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Author(s): **Coordinator of the Project: C. Chauliac (CEA)**
Coordinator of SP1 (core physics): JM Aragones (UPM)
Coordinator of SP2 (thermal-hydraulics): D. Bestion (CEA)
Coordinator of SP3 (multi-physics): M. Zimmermann (PSI)
Coordinator of SP4 (sensitivity and uncertainty): D. Cacuci (UniKa)
Coordinator of SP5 (integration): N. Crouzet (CEA)

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NURESIM

ABSTRACT

This report is the Final Activity Report (Publishable Report) of the NURESIM Integrated Project (2005-2008) in charge of the development of a Common European Standard Software Platform for Nuclear Reactor Simulations.

It presents a summary of the salient results obtained by the 18 Partners during the project.

**This document is available on the
NURESIM-NURISP Open Web Site:**

www.nurisp.eu



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1 EXECUTIVE SUMMARY

The objective of the NURESIM Integrated Project (FP6) which lasted from 2005 to 2008, with contributions of 18 organizations from 13 European countries, was to start the development of a European Reference Simulation Platform for Nuclear Reactors (so-called NURESIM) and to deliver its first versions.

This development has followed a roadmap which is consistent with the SRA (Strategic Research Agenda) of the European SNE-TP (Sustainable Nuclear Energy Technology Platform) and resulted in the delivery of two successive versions during the course of the project. Consistently with the NURESIM roadmap, the development of the platform goes on now in the frame of the NURISP European Collaborative Project (FP7), which includes 22 organizations from 14 European countries.

NURESIM intends to be a reference platform providing high quality software tools, physical models, generic functions and assessment results.

The NURESIM platform provides an accurate representation of the physical phenomena by promoting and incorporating the latest advances in core physics, two-phase thermal-hydraulics and fuel modelling. It includes multi-scale and multi-physics features, especially for coupling core physics and thermal-hydraulics models for reactor safety. Easy coupling of the different codes and solvers is provided through the use of a common data structure and generic functions (e.g., for interpolation between nonconforming meshes).

More generally, the platform includes generic pre-processing, post-processing and supervision functions through the open-source SALOME software, in order to make the codes more user-friendly.

The platform also provides the informatics environment for testing and comparing different codes. For this purpose, it is essential to permit connection of the codes in a standardized way. The standards are being progressively built, concurrently with the process of developing the platform.

The NURESIM platform and the individual models, solvers and codes are being validated through challenging applications corresponding to nuclear reactor situations, and including reference calculations, experiments and plant data. Quantitative deterministic and statistical sensitivity and uncertainty analyses tools are also developed and provided through the platform.

A Users' Group of European and non-European countries, including vendors, utilities, TSO, and additional research organizations (beyond the current partners) has also been established in order to enhance the role of the platform in meeting the needs of the nuclear industry, as applied to current and future nuclear reactors.

This Final Activity Report summarizes the achievements of the platform in core physics, thermal-hydraulics, multi-physics, uncertainties and code integration at the end of the NURESIM project.



2 OBJECTIVES AND ROADMAP OF THE NURESIM PLATFORM

2.1 *The objectives of the NURESIM platform*

The NURESIM platform intends to be a European reference platform for nuclear reactor applications supported by a united European team of experts.

A reference platform

In order to become a reference, 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 capacity 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 meshes.
- to provide generic pre-processing and post-processing and supervision functions through the SALOME open source tool (www.salome-platform.org).
- 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.

A platform for nuclear reactor applications

The NURESIM platform is designed to meet the needs of the nuclear industry and it will be applied to current and future nuclear reactors. The Users' Group will help in this process.

A European platform supported by a European united team

The NURESIM-Platform aims to be a European platform, integrating the products and the knowledge of the European countries and easing collaborative work between them thanks to standards.

From the management point of view, an essential way to build the European platform was to federate the European competence within a single project and towards a common objective contrary to the past situation of skills fragmented between countries, organizations and scientific disciplines. 18 organizations were involved in the NURESIM project: ASCOMP, CEA, EDF, FZD, GRS, INRNE, JSI, KFKI, KTH, LUT, NRI, PSI, TUDELFT, UCL, UNIKA, UPISA, UPM, and VTT. They came from 13 countries: Belgium, Bulgaria, Czech Republic, Finland, France, Germany, Hungary, Italy, Netherlands, Slovenia, Spain, Sweden, and Switzerland.



2.2 The roadmap of the NURESIM platform

The development of the NURESIM Platform is a long term task which follows a general roadmap.

