Advanced Numerical Simulation for Reactor Safety

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Summary

The numerical simulation tools used for the design and safety evaluation of nuclear reactors are under continuous development, improvement and validation. As an example, in the last years several ambitious projects to develop powerful simulation platforms for LWR reactor multi-physics analyses were launched, such as, NURESIM platform in Europe, or the Numerical Nuclear Reactor and CASL program in the United States. One of the main objectives of the research in this area is to enhance the prediction capability of the tools used for safety demonstration of the current LWR Nuclear Power Plants (NPP) through the dynamic coupling of the codes simulating the different physics of the problem into a common multi-physic simulation scheme. Another main objective is to develop those tools in a way that they can be applied not only to Gen-II LWR but also for the safety evaluation of Gen-III, Gen-IV NPP designs and other innovative nuclear systems, like Accelerated Driven System (ADS). At last but not least, in the actual environment where the computational power is increasing at giant steps, the development of these software platforms is being oriented towards High Performance Computing Standards. Just to give an example, highly detailed two-phase CFD (Computational Fluid Dynamics) computations are becoming practical daily use applications in all engineering fields bringing to reality what was science fiction ten years ago.

1. Introduction

Advanced Numerical Simulation for Reactor Safety is being supported by the Euratom fission research program within the 7th Framework Program (FP7). The current NURESAFE project aims at delivering to the European stakeholders a reliable software capacity usable for safety analysis needs and developing a high level of expertise in Europe in the proper use of the most recent simulation tools including uncertainty assessment to quantify the margins towards regulatory and safety limits occurring during an accident. This software capacity is based on the NURESIM European simulation platform created during the FP6 NURESIM project (2005-2008) under the context of the SNETP (Sustainable Nuclear Energy Technology Platform). The NURESIM platform was conceived as a joint European effort to develop an integrated software platform with common functions, which allow conducting multi-scale and multi-physics calculations in a user friendly environment. This platform was further developed during the FP7 NURISP project (2009-2012). NURISP achieved its goal by making available an integrated set of software at the state-of-the-art. NURESAFE started in early 2013 and the objective is now to further develop, validate, and deliver to end-users fully integrated industry-like applications to perform reactor safety analysis, and to support flexible operation and design optimization.

The High Performance Monte-Carlo (HPMC) project was launched in the FP7 complementary to NURESAFE to further develop neutronic Monte Carlo methods. The HPMC project methodology consists in the combination of a state-of-the-art Monte Carlo codes review of the current modelling capabilities regarding safety relevant simulations, together with innovative model developments towards higher-fidelity simulations. These high-fidelity simulations are based on coupled neutronic/thermal-hydraulic solutions, including time-dependent Monte Carlo methods and improved stable burn-up approaches, at both fuel assembly and pin level making use of high-performance computing (HPC). First of all, new methodologies and code developments are implemented regarding the topics listed above. Then, the demonstration and application of the extended code capabilities for safety relevant cases taking profit of existing computer clusters are being performed. Hence, reference solutions for any kind of reactor systems, for safety-relevant scenarios and for problems where no experimental data is available, can be provided by the developed tools.

For the long-term development of nuclear power, innovative nuclear systems such as Gen-IV reactors and transmutation systems need to be developed for meeting future energy challenges. Thermal-hydraulics is recognized as a key scientific subject in the development of innovative reactor systems. The THINS project is devoted to crosscutting thermal-hydraulic issues encountered in various innovative nuclear systems cooled by liquid metals, gases or water, such as advanced core thermal-hydraulics, single phase mixed convection and turbulence, specific multiphase flow, and multi-scale code coupling and qualification. A list containing all the partners involved in the mentioned projects can be found as an appendix to this paper.

2. Advanced Numerical Simulation

2.1 The NURESIM platform

Under the context of the SNETP (Sustainable Nuclear Energy Technology Platform), the NURESIM (NUmerical REactor SIMulation) platform [1], [2] was conceived as a joint European effort to develop an integrated software platform with common functions, which allow conducting multi-scale and multi-physics calculations in a user friendly environment. The platform is supported by a united European team of experts.

In order to become a platform for providing reference solutions, the NURESIM platform is developed with the following objectives:

- To provide an accurate representation of the physical phenomena by promoting and incorporating the latest advances in reactor and core physics, two-phase thermal-hydraulics and fuel modelling (with a focus on its mechanical behaviour during accidents).
- To offer capability for multi-scale and multi-physics computations, especially for coupling core physics and thermal-hydraulics models for reactor safety; to provide easy coupling of the different codes and solvers through the use of a common data structure and generic functions, for instance for interpolation between non-conforming calculation meshes.
- To provide generic pre-processing and post-processing and supervision functions through the SALOME open source tool (<u>www.salome-platform.org</u>).
- To validate the individual models, solvers, codes and the platform through challenging applications corresponding to nuclear reactor situations and including reference calculations,

experiments and plant data; to complement the validation by using quantitative deterministic and statistical sensitivity and uncertainty analyses.

In Figure 1, the overall roadmap of the NURESIM simulation platform is presented showing the time allocated for each project. The first project, NURESIM, established the basic architecture of the platform and resulted in a first prototype of a truly integrated multi-physics simulation environment. The NURISP project was conceived as a consolidation of the platform together with an extension of the simulation capabilities towards higher-resolution both in space and time. The NURESAFE project will show the extended capabilities of the platform and demonstrate the readiness of the tool for industrial design, new developments and safety applications.



