incomplete mixing in the downcomer and the lower plenum leading to a sector-shaped distribution of the coolant temperature in the core inlet plane. Moreover, the simulation produced a three-dimensional flow field in the reactor core, which leads to lateral mixing of coolant on its passage through the core. It was shown that slight variations of feedback parameters at the inlet boundary produce a measurable effect on the reactor power. Coupled, whole pressure vessel simulations can help to provide the neutronic simulation part with more accurate boundary conditions.

# V. ACKNOWLEDGMENTS

The presented work was financed by the European Union within the FP7 NURESAFE project.

#### REFERENCES

- 1. S. KLIEM, S. MITTAG, U. ROHDE, and F.-P. WEISS, "ATWS analysis for PWR using the coupled code system DYN3D/ATHLET," *Annals of Nuclear Energy*, **36**, 1230–1234 (2009).
- F. MORETTI, D. MELIDEO, F. D'AURIA, T. HÖHNE, and S. KLIEM, "CFX Simulations of ROCOM Slug Mixing Experiments," *Journal of Power and Energy Systems*, 2, 2, 720– 733 (2008).
- T. HÖHNE, S. KLIEM, U. ROHDE, and F.-P. WEISS, "Boron dilution transients during natural circulation flow in PWR—Experiments and CFD simulations," *Nucl. Eng. Design*, 238, 1987–1995 (2008).
- T. HÖHNE, "CFD-simulation of the VVER thermal hydraulic benchmark V1000CT-2 using ANSYS-CFX," Science and Technology of Nuclear Installations, 2009 (2009).
- S. KLIEM, T. SÜHNEL, U. ROHDE, T. HÖHNE, H.-M. PRASSER, and F.-P. WEISS, "Experiments at the mixing test facility ROCOM for benchmarking of CFD-codes," *Nucl. Eng. Design*, 238, 566–576 (2008).
- P.-E. ANGELI, U. BIEDER, and G. FAUCHET, "Overview of the TRIOCFD code: main features, v&v procedures and typical applications to nuclear engineering," in "NURETH-16," (2015).
- U. ROHDE ET AL., "The reactor dynamics code DYN3D models, validation and applications," *Progress in Nuclear Energy*, **89**, 170–190 (2016).
- A. GRAHN, A. GOMMLICH, and S. KLIEM, "Application of the TRIO\_U-DYN3D coupling," Tech. Rep. NURESAFE D11.112, European Commission (2015).
- 9. E. DEVILLE and F. PERDU, *Documentation of the Interface* for Code Coupling: ICoCo, CEA, Paris (2012).
- T. KOZLOWSKI and T. J. DOWNAR, "OECD/NEA and US NRC PWR MOX/UO<sub>2</sub> core transient benchmark, final specifications, Rev. 2," Tech. Rep. NEA/NSC/DOC(2003)20,

NEA (2003).

 S. KLIEM, T. HÖHNE, U. ROHDE, and F.-P. WEISS, "Experiments on slug mixing under natural circulation conditions at the ROCOM test facility using high resolution measurement technique and numerical modeling," *Nucl. Eng. Design*, 240, 2271–2280 (2010).