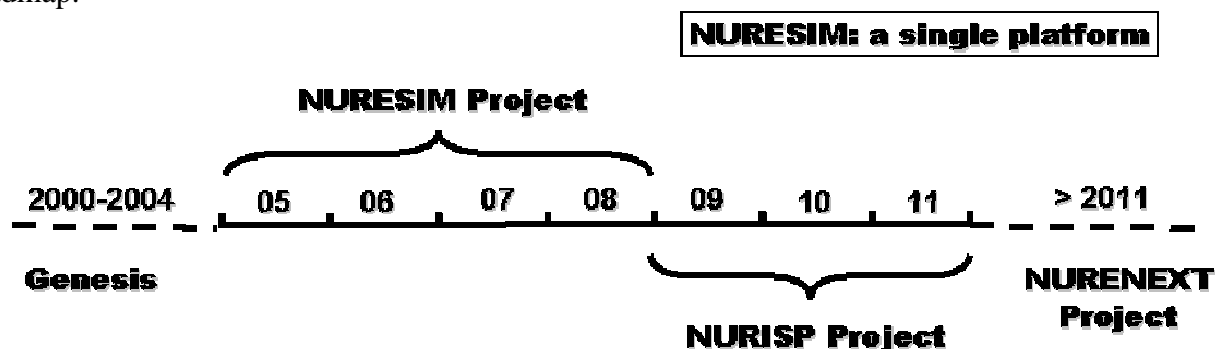


Fig. 1: the NURESIM Roadmap

Before NURESIM (genesis)

The FP6 NURESIM project was based on the results of several actions of FP5. Among them, EUROFASTNET made an analysis of the state-of-the-art in thermal-hydraulics, identified the limitations of the models and codes, listed 44 industrial needs ranked according to their industrial priority (based on information provided by the nuclear industry), and elaborated an R&D program.

The NURESIM project: a basis towards the target with first significant possibilities

The FP6 NURESIM project (2005-2008) has extended the EUROFASTNET approach to core physics, multi-physics and S&U (sensitivity and uncertainty) and proposed a platform to integrate the codes and the methods. This Integrated Project has provided the initial step towards the European Simulation Platform and demonstrated the potential of the proposal (www.nuresim.eu).

The following main results were obtained: improvement of models and/or methods in core physics and thermal-hydraulics, a first demonstration of a generic method for multi-physics coupling, the delivery of advanced S&U methods, a first integration of codes into the NURESIM platform, benchmarking results.

The NURISP project: consolidation and extension

The present FP7 NURISP project (2009-2011) is consolidating and extending the results of the FP6 NURESIM project with new codes connected to the platform and new steps made for integration, model development (including fuel), coupling, S&U and validation. The focus is on present (GEN-II) and future (GEN-III) PWR, VVER and BWR, but care will be taken to use generic methods so that future extension to GEN-IV reactors will be possible.

Long term development after NURISP: confirmation, rationalization and further extension

In the longer term, the NURESIM-platform will be developed consistently with the roadmap of the SRA (Strategic Research Agenda) of SNETP (Sustainable Nuclear Energy Technology Platform) and through close connection with the Users' Group.

The main objective will be to improve the NURESIM-platform and to further meet the needs of the European nuclear industry. The developments will be deepened and made more robust based on industrial feedback. Extension of the platform to Gen-IV requirements will be a new important and challenging target. The opportunity of extending the platform to severe accidents will be studied.

Another important objective of NURISP in the future will be to choose an "optimum set" of codes, not necessarily the same set for every partner, but a limited number of codes to avoid dispersion of effort. In these conditions, it should be possible to progressively move away from the present set of codes (which are dispersed, redundant, difficult to link to one another and where certain weaknesses persist) and work towards a European optimum suit of codes coupled together within the framework of the NURESIM-Platform.



3 OVERVIEW OF OBJECTIVES AND RELATION TO THE STATE-OF-THE-ART

3.1 Overview of objectives and relation to the state-of-the-art for SP1 (Core Physics)

Innovative activities within the NURESIM Core Physics (CP) Subproject SP1 aimed at solving the following important outstanding issues:

- For *Monte-Carlo codes*, control of the convergence of sources in eigenvalue calculations in order to perform coupled thermal-hydraulics/neutronics or coupled depletion/neutronics computations.
- For *deterministic codes*, extension of the treatment of self-shielding for intermediate mass isotopes that have diffusion resonances (e.g., iron). By fully coupling the lattice and the core codes, it would be possible to perform lattice-scale calculations with realistic core boundary conditions. Further improving the acceleration techniques is fundamental for all solvers.
- 3-D full-core integrated Neutronics-Thermalhydraulics LWR nodal simulation with fast execution of the *neutron kinetics modules*
- *Validation* with experiments and *benchmarks* of both well-separated and clean integral steady-state and transient effects.

The main objective was to integrate the most advanced software (physical modelling and numerical techniques) for reactor core physics, in a new standardized, common European software platform.