Figure 1: NURESIM platform roadmap

In overall, the development of the NURESIM platform involved 14 countries and 24 organizations from the European Union in the last years.

2.2 NURISP (Nuclear Reactor Integrated Simulation Platform) project

The NURISP project (2009-2011) was a Collaborative Project funded by the 7th EU Framework Program which aimed at consolidating and extending the results of NURESIM project. New codes were connected to the platform and new steps were made for integration, model development (including fuel), coupling schemes, sensitivity and uncertainty analysis and validation, with broader applications. NURISP focused on present (GEN-II) and future (GEN-III and GEN-III+) PWR, VVER and BWR, but care was taken to develop methods as generic as possible so that future extension to GEN-IV reactors would be possible.

As already mentioned, the European Project NURESIM included five subprojects, namely: Core Physics (SP1), Thermal-hydraulics (SP2), Multi-physics (SP3), Uncertainty and sensitivity (SP4), and Integration (SP5), plus the Users Group to supplement the project with feedback from the industry and TSOs (Technical Support Organizations). The overall objective of the Multi-Physics subproject (SP3) was the development of generic coupling interfaces to be applied on the neutronics and thermal-hydraulics solvers developed by the SP1 and SP2, in order to enable coupled neutron-kinetics/thermal-hydraulics (NK/TH) transient simulations of LWR's (PWR, BWR, VVER).

During the NURISP project, advanced LWR neutronics calculation schemes for pin-by-pin core calculations have been developed and successfully tested against experiments. They are based on a two-step approach with a self-shielding collision probability (PIJ) approach followed by a method of characteristics (MOC) flux calculation applied on an unstructured mesh.

Multi-scale thermal-hydraulic analyses of critical heat flux (both DNB (Departure from Nucleate Boiling) & Dry-Out), LOCAs (critical flow, reflooding, 3-field modelling), PTS (Pressurized Thermal Shock), DCC (Direct Contact Condensation), are being continued with advanced system

codes, two-phase CFD codes and with support of some DNS (Direct Numerical Simulation) tools. An extensive validation of the NURESIM TH codes includes many data sources. Uncertainty methods for system and CFD codes are applied and further developed. The coupling technique was developed using the SALOME software, which is the base infrastructure of the NURESIM Simulation Platform. SALOME is open source software that offers an environment including all the necessary tools for the definition, solution and post-processing of scientific analysis (Graphical User Interface, meshing tools, code execution supervision tools, 3D graphical pre-and-post-processors, etc.).

In addition, neutronics/thermal-hydraulics coupling applications were developed in order to model PWR boron dilution accidents or steam line breaks. These developments are pursued within NURESAFE in order to progress towards higher fidelity pin-by-pin modelling and to validate the models.

2.3 NURESAFE (NUclear REactor SAFEty Simulation Platform) project

The NURESAFE project started in early 2013 continuing with the development line of the NURESIM platform. The main objective is to develop, validate, and deliver to end-users fully integrated practical applications relevant to reactor safety analysis, operation and design. With regards to the two previous projects, the Users Group has been extended to more partners including non-European institutions and the industrial representation has been strengthen with the incorporation of AREVA NP. More information about this project can be found in the homepage: http://www.nuresafe.eu/

The objectives under the work program are to develop practical applications usable for safety analysis or operation and design, and to expand the use of the NURESIM platform. Therefore, the NURESAFE project concentrates its activities on several safety relevant 'situation targets'. The main outcome of NURESAFE will be the delivery of multi-physics and fully integrated applications. The objectives of NURESAFE will be achieved through six sub-projects:

- Sub-Project 0 (SP0): Networking
- Sub-Project 1 (SP1): Multi-physics applications involving core physics
- Sub-Project 2 (SP2): Multi-scale analysis of core thermal-hydraulics from DNS to subchannel modelling
- Sub-Project 3 (SP3): Multi-scale and multi-physics applications of thermal-hydraulics
- Sub-Project 4 (SP4): Platform support
- Sub-Project 5 (SP5): Education and training

2.4 THINS (Thermal-Hydraulics of Innovative Nuclear Systems) project

Thermal-hydraulics is recognized as a key scientific subject in the development of the different innovative reactor systems. The overall objectives of the THINS project are the development and validation of new physical models and, the improvement and qualification of numerical analysis tools [3], [4], [5]. Specific objectives are:

• Establishment of a *data base* for the development and validation of new physical models and numerical codes for a more accurate description of the selected crosscutting thermal-hydraulic phenomena.

- Establishment of an *experimental platform* for the thermal-hydraulic research of the innovative nuclear systems. The THINS project will make the optimum usage of the available European experimental facilities and expertise, combine the resources available and establish a European experimental platform.
- Establishment of a *numerical platform* for the design analysis of the innovative nuclear systems. Numerical codes for covering various classes of spatial scales, i.e. system analysis based mainly on lumped parameter approach and CFD codes for detailed local flow behaviour will be considered and coupled.

To achieve the objectives described in the previous paragraph, the THINS project is structured with six work packages (WPs). The six work packages are:

- WP1: Advanced reactor core thermal-hydraulics
- WP2: Single phase mixed convection
- WP3: Single phase turbulence
- WP4: Multi-phase flow
- WP5: Code coupling and qualification
- WP6: Education and training

The first five WPs are devoted to the individual cross-cutting issues. Experiments are foreseen to provide experimental evidence and a fundamental test data base. New physical models will be developed to improve codes. The models will be validated for each individual cross-cutting issue. The fifth issue is the coupling of numerical codes of various scales to build a reliable numerical platform for thermal-hydraulic analysis of innovative nuclear systems. The last WP is devoted to the education and training of young nuclear engineers and researchers.

The methodology used in the THINS project is indicated in Figure 2. Based on phenomenological analysis of the identified cross-cutting phenomena, experimental programs will be defined with the purpose to provide experimental evidence to a better understanding of physical phenomena and test data for the development of models and validation of codes. Totally, 13 experiments have been defined. Due to limited possibility of experiments with low Prandtl number fluids, direct numerical simulation (DNS) will be carried out, to provide additional data for the data base. In parallel, numerical investigation are carried out with three different scales of codes, i.e. system analysis, sub-channel analysis and CFD codes [6]. Numerical support will be provided to experimental work in various phases, such as selection of measurement techniques, design of test facilities, definition of test matrix and experimental data analysis.

The data base consisting of both experimental and numerical results can be then applied for the development of physical models and validation of simulation codes. The models considered in this project are for both system analysis codes and CFD codes, e.g. heat transfer and friction pressure drop in liquid metal for system analysis codes, and dynamic turbulent Prandtl number for CFD simulations. To achieve this target benchmarks are organized for various classes of codes and different applications.



Figure 2: Approach applied in THINS project (Cheng et al. 2013, [7])

2.5 HPMC (High Performance Monte Carlo Reactor Core Analysis) project

Design and safety analysis of nuclear reactors is based on extensive use of computer codes for the coupled calculation of time-dependent neutron transport, thermal-hydraulics and fuel burn-up. State-of-the-art methods use deterministic techniques to solve the neutronics equations, which require various approximations for a full core: a limited number of energy groups, application of diffusion theory instead of transport theory, homogenization of fuel cells and fuel assemblies, pin power reconstruction, etc.

These approximations can be overcome by the stochastic Monte Carlo (MC) method for neutron transport [8], [9]. The HPMC project aims at developing and demonstrating the application of full-core Monte Carlo calculation for time-dependent safety analysis with thermal-hydraulic feedback and burn-up using high performance computing taking into account the most appropriate parallelization approach [10]. To achieve the goals, the HPMC project is organized in the following technical work packages:

- WP1: Optimum Monte Carlo- Thermal Hydraulic Coupling
- WP2: Optimum Monte Carlo- Burn-up Integration
- WP3: Monte Carlo Time-dependence
- WP4: Integration of high-performance parallel Monte Carlo
- WP5: Dissemination and Training

The main elements of advanced MC/TH coupled simulations within the HPMC project are represented in Figure 3.



Figure 3: Major areas interrelation where the HPMC project will provide solutions

The project will provide the general tools for reference calculations, applicable to different reactor types, to test the accuracy of current and future deterministic analysis methods. The methods and

codes under development are tailored to reactor core calculations and highly optimised to run on massively parallel supercomputers [11], [12], [13], [14], [15], [17], [18], [19], [20] and [21].

Using a flexible and efficient coupling scheme, coupled Monte Carlo/thermal-hydraulic calculations for fuel assemblies and whole cores at pin level can be done taking into account the feedback effect of temperatures and coolant densities for all coolant channels in the reactor with high accuracy but in reasonable and acceptable execution time (relevant for industry, regulators, TSO and other potential users).

Within the framework of the project, dynamic calculations with feedback will be performed to analyse effects of reactivity insertion due to control rod movements and for loss-of-coolant accidents (LOCAs) situations. As the Monte Carlo method is not restricted to specific reactor types, the resulting code combinations can also be applied to new reactor designs. More information about this project can be found in the homepage: www.fp7-hpmc.eu.

3. Results from the research activities

In this section, selected results provided by those projects are presented.

3.1 Selected results from the NURISP project

(A) Coupling schemes between Thermo-hydraulics system codes and CFD codes

This task aims at developing new coupling schemes between system and CFD codes. First, a comprehensive study on the state-of-the-art on available coupling schemes has been carried out. An Application Protocol Interface, named ICOCO, has been implemented in the system code CATHARE and in the CFD Trio_U [22] and integrated in SALOME (Figure 4). This development has been used for several System-CFD coupling exercises involving CATHARE (in sequential mode) and Trio_U (in parallel mode) in order to analyse various coupling schemes including overlapping and non-overlapping schemes, and synchronous or asynchronous time stepping coupling schemes.



Figure 4: Architecture of the coupled system

In a first phase, only single phase flows where dealt with. This single phase coupling scheme has been also successfully used within the THINS project. In a second phase, an extension of the coupling scheme to two-phase flows has been developed and encouraging results have been obtained.