The final SP1 Core Physics codes available as deliverables at the end of the NURESIM project were:

- *Advanced Monte Carlo*: TRIPOLI-4 (CEA) with links to adjoint transport fluxes and modules for accelerated convergence of sources (CEA, TUD, KTH)
- *Lattice Level Transport*: APOLLO2.7 (CEA) with XS libraries, resonance and transport solvers and links to DKLib.
- *Core Level Transport and Diffusion*: DESCARTES System (CEA) with advanced 3D diffusion and SPN solvers (MINOS), which also includes now the analytical diffusion nodal solver ANDES (UPM), for eigenvalue and source-transient problems.
- *Core-Lattice Multiscale Diffusion*: COBAYA-3 (UPM) integrating the lattice (pin-cell scale: ALPES) and core (nodal scale: ANDES) solvers for whole 3D LWR cores by multigroup diffusion.
- *Advanced Kinetics Methods*: DYN-3D (FZD) with SP3 multigroup; in addition to DESCARTES (CEA) and COBAYA-3 (UPM).

The final result of the integration of the three code systems from CEA, UPM and FZD was the following one:

- The CEA system (TRIPOLI, APOLLO and DESCARTES) is the reference one in NURESIM, covering all the steps in reactor simulation.



- The UPM and FZD codes (COBAYA-3 and DYN-3D) are alternative codes which provide complementary LWR simulation capabilities, with quite effective and validated performance, that are covered in a different way, by the DESCARTES system.
 - Some of the solvers of COBAYA-3 are planned to be included in DESCARTES (such as the analytical nodal diffusion solver ANDES), but others are not so amenable to integration, so that the full COBAYA-3 code (that integrates a 3D multi-scale lattice-core multigroup diffusion scheme, with TH couplings at the sub-channels and core-channels levels, as well as a domain-decomposition scheme for parallel computation) offers a quite interesting RTD tool.
 - The DYN-3D code can be considered as a reference for 3D core nodal simulations for VVERs, because of its extensive validation applications.

The benchmarking of this NURESIM Core Physics platform of codes was very extensive, with the application of the main codes (TRIPOLI4, APOLLO2, COBAYA3 and DYN3D) by several partners to a wide and consistent range of PWR and VVER benchmarks, obtaining quite good results that provide a broad database for their verification and demonstration.

Hence it can be concluded that the NURESIM Core Physics simulation platform is at the state-of-the-art upper level for the design and safety analysis of PWR and VVER; showing significant potential, demonstrated at least at the proof-of-principle level, with capabilities and performance beyond the state-of-the-art codes and platforms for LWR and future reactors (as Gen.IV), such as the enhanced convergence of the fission sources in the Monte Carlo TRIPOLI4 code, the accuracy of the new MOC schemes for heterogeneous multigroup transport of whole 2D LWR cores in the APOLLO2 code, the 3D nodal and pin-by-pin parallel performance of the multigroup diffusion COBAYA3 code, the SP3 extension of the DYN3D code and the integration of these codes into the SALOME platform of NURESIM.

3.2 Overview of objectives and relation to the state-of-the-art for SP2 (Thermalhydraulics)

The general objectives of the NURESIM SP2 were:

- to progress significantly in the reliability of CFD simulations for key two-phase flow thermal-hydraulic processes that can occur in nuclear reactors, focussing on two high priority issues, the Pressurised Thermal Shock (PTS) and the Critical Heat Flux (CHF) (DNB and Dry-Out). This will be obtained by validating the models against available experimental data, developing and implementing new specific models, benchmarking NURESIM-CFD with other codes, and using fine scale simulations (DNS, LES, etc.) in a multi-scale approach.
- to implement the latest advances in thermal-hydraulics modelling in a shared platform, consistently with the general NURESIM objective to build a Common European Standard Software Platform for nuclear reactors simulations. This NURESIM TH platform will be coupled to SALOME. It will benefit from maintenance, and assistance and training will be provided to users.

The initial framework for performing these tasks was the NEPTUNE two-phase CFD module.

The specific objectives for PTS (Pressurized Thermal Shock) were:

- To use two-phase CFD to simulate all basic flow processes involved in two-phase PTS scenarios by developing and validating adequate models



- To develop better predictions than previous engineer methods based on experiments.
- To develop condensation models for large interfaces (free surface, liquid jet interface, steam jet interface, for PTS, K-H instability and steam injection in a pool)

The specific objectives for CHF (Critical Heat Flux) were:

- To use two-phase CFD as a tool for understanding boiling flow processes, in order to subsequently help new fuel assembly design and to develop better CHF predictions in both PWR and BWR.
- To envisage a “Local Predictive Approach” for the long term, where CHF empirical correlations would be based on local (meso-scale) T/H parameters provided by CFD

Common objectives for PTS and CHF for the end of the three year period.