The coupling interface between CFD code Trio_U and the system thermal-hydraulic code CATHARE was tested on a numerical benchmark based on an actual main-steam-line-break (MSLB) accident scenario. A simplified model of primary circuit of VVER-1000 nuclear reactor

(including 4 loops and primary sides of steam generators) was created in CATHARE. Trio_U computational domain covered the reactor downcomer (Figure 5), and the lower plenum was overlapped over the CATHARE model of the primary circuit so as to properly simulate the mixing in the reactor inlet part. This work demonstrated that the coupled system of Trio_U and CATHARE codes can be used in a satisfactory way to simulate the coolant mixing in the downcomer and the flow reversal in the afflicted loop during the MSLB event in a VVER-1000 nuclear power plant.



Figure 5 : Trio_U solution domain of a VVER-1000 primary circuit for coolant mixing calculations

(B) CFD model of heat transfer in LOCA situation

During the reflooding phase of a LOCA, core cooling is provided by a super-heated vapour flow carrying water droplets, which experience breakup, coalescence and may impact the ballooned fuel cladding. This work aimed at building a general-purpose CFD model of heat transfer for such a flow regime. This model comprises an Eulerian description of the continuous vapour field coupled with Lagrangian tracking of the droplet population.

In the first stage of the work, the models governing the dynamics of the motion of droplets according to the external forces acting upon them have been assembled. The second stage of the work was the implementation of the heat transfer models for the droplet phase (Figure 6). The principal heat transfer mechanisms are (i) wall-to-vapour (this is a standard feature in all general-purpose CFD codes, and no extra programming is required); (ii) vapour-to-droplet (this will result in droplet evaporation, which will feed back into mechanical equations of motion); (iii) wall-to-droplet by radiation (The analysis performed within NURISP project concluded that this heat transfer is of the order of magnitude of the convective heat transfer in LOCA conditions and cannot be neglected); and (iv) wall-to-droplet heat transfer as a result of direct droplet impact.



Figure 6: Principal heat transfer mechanisms in LOCA

All models have been tested by comparing code predictions against analytical solutions in simple, though relevant, situations. Implementation of models into the NEPTUNE_CFD code is ongoing as well as sensitivity studies involving various flow features. In the framework of NURESAFE, the physical bases of the models will be examined by direct comparison of numerical results against measured data.

3.2 Selected results from the HPMC project

(A) High-fidelity Simulation of a PWR Fuel Assembly with coupled Monte Carlo / Thermal-Hydraulic Codes (PIRS, MCNP5/SUBCHANFLOW)

To demonstrate the prediction capability of the coupled codes PIRS (external coupling) and MCNP/SUBCHANFLOW (internal coupling), a PWR fuel assembly consisting of 264 UOX pins with 4.2% enrichment and 25 guide tubes has been studied. This problem was analysed with the advanced MC/TH coupling schemes developed within HPMC project [11], [12], [13], [14] and [15].

As clearly shown in Figure 7, the old relaxation scheme has a convergence limit given by the statistical uncertainty of the MC method. It starts oscillating in the limit of \mathcal{E} (relative difference between iterations) approaching the values for the tally relative errors. This oscillation will not disappear even when running very large number of iterations, unless the number of histories is increased. On the other hand, by using the stochastic approximation method to the relaxation scheme, the convergence parameter exhibits 1/N behaviour. Using the new scheme, it was possible to achieve very fine convergence $\mathcal{E}=0.04\%$ while the old method was badly converged after 18 iterations with a convergence criteria of $\mathcal{E}=0.54\%$ (see Figure 7).

In Figure 8, the 3D fuel temperature distribution within the PWR FA as predicted by the coupled system for 200k histories, 600 active cycles and using 48 processors is shown. The dark blue positions are representing the guide tubes where no fuel pin is present. The coupled system converged after 16 iterations using a convergence criterion of $\mathcal{E}=0.04$ [14].



Figure 7: Improved behaviour of the coupled Figure 8: Predicted 3D fuel temperature system based due to the new relaxation scheme distribution within the PWR FA

(B) Optimum Monte Carlo Burn-up [16], [17], [18], [19]

Previous studies have shown that basic coupling schemes in the existing Monte Carlo burn-up codes are numerically unstable, and within HPMC it was shown that the same applies to the popular predictor-corrector scheme, see [16]. The numerical instability is visible when analysing the Xenon spatial distribution on each burn-up steps as it does not follow the cosine law of the power profile. HPMC aims to achieve an optimum MC-burn-up integration; therefore one major task was to derive, implement and test a stable coupling scheme for Monte Carlo burn-up calculations.

This goal has been accomplished with the Stochastic Implicit Euler (SIE) method, see [17]. The SIE method has been derived as a stable method in theory, and this has been confirmed by our test calculations. Also, the SIE method is more efficient than other existing coupling schemes since all neutron histories contribute to the final solution.

The performance of the SIE based Monte Carlo burn-up coupling scheme was also tested on a burnup calculation of a standard 17×17 PWR fuel assembly, see [19]. The test results of the SIE method have been compared to those obtained from the standard predictor-corrector method as depicted in Figure 9 and Figure 10. The results confirm that the SIE based Monte Carlo burn-up coupling scheme is numerically stable even with large time steps of several months; the conventional burn-up calculation reveals strong numerical instability on Figure 9, while the new SIE-based burn-up calculation on Figure 10 is stable.