For each application (PTS, DCC, DNB, Dry-Out) answers to the following questions were expected:

- Identification of all important flow processes of the application: how exhaustive is our identification and are there still some phenomena to identify?
- Selecting a Basic model: If a choice is made, how is it justified? If the choice is fully or partly open, what did we learn from benchmarking of various options?
- Filtering turbulent scales and two-phase intermittency scales: If a choice is made, how is it justified? If the choice is fully or partly open, what did we learn from benchmarking of various options?
- Identification of Local Interface structure: If a choice is made, how is it justified? If the choice is fully or partly open, what did we learn from benchmarking of various options?
- Modelling interfacial transfers: what are the most important and sensitive interfacial transfers to be modelled? Are the present available models validated on a Separate Effect Test (SET) basis and are the results satisfactory? Are further improvements or further validation work necessary?
- Modelling Turbulent transfers: what are the most important and sensitive turbulent transfers to be modelled? Are the present available models validated on a Separate Effect Test (SET) basis and are the results satisfactory? Are further improvements or further validation work necessary?
- Modelling Wall transfers: what are the most important and sensitive wall transfers to be modelled? Are the present available models validated on a Separate Effect Test (SET) basis and are the results satisfactory? Are further improvements or further validation work necessary?
- Use of finer scale simulations: what finer scale simulations were used and what did we learn from them?
- Demonstration test cases: what are the results of demonstration test cases in conditions close to the industrial application? What did we learn from them?
- Numerical Verification: What are the results of the Verification tests cases? Are the conditions for a good mesh and time step convergence clarified?

The achievement of these objectives is presented in section 4.2.



3.3 Overview of objectives and relation to the state-of-the-art for SP3 (Multiphysics)

The main objective of this subproject was to implement and test coupling between available neutronic and thermal-hydraulic solvers. To this aim, first the coupling scheme i.e. interface structure and data exchange had to be defined. Second, the established coupled codes had to be tested against known solutions. Two OECD/NEA benchmarks were selected: PWR MSLB and Peach Bottom Turbine Trip.

The subproject was organized into 3 situation targets: PWR, BWR and VVER. For each of these, the coupling scheme needed to be established.

At the beginning of NURESIM, state-of-the-art simulations were based on 2-group diffusion codes (with, generally, one node per assembly) coupled to reactor system codes, which usually represent a group of fuel assemblies by one thermal-hydraulic node (particularly for large BWRs with many hundreds of assemblies).

An important advancement was to increase the level of detail in the modeling of a reactor core. This meant to extend the current state-of-the-art simulation capabilities described above to a much more detailed, pin-based simulation. In this perspective, a pin-based deterministic transport calculation with a full CFD-thermal-hydraulics (2-phase) core-wide sub-channel simulation was to be coupled.

In light of the limited resources available, this concept was implemented only for a hot channel in a PWR application, resulting in a so-called 2-level coupling scheme.

The following work program was followed:

- Specification, review and integration within the NURESIM platform of coupling schemes for core analysis based on existing codes (CRONOS - FLICA) at the nodal (fuel assembly) and sub-node (pin) level. Evaluation of the future requirements i.e. for those codes expected to be available during the time frame of the project, e.g., TRIPOLI, CATHARE, etc. This review will need to account for the different core features of PWRs including VVERs and BWRs.
- Development and integration within the NURESIM platform of interpolation and averaging schemes, and data transfer based on the existing codes at the nodal (fuel assembly) and sub-nodal (pin) level
- Development of LWR Core model taking advantage of previous OECD/NEA benchmarks.

3.4 Overview of objectives and relation to the state-of-the-art for SP4 (Sensitivity and Uncertainty analysis)

In general, a physical system and/or the result of an indirect experimental measurement can be modelled mathematically in terms of:

- (a) linear and/or nonlinear equations that relate the system's independent variables and parameters to the system's state (i.e., dependent) variables,
- (b) inequality and/or equality constraints that delimit the ranges of the system's parameters,
- (c) one or several quantities, customarily referred to as system responses (or objective functions, or indices of performance) that are to be analyzed as the parameters vary over their respective ranges.

The objective of local sensitivity analysis is to analyze the behaviour of the system response locally around a chosen point or trajectory in the combined phase space of parameters and state variables.



On the other hand, the objective of global sensitivity analysis is to determine all of the system's critical points (bifurcations, turning points, response maxima, minima, and/or saddle points) in the combined phase space formed by the parameters and dependent (state) variables, and subsequently analyze these critical points by local sensitivity analysis.

Large-scale models of complex physical systems usually involve two distinct sources of uncertainties, namely:

- (i) stochastic uncertainty, which arises because the system under investigation can behave in many different ways,
- (ii) subjective or epistemic uncertainty, which arises from the inability to specify an exact value for a parameter that is assumed to have a constant value in the respective investigation.

A typical example of such a complex system is a nuclear power reactor plant: in a typical risk analysis of a nuclear power plant, stochastic uncertainty arises due to the many hypothetical accident scenarios which are considered in the respective risk analysis, while epistemic uncertainties arise because of the many uncertain parameters that underlie the estimation of the probabilities and consequences of the respective hypothetical accident scenarios.

A further classification can be introduced by distinguishing between sensitivity and uncertainty analysis methods that are conceptually based on deterministic procedures versus methods based on statistical procedures. Note that although both the deterministic and statistical methods can be used for both local and global sensitivity and uncertainty analysis, a survey of the literature clearly indicates that the deterministic methods are used overwhelmingly for local analysis while statistical methods are overwhelmingly used for global analysis.

Statistical methods bring with them at least two major, inherent, disadvantages, as follows:

- (i) since many thousands of simulations are needed, statistical methods are at best expensive (for small systems), or, at worst, impracticable (e.g., for large time-dependent systems);
- (ii) since the response sensitivities and parameter uncertainties are amalgamated, improvements in parameter uncertainties cannot be directly propagated to improve response uncertainties; rather, the entire set of simulations must be repeated anew.

For large-scale systems, in which the number of system parameters and/or parameter variations to be considered exceeds the number of responses of interest, the Adjoint Sensitivity Analysis procedure (ASAP) is the most advantageous method to employ, even though its implementation requires the development of an appropriately constructed adjoint system. This is because the adjoint sensitivity equation is linear in the adjoint function, and is independent of any parameter variations. Hence, the adjoint sensitivity equation needs to be solved only once in order to obtain the adjoint function.

For linear systems, the adjoint sensitivity equation can be solved independently of the original equation. In turn, once the adjoint function has been calculated, it is used to obtain the sensitivities to all system parameters, by simple quadratures, without needing to solve repeatedly differential and/or integral equations.

The exact local sensitivities obtained by using deterministic methods can be used for the following purposes:

- (i) understand the system by highlighting important data;
- (ii) eliminate unimportant data;
- (iii) determine effects of parameter variations on system behaviour;
- (iv) design and optimize the system (e.g., maximize availability/minimize maintenance);



- (v) reduce over-design;
- (vi) prioritize the improvements effected in the respective system;
- (vii) prioritize introduction of data uncertainties;
- (viii) perform local uncertainty analysis.

The objectives of the two workpackages of the Sub-Project SP4 are briefly recalled in the following.

- ***Sensitivity and Uncertainty Analysis of Core Physics Modules (NURESIM-S&U-CP)***

The aim of this work package was to develop new software modules that extend the methods for propagation of uncertainties significantly beyond the current state-of-the-art, by using the CEA-based software platform KALIF. Implementation of KALIF in the NURESIM platform was to lead to significant new capabilities (e.g., network of computers/nodes, grid computing, implementation of statistical tests via R language, and graphical user interface of SALOME for statistical post processing). Furthermore, new deterministic optimization methods to find extremas of model responses were to be developed based on GASAP method, and be implemented in KALIF as generic components.

- ***Sensitivity and Uncertainty Analysis of Multi-Physics Modules (NURESIM-S&U-MP)***

The aim of the first task was to implement uniformly in NURESIM the state-of-the-art in the area of uncertainty and sensitivity, including clarification of the nomenclature, identification & characterization of sources of uncertainty, and the evaluation of application results available from the industry, considering accident scenarios described in recent IAEA guidelines, and to write a state-of-the-art report on uncertainty and sensitivity analysis.

The aim of the second task was to evaluate and characterize the features of the GASAP (Global Adjoint Sensitivity Analysis Procedure) method, and to prepare a summary report that describes the GASAP and the other connected fundamental methods for commuting sensitivities exactly, namely the Forward Sensitivity Analysis Procedure (FSAP) and the Adjoint Sensitivity Analysis Procedure (ASAP), respectively, adopting the typical nomenclature currently used for the analysis of thermal-hydraulic system codes. This report had to prepare the basis for a step-by-step comparison between the CIAU method of Uni. Pisa, on the one hand, and the GASAP method.

3.5 Overview of objectives and relation to the state-of-the-art for SP5 (Integration)

The aim of the "Integration" Sub-Project was to develop the generic functions of the platform, to deliver them to the NURESIM partners, and to integrate the developments undertaken within RTD-SP1 through SP4.

In particular, SP5 had to assist the NURESIM participants to integrate modules, codes and deliverables into the SALOME platform, and provide specific training on the SALOME platform.

Furthermore, the platform had to be adapted to meet the needs of the other SPs.