Figure 9: Spatial distribution of Xe-135 as function of the burn-up step in a conventional predictor-corrector based MC-burn-up calculation with 10.0 MWd/kgU step length.



Figure 10 : Spatial distribution of Xe-135 as function of the burn-up step in the SIE-based MCburn-up calculation with 10.0 MWd/kgU step length.

(C) High-Fidelity MC/TH Coupled Simulations and High Performance Computing

The coupled Monte Carlo/Thermal-Hydraulics system developed within HPMC [8], [11] is designed as a reference calculation tool for high-fidelity simulations of whole cores with advanced features e.g. an innovative technique of on-the-fly material definition that enabled the direct treatment of thermal-hydraulic feedback. This is realized by supplying continuous information to the particle tracking subroutine, enabling it to compute the macroscopic cross-sections at the proper temperature. Therefore, the original input parameters are overwritten, and the effective distribution of density and temperature is introduced. This technique greatly simplifies the neutronic input, and enables the simulation of large problem consisting of hundreds of thousands of cells. Therefore, the new methodology has opened many new possibilities including the analysis of full core problems which is of high interest for core design optimization and safety evaluations.

The coupled calculation scheme have been developed having in mind the MPI-OpenMP hybrid parallelisation approach. Since each MPI process operates on its own memory space, the thermal-hydraulic feedback has to be send to all slave processes. Special care must be taken to enable OpenMP threading and prevent data override. To demonstrate the capabilities of the newly developed methodology, a 3x3 PWR fuel assembly problem has been selected. It has had 104040 cells with thermal-hydraulic feedback. Two types of fuel fresh UOX and low enriched MOX has been used. Each assembly has been divided into 20 axial nodes. Such a calculation would have been impossible with the coupled schemes used in the past.



Figure 11: 3D power distribution within the 3x3 fuel assembly power predicted by the coupled MCNP5/SUBCHANFLOW system

To reduce the variance in the global power and accelerate the solution an iterative Weight-Window technique has been applied. This technique resulted in a rather uniform distribution of the relative error, by producing about equal particle population in all cells. In Figure 11, the normalized power distribution is depicted. The coupled scheme was run on computer nodes with 8 cores running 7 MPI jobs on each node. One core was left unused to increase the communication speed between processor cores. Based on the experience gained, a PWR quarter core, consisting of 647360 cells, is being prepared for calculation.

Special attention is given to improve the speedup of a parallel calculation with MCNP using large numbers of cores on a supercomputer cluster by a hybrid MPI and OpenMP parallelization. A simulation of a 3x3 pin cluster in the HPC supercomputer Juqueen at the Forschungszentrum Jülich was done for a criticality problem with MCNP using a total of 8192 cores. A speedup factor of about 2200 was reached. But if a 4-way Symmetric MultiThreading (SMT) on each core is used, an additional factor of about 2 can be gained in speedup.

For the development of a dynamical form of MCNP [21], capable of dealing with time-dependent problems with thermal-hydraulic feedback for safety calculations, the behaviour of precursors of delayed neutrons was implemented. The inherent statistics in the chain length of prompt neutrons and the large difference in lifetime of a prompt neutron chain (less than 1 ms) and the decay time of neutron precursors (0.1 to 100 s) presents major problems in the statistics of the estimated power as a function of time. New techniques like forced decay of precursors in each time interval and the branchless collision method allowing always a single neutron continuing after a collision (either from scattering or fission) are introduced to reduce the variance. A new and accurate technique was implemented to deal with moving control rods or control rod banks. The methods are about ready to demonstrate the calculation of time dependence in the time domain of seconds with a Monte Carlo code without any approximation to the physical modelling.

3.3 Selected results from the THINS project

In this section, two selected results from the THINS project are presented. Those correspond to the results from the code validation based on Phénix Natural Convection Test (NCT) and CFD analysis of LBE cooled fuel bundle heat transfer.

(A) Simulation of the SFR Phénix Natural Convection Test (NCT) [6], [22], [24]

Figure 12 shows the scheme of the Phénix primary system. The calculation of the NCT by coupling the 3D computational fluid dynamics (CFD) code TRIO_U with the best-estimate thermal-hydraulic system code CATHARE is presented.

The transient involves both system scale, with flows and temperatures varying in different components and circuits, and local 3D effects where fluid behaviour can't be modelled by 1D approach. Local simulation accuracy is usually limited by the applied boundary conditions, but it is impossible to model the whole reactor using only CFD tools. On the other hand, system codes do not provide capabilities to account for local fluctuations. Therefore, it appears necessary to couple a system code with a CFD code for detailed TH analyses in the primary circuit.

The first phase of the Phénix NCT, a steam generator drying operation, is characterized by a hotshock occurring at the intermediate heat exchanger (IHX) primary outlet window. During this unprotected phase of the transient, the temperature at the pump inlet is a key physical parameter for the determination of the core inlet temperature and consequently on the core neutronics. Physically, this parameter is determined by the complex 3D flow paths of the cold pool, which are likely to evolve during the transient due to buoyancy forces. After the reactor scram, the second phase begins and natural circulation rapidly takes place in the primary sodium system. Physically, the IHX primary inlet temperature is again determined by 3D complex thermal-hydraulic effects occurring in the hot pool. It seems therefore reasonable to prescribe the use of a CFD model for both cold and hot pool.