To integrate new developments into the NURESIM platform, a strict protocol had to be set up. Thus, softwares proposed for integration have been subject to passing acceptance tests, to ensure their compatibility with the SALOME platform without degrading previously achieved results and performances.



4 MAJOR ACHIEVEMENTS DURING THE PROJECT

4.1 Major achievements during the project for SP1 (Core Physics)

The major achievements accomplished and demonstrated in the NURESIM SP1 Core Physics subproject, based in the proof-of-principle and first significant milestones achieved in the first two years, were completed and documented in the third reporting period, including significant advancements in the state-of-the-art of Monte Carlo methods (TRIPOLI code in WP1.1, done by CEA, TUD and KTH), deterministic diffusion and transport methods (APOLLO2, DESCARTES1 and COBAYA3 codes in WP1.2, done by CEA and UPM) and neutron kinetics methods (DYN3D, DESCARTES1 and COBAYA3 codes in WP1.3, done by FZD, CEA and UPM).

All of the new codes development, implementation and documentation were achieved and documented as milestones and deliverables of the tasks, with the codes and solvers released to the interested partners. The final implementation and testing of some advanced modules and options, as well as the revision and completion of the documentation for the final deliverables, were completed and revised in the last reporting period of the project.

In conclusion, the advanced codes of the NURESIM Core Physics platform were released and documented and the Core Physics benchmarks for PWR and VVER were completed and documented.

On other hand, the coordination and the setup of guidelines for the utilization and benchmarking of the NURESIM Core Physics computational platform created a team of partners which accomplished the training on the use of the SALOME platform, started the in-house implementation and use of the CEA codes included in the NURESIM Core Physics platform (APOLLO2, CRONOS2, CEA93-Lib, SILENE, FLICA4 and DESCARTES-Core) after signing the ad-hoc bilateral *SOFTWARE USE LICENSE AGREEMENTS in the frame of the European NURESIM Project* in December 2005, as extensions of the Consortium Agreement (in WP1.4, done by CEA, TUD, KTH, EDF, FZD, PSI, UPM, INRNE, NRI and KFKI). Several hands-on training seminars on the APOLLO2 and CRONOS2 codes with auxiliary tools and codes, of one week duration each, were done in the last quarter of 2006 with the assistance of the technical staff of the partners. Moreover, a support for the use of these codes has been continuously delivered for the achievement of the different benchmarks.

A detailed presentation of the NURESIM Core Physics codes including presentation of physical models, mathematical methods and description of input decks was performed during the final NURESIM workshop training sessions on the TRIPOLI4, APOLLO2 and CRONOS2, COBAYA3 and ANDES and DYN3D-SP3 codes, which took place in Madrid, before the General NURESIM Seminar in November 2008.

The detailed list and specifications of the PWR and VVER benchmarks, achieved by the partners using the NURESIM CP platform, was released and documented after being elaborated, discussed and agreed between the task coordinators (EDF and FZD) and the partners (CEA, PSI, UPM, INRNE, NRI and KFKI), with the overview of the WP and SP coordinators (CEA and UPM) for quality assurance.



4.1.1 WP 1.1: “Advanced Monte Carlo Methods”

4.1.1.1 - Steady state calculations

The general-purpose Monte Carlo transport TRIPOLI-4 modules (CD-ROMs with code and documentation) was released, and a first necessary step was to familiarise with the code, its installation procedures and its programming as well with the C++ programming language used in the code. Feedback to CEA has been given on several occasions, both with respect to the installation procedures and the code itself and some code improvements were suggested.

A report with findings on the installation procedure for the TRIPOLI-4 Monte Carlo code was produced, as well as compilation and use of the code. New versions of TRIPOLI-4.4 were received, and a number of new features were provided.

A methodology for efficient computing of the steady state core conditions by Monte Carlo method suitable for TRIPOLI-4 was prepared. It was done efficiently by the stochastic approximation process with variable step size and variable sample size of MC eigenvalue calculations. A report was issued, and a journal paper “Stochastic Approximation for Monte Carlo Calculation of Steady-State Conditions in Thermal Reactors” was published in NSE in March 2006.

4.1.1.2 - Benchmarking

First of all the Specifications of the PWR and VVER cell-lattice benchmark problems for TRIPOLI-4 were done.

The work started with the execution of the PWR benchmarks, especially the pin cell and assembly benchmarks. Input files were generated as well as cross section files at the required temperatures, which were not available in the TRIPOLI-4 package.

To carry out the benchmark problems for PWR geometries, inputs were created to TRIPOLI-4 and MCNP5 for the pin cell and assembly benchmarks at zero burn-up. As the benchmark specifications defined specific temperatures of materials, cross section data files had to be generated at those specific temperatures as they are not available with the TRIPOLI-4 or the MCNP5 code packages. After correcting the cross section libraries generated for the MCNP5 code for thermal scattering at the relevant temperatures good agreement was found between TRIPOLI-4 and MCNP5. A report was written documenting the results.