Figure 12: Phénix primary system scheme [22]

The coupling methodology used is of the domain-overlapping type associated to a Defect Correction (DeC) method [23]. The coupling software architecture relies on a common application programming interface (API) named ICoCo developed by CEA for coupling activities under NURISP project. The methodological aspects related of this work are detailed in [6]. Figure 13 presents the velocity and thermal fields during the first phase of the NCT obtained by the 1D/3D coupled model.



Figure 13 - Temperature and velocity fields in the primary circuit at t_0+250s [6].

Numerical vs. experimental comparison has been performed against measured quantities consisting of inlet/outlet primary and secondary IHX temperatures, primary pump inlet temperature, core outlet temperature, primary sodium mass flow-rate as well as level measurements in the hot pool, the cold pool and in the main vessel cooling system. An interested reader can refer to (Baviere et al. 2013, [6]) to have a better insight into the predictions of the 1D/3D coupled calculation. It was chosen here to present the evolution of the primary IHX outlet temperature, which illustrates the interest of thermal-hydraulic multi-scale coupling for addressing SFR transient analysis.

Obtaining the steady state requires several thousand seconds CFD/system coupled calculation in order to correctly evaluate the cold pool thermal stratification. Stratification originates from both the heating by the hot pool and the cooling by the main vessel cooling system. It occurs at elevations where sodium is poorly mixed by the primary flow, i.e. above the top of the IHX outlet windows. Thermal stratification of the cold pool was found to significantly alter the sodium temperature at pump inlet during phase 1 of the NCT.

During the initial steady state, the primary mass flow-rate, as well as the temperature at the inlet/outlet of the main components provided by the CFD/system coupled calculation where found to be very similar to that of the system stand-alone calculation.

The transient evolution of the primary IHX outlet temperature, as measured by a sensor located at the bottom of the IHX outlet window is shown in Figure 14. This sensor is immersed in the sodium stream exiting the IHX in the forced convection regime. The 60 K increase, resulting from the steam generator dry out during phase 1 and during the beginning of phase 2, is very well reproduced by the CFD/system coupled calculation. A 15 K temperature drop is then observed (at t = 5490 s), 24 s after the primary pump trip. Visualization of 3D temperature and velocity fields have revealed that this temperature drop originates from the transition between the forced convection to the natural circulation regime. Indeed, when buoyancy forces become predominant, the sodium stream exits the IHX at the top of the outlet window and the measurements of the sensor experiences a sudden shift from the average outlet temperature of the IHX to the local temperature of the cold pool which happens to be 15 K lower than the former one at this stage. The predictions of the CFD/system coupled calculation are also in very good agreement with the measured values during phases 2 and 3.



Figure 14 - Short- (left) and long- (right) term evolutions of the IHX primary outlet temperature (transient starts at to = 5000 s) [6].

To illustrate the effectiveness of coupling CFD and system codes in addressing SFR transient analysis, the predictions of the system code alone were also shown in Figure 14. Three liquid temperatures corresponding to the 0D elements located at the elevation of the sensor are presented

(the system code model of the cold pool is azimuthally sectorized into three equal parts). More generally, the spatially averaged quantities calculated by the system code present smoother evolutions than the experimental values obtained from local measurements. If correct, the temperature field obtained from the CFD/system coupled calculation may eventually be used to define the spatially averaged quantities that could be directly compared to the results of a system code. This leads to a more accurate validation procedure for the use of system codes to simulate the complex in-vessel flow of innovative reactors such as SFR and LFR.

(B) Simulation of LBE cooled rod bundle heat transfer [25]

In the Karlsruhe Liquid Metal Laboratory (KALLA) at KIT testing of rod bundle configurations is performed, to investigate the heat transfer in Lead-Bismuth Eutectic (LBE) cooled rod bundle and to quantify the influence of the spacers. The tested bundle consists of 19 rods with a diameter of 8.2 mm and a pitch of 11.48 mm in hexagonal arrangement. The length of the bundle is about 1.3 m. The 19 rods can be electrically heated with heat fluxes at a maximum of 106 W/m². The experiments are performed at coolant temperatures from 190°C to 450°C and at average flow velocities up to 1.8 m/s, i.e. Reynolds numbers close to 80000. For the test bundle 3 spacers are installed. The spacers have a length of 25 mm with a variable wall thickness from 0.5mm upstream to 1 mm at downstream. The bundle configuration of the numerical model is presented by Figure 15.



Figure 15: The rod bundle configuration

Because of symmetry conditions only a 60° part of the bundle is considered for numerical analysis. In vicinity of spacers large variations of the heat transfer conditions are expected, therefore the quality and the spatial resolution of the grid have significant influence on the accuracy of the simulations. In order to minimize the number of cells and mainly the numerical diffusion a full structured mesh consisting of 22 million cells was created. The difficulty for the meshing was to find an appropriate topology for a structured mesh and mainly to keep the cell angles within a reasonable range.

Standard turbulence models based on dissipation rate failed, also the application of scalable wall functions. The simulations could be performed with an omega Reynolds stress model and automatic wall functions with low Re formula taking viscous sub-layer resolution into account. Also the calculation of heat transfer in liquid metal flow is problematic because of the very low Prandtl number Pr<0.018. In most commercial CFD tools – the presented simulations are performed with ANSYS CFX - the calculation of the turbulent heat transfer is based on Re analogy, which means that the thermal boundary layer is balanced with the momentum layer and has the same thickness. The turbulent thermal diffusivity and the turbulent eddy viscosity are coupled by the so called turbulent Prandtl number Pr_{turb} , such as

$$Pr_{turb} = \frac{\mathbf{v}_t}{a_t},$$

which is assumed to be a constant close to 1. In this work, based on DNS/LES simulations on liquid metal flows in heated rectangular channels, the turbulent Prandtl number is considered as dependent on Re, y^+ and Pr. Figure 16 presents the distribution of Pr_{turb} in central position of spacer 2. At the walls Pr_{turb} approaches values close to 3, while towards the centre of the subchannels values of about 1.4 are reached. Away from the spacer at the centre of the subchannels Pr_{turb} decreases to values of 0.9, which is usually used as constant value for conventional fluids such as air and water.



Figure 16: Cross section showing the turbulent Prandt number at Re=78000

In Figure 17, a detailed analysis of local Nusselt numbers along two straight lines in axial direction on the heaters surface is presented. Line **a** is denoted as touched and passes through the centre of the fixing elements, while line **b** (untouched) is located with a circumferential displacement of 60° towards **a**. The heating of the bundle starts at z = 0.20m and ends at z = 1.08m with a constant heat flux. The origin of z is located at the model inlet, see Figure 15.



Figure 17: Analysis of the local Nusselt numbers

An analysis for two different Re numbers is presented, where Re=78000 is reached at an average coolant velocity of 1.8 m/s. Higher velocities lead to corrosion problems especially at the spacers made of steel. The local distributions are compared with a correlation taken from an OECD handbook for liquid metal rod bundle flows [26]. At the beginning of the heating the temperature

differences between the heater rod surface and coolant are low therefore Nu has a local maximum. Further downstream to the first spacer the flow develops towards an equilibrium state and the predicted Nusselt numbers are rather close to the OECD correlation.

The spacers are blocking the cross section, therefore the average cooling velocities are increasing and the conditions for heat transfer are improved. So at the entrance of a spacer the Nusselt numbers are locally increasing by about 80%. Along the touching lines inside the spacers the local heat transfer conditions are varying significantly, because in upstream position of a touching point the heat transfer conditions are improving rapidly due to stagnation point conditions while downstream a touching point the flow separates and offers poor conditions in terms of local heat transfer. So near touching points strong local fluctuations for the Nusselt numbers are predicted. For Re=7800 the turbulent heat transfer is significantly lower (against conduction), therefore the amplitude of the fluctuations are lower. Additionally for Re=7800 we are in the transitions region to laminar flow together with upcoming buoyancy effects which are yet not included in the numerical model. So in equilibrium regions in upstream positions of the spacers the agreement with the OECD correlation is lower. On the other hand for liquid metal flows especially for heat transfer there is a wide range of uncertainty for the experimental values from which correlations are derived. Therefore the overall agreement between simulation and the OECD correlation for the entire Re range can be designated as good.

4. Conclusions

The NURESIM roadmap started in 2005. Its target was to build and validate a European software platform for advanced core physics, thermal-hydraulics and multi-physics coupling, also including uncertainty and sensitivity tools. The NURESAFE project (2013-2015) should demonstrate that this target has become a reality by providing an exhaustive set of state-of-the-art software integrated in the platform and by running higher fidelity simulations of some LWR typical accidental transients at the full core scale. A European community of experts was created through the collaborative work within the NURESIM roadmap. Knowledge, best practices, modules are shared within this European community. In addition, the User's Group, consisting of partners from Europe, Asia and USA, are using and benchmarking the simulation platform against their own tools. The integration of codes into generic standardized tools for coupling or data processing also enhances the flexibility and effectiveness of the software platform.

As complement to the deterministic tools being developed at the NURESAFE project, the HPMC project, started in 2011, focused on the development of higher-fidelity numerical tools for design improvement and safety evaluations of any kind of reactors. To achieve these goals, a coupling of Monte Carlo methods with detailed thermal-hydraulic codes (subchannel codes), time-dependent Monte Carlo methods and stable MC-based depletion schemes are being developed. Due to the complexity of the problems to be solved and the degree of details (pin level) of the core simulations envisaged within the HPMC project, the use of high performance computers is a must, and to do so, modifications and new approaches for parallelization, converged solutions, reduced variance and high statistics are of paramount importance to be able to solve safety-relevant problems with the HPMC tools. In addition, the HPMC tools are definitely very much appropriate to deliver reference solutions to the ones of the NURESAFE codes (deterministic), especially in case where no experimental data is available. Hence, the HPMC and NURESAFE projects are very much complementary and will contribute to substantially improve the design and safety analysis methodologies of reactors cores. Regarding thermal-hydraulics, such an objective can rely on the THINS achievements.