The VVER-1000 cores are characterized by high dominance ratio which is a challenging issue in criticality calculations. The solutions were obtained by 64-processor runs using “super cycle” techniques for post-processing to account for the cycle to cycle correlations and to estimate the real (not apparent) deviations.

The TRIPOLI4 solutions for pin cell and lattice problems were tested against consistent MCNP calculations. The results for fresh and depleted VVER cores were compared with well converged solutions by the higher-order MOC in APOLLO2. Good overall agreement was displayed.

The detailed achieved results are the following ones:



- Production of cross section data files for TRIPOLI-4 at the required temperatures for the PWR and VVER benchmarks.
- Results of the PWR pin cell and cell-lattice benchmark problems.
- Results of the VVER-1000 LEU and MOX assembly benchmarks.
- Results of the *VI000-2D-C1-tr* and *VI000CT2-EXT1* whole core benchmarks.

4.1.1.3 – Variance reduction and accelerated convergence

The adjoint methods for automated variance reduction and accelerated convergence of sources distribution in Monte Carlo calculations have been developed and tested, in order to introduce the results in the TRIPOLI-4 code for the NURESIM platform.

Building on the theory of zero-variance Monte Carlo schemes for source-detector problems, a theory has been developed for a zero-variance scheme for criticality problems. The theory is based on biasing the neutron transport process to determine the next collision site as well as the collision process to determine energy and direction after scattering by appropriate adjoint functions.

For verification purpose, this theory has been implemented in a separate program using the simplified one-group two-direction transport model, in which case analytic solutions of the neutron flux distribution, k_{eff} eigenvalue and necessary adjoint functions can be obtained for a simple slab reactor. The implementation shows clearly a limit to zero variance if the Russian roulette threshold goes to zero. However, this requires that the eigenfunction of the fission source distribution is known in analytical form, which is only possible for such a simplified system. A report was issued describing the analytical solutions of the adjoint functions for such a system as well as the results of the Monte Carlo program showing the approach to zero variance.

If the fission source distribution is not known, it must be derived by sampling successive generations of neutrons until a converged source distribution is obtained. If the adjoint function is known exactly, the effective multiplication factor for a single generation can still be obtained with zero variance. However, due to the generation of zero, one or more new fission neutrons at each collision there is a lower limit to the variance that can be obtained for the effective multiplication factor over various generations. During the project no method was found to eliminate this residual variance. It was also found that biasing of the transport kernel in the Monte Carlo calculation also accelerates the convergence of the fission source distribution.

The program has been extended to read in and use the adjoint function from a 1-D discrete ordinates calculation with discrete directions. Studying the separate effect of biasing the transition kernel and the collision kernel showed that implementation of optimum biasing of the transition kernel takes much additional CPU time and is therefore not always effective. It depends strongly on the way of implementation and the geometrical complexity of the system. In contrast, the optimum collision kernel biasing not only reduces the variance but also increases the total efficiency of the Monte Carlo calculation.

As a first step to realistic neutron transport models the multi-group case was implemented. Adjoint functions for the one-dimensional plane geometry with the two-direction model were obtained from the deterministic code XSDRN. As the adjoint calculation must be performed for the system neglecting fission reactions, the cross section library has to be adapted.

The theory of zero-variance Monte Carlo schemes for criticality problems was further developed for realistic applications. As the adjoint functions are obtained from a deterministic multi-group discrete-ordinates calculation, extensions of the theory were developed for application to continuous



directions as used in the Monte Carlo modelling. Much effort was spent on the implementation of the zero-variance biasing technique in the general purpose Monte Carlo code TRIPOLI-4. To that end the most recent development version of the code was obtained from CEA which included the option for multi-group treatment of the neutron transport. The implementation in TRIPOLI-4 was realized in close cooperation with CEA. A report was written to document the methods used and some implementation details.

The method was applied to an existing benchmark test problem consisting of a 1-D slab system with two fuel zones separated by a water zone. This system forms a loosely coupled core and therefore it may be problematic to reach a converged source distribution in a Monte Carlo calculation. The zero-variance based biasing scheme could be successfully applied, resulting both in a faster source convergence and a reduction in variance of the effective multiplication factor.

A special issue is the generation of the appropriate adjoint function from a deterministic transport code. It turned out that the TORT code was not reliable for generating the angular adjoint function. Therefore the PARTISN code was obtained from the NEA Data Bank which could be used satisfactory to generate the angular adjoint function for 1, 2 and 3-D systems with arbitrary number of energy groups and directions. With the PARTISN code the necessary adjoint functions were obtained for the 3-zone loosely coupled core system used for testing purposes and for a realistic PWR 17x17 fuel assembly for a demonstration calculation.