The considered GEN-IV and ADS (Accelerator-Driven Systems) innovative reactor designs are from the thermal-hydraulic point of view mainly characterized by their coolants (gas, water and liquid metals). Many common thermal-hydraulic issues are identified among various innovative nuclear systems. Such thermal-hydraulic issues are the subject of the THINS (Thermal-Hydraulics of Innovative Nuclear Systems) project. The top target of the THINS project is the development of new and more accurate physical models and numerical simulation tools. To achieve this target thirteen experimental studies are included in this project and provide test data. Hence, a tight interaction between experimental and numerical activities is established. Numerical simulation provides support to experiments, and receives test data for the improvement of numerical simulation tools. Three years after the start of the THINS project, construction of most test facilities is finished. Most of them are in the phase of test data production and the project has been recently extended an additional year.

For the medium term, a tighter interaction with the NUGENIA (Nuclear Generation II & III Association) organization should allow industrial actors to acquire the NURESIM tools and methods in order to integrate them in their respective software systems. Also there is a will of integrating the HPMC-tools and methods in different NUGENIA areas, such as, Core and Reactor Performance (Area 3), Fuel Development, Spent Fuel and Decommissioning (Area 5) and Innovative LWR (Area 6). Another area for improvement would be to extend the software NURESIM platform to the GEN-IV reactors in the framework of ESNII and Horizon 2020, so that GEN-IV development can benefit from the generic developments achieved within those projects.

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Appendix: List of partners involved

The project partners are organized as follows: NURISP¹, NURESAFE², HPMC³ and THINS⁴

Name	Short Name	Country
AGENZIA NAZIONALE PER LE NUOVE TECNOLOGIE, L'ENERGIA E LO SVILUPPO ECONOMICO SOSTENIBILE ^{2, 4}	ENEA	Italy
ANSALDO NUCLEARE S.P.A. ⁴	ANSALDO	Italy
AREVA NP SAS ²	AREVA	France
ASCOMP GmbH ^{1, 2, 4}	ASCOMP	Switzerland
CENTER FOR ADVANCED STUDIES, RESEARCH AND DEVELOPMENT IN SARDINIA $^{\rm 4}$	CRS4	Italy
CHALMERS UNIVERSITY OF TECHNOLOGY ¹	CHALMERS	Sweden
COMMISSARIAT A L'ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES ^{1, 2, 4}	CEA	France
COMPUTATIONAL DYNAMICS LIMITED ⁴	CD-ADAPCO	Great Britain
DELFT NUCLEAR CONSULTANCY V.O.F ³	DNC	Netherlands
ELECTRICITE DE FRANCE S.A. ^{1,2}	EDF	France
GESELLSCHAFT FUER ANLAGEN- UND REAKTORSICHERHEIT (GRS) MBH ^{1, 2, 4}	GRS	Germany
HELMHOLTZ-ZENTRUM DRESDEN-ROSSENDORF EV ^{1, 2, 4}	HZDR	Germany
IMPERIAL COLLEGE OF SCIENCE, TECHNOLOGY AND MEDICINE ^{1, 2, 4}	ICL	United Kingdom
INSTITUT DE RADIOPROTECTION ET DE SURETE NUCLEAIRE ^{1, 2, 4}	IRSN	France
INSTITUT JOZEF STEFAN ^{1, 2, 4}	JSI	Slovenia
INSTITUTE FOR NUCLEAR RESEARCH AND NUCLEAR ENERGY - BULGARIAN ACADEMY OF SCIENCES ^{1,2}	INRNE	Bulgaria
KARLSRUHER INSTITUT FÜR TECHNOLOGIE ^{1, 2, 3, 4}	KIT	Germany
KUNGLIGA TEKNISKA HOEGSKOLAN ^{1, 2, 3, 4}	KTH	Sweden
LAGRANGE SARL ²	LGI	France
LAPPEENRANNAN TEKNILLINEN YLIOPISTO ^{1,2,4}	LUT	Finland
MAGYAR TUDOMANYOS AKADEMIA ENERGIATUDOMANYI KUTATOKOZPONT ^{1, 2}	KFKI	Hungary
NARODOWE CENTRUM BADAN JADROWYCH ²	NCBJ	Poland
NUCLEAR RESEARCH AND CONSULTANCY GROUP ⁴	NRG	Netherlands
PAUL SCHERRER INSTITUT ^{1, 2, 4}	PSI	Switzerland
STUDIECENTRUM VOOR KERNENERGIE - CENTRE D'ETUDE DE L'ENERGIE NUCLEAIRE ⁴	SCK-CEN	Belgium
TECHNICAL UNIVERSITY MUNICH ⁴	TUM	Germany
TECHNISCHE UNIVERSITEIT DELFT ^{1,4}	TU-Delft	Netherlands
TEKNOLOGIAN TUTKIMUSKESKUS VTT ^{1, 2, 3}	VTT	Finland
TEXAS A&M UNIVERSITY ⁴	TAMU	USA
UNIVERSIDAD POLITECNICA DE MADRID ^{1,2}	UPM	Spain
UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA ⁴	UNIMORE	Italy
UNIVERSITA DI PISA ^{1, 2, 4}	UPISA	Italy
UNIVERSITE CATHOLIQUE DE LOUVAIN ^{1, 2, 4}	UCL	Belgium
UNIVERSITY OF BOLOGNA ⁴	UNIBO	Italy
USTAV JADERNEHO VYZKUMU REZ A.S. ^{1,2}	UJV	Czech Republic