The variance reduction technique developed for criticality calculations was also used for calculating the response of an ex-core detector. To this end the eigenfunction source distribution in the core has to be obtained first and next the ex-core detector response is estimated using a biased neutron transport run without taking into account fission. The biased transport run requires an additional preparation step to start from a source distribution with particle weights inversely proportional to the detector adjoint function. A report was issued with a description of the method and a demonstration case.

Several papers about the main research results were published at international conferences and in international journals (see section 7.1).

The detailed achievements were the following ones:

- Development of a Monte Carlo program applying the two-direction transport model to demonstrate the variance reduction when the transport kernel is biased based on the zero-variance scheme.
- Extension of the demonstration program to multiple energy groups.
- Proof that biasing of only the collision kernel results in the highest efficiency gain.
- Acceleration of fission source convergence due to optimum biasing.
- Reporting the results of a study of various source convergence acceleration methods encountered in the literature.
- Demonstrating with a simplified test program the performance of the fission matrix method for accelerating the fission source distribution convergence in Monte Carlo calculations.



4.1.2 WP 1.2: “Advanced Deterministic Diffusion and Transport Methods”

4.1.2.1: Integration of the advanced data model and lattice scope tools.

First of all, the advanced data model and lattice scope tools were specified and described.

Then, the following software modules were released: libraries containing the modules for the target platforms, Python interface of the modules, and HTML documentation of the modules, the cross sections libraries for core calculations and advanced lattice scope tools: resonance and flux transport solvers integrated in the common platform.

Three two-week hands-on seminars on the APOLLO2 and CRONOS2 codes have been organized, and some of the new investigation results and an overview of the computational characteristics of DESCARTES were also presented. Finally, tools have been implemented in order to have a direct link between APOLLO2 libraries and DESCARTES

4.1.2.2: Integration of the advanced core scope tools.

The following developments were done and integrated into Descartes and delivered with links to the SALOME platform:

- A diffusion eigenvalue solver in x-y-z geometry compatible with discontinuity factors and without energy group or approximation order limitations (mixed dual finite element solver MINOS)
- A simplified transport SPN solver based on mixed dual finite elements, with flux angular discretization and scattering anisotropy determined by user cross section library.
- A transport SN solver, with flux angular discretization and scattering anisotropy determined by user specifications according to cross section library capability.
- The capacity to deal with adjoint problems for critical and source equation diffusion, and SPN and source problem solution for diffusion and SPN solvers.
- The development and testing of the generalized analytical nodal method for multi-group and 3D geometries in the ANDES analytical nodal solver for 3D rectangular and triangular nodes.

4.1.2.3: Integration of the advanced core-lattice methods.

The advanced core-lattice method developed by UPM has been implemented in the full COBAYA-3 code, in multigroup diffusion for 3D rectangular geometry (PWR cores) and steady-state eigenvalue problems. That is a scheme with a Domain Decomposition by alternate core dissections for the local 3D fine-mesh problems with synthetic nodal acceleration, which has been perfected with cyclic overlapping in four dissections.

The domain decomposition method was developed and tested with four alternate 3D dissections in the COBAYA-3 code for lattice-core multi-scale 3D rectangular geometry, including positive verification results and integration into the SALOME platform

The scheme has been extended to source and kinetics problems.

The report and sample/test problems for use of this advanced core-lattice methods integrated in NURESIM have been released: COBAYA3 and ANDES Users Guide



4.1.3 WP 1.3: “Advanced Neutron Kinetics Methods”

The particular objectives of this Work Package were the improvement of physical models and numerical techniques as well as the validation of the models and implementation of interfaces to Thermal-Hydraulics.

First of all the release of the neutron kinetics modules of DESCARTES (including the SPN approach) forming the initial basis of the common software platform was done, as well as the description of models and methods and the Code Manual and Input Data Description.

The main achievements are:

- All kinetics modules, including multi-group and analytical coarse-mesh finite-difference solvers, were embedded in the common software platform architecture by linking via SALOME. Thus, data exchange between kinetics and other solvers of the software platform are accomplished using the common data structure.
- The advanced kinetics modules of DYN3D for hexagonal core geometry were further developed, including descriptions of the improved physical and mathematical models.
- The multi-group SP₃ transport version of 3D steady-state and transient reactor core analysis code DYN3D was developed.
- The multi-group SP₃ solver was validated against OECD/NRC PWR MOX/UO₂ transient benchmark (Beckert and Grundmann, 2007 and 2008). The SP₃ solver comprises versions for both node-wise and pin-wise resolution of the neutron flux and power distribution.
- Description of models, methods and input data for the basic version of the DYN3D code which was put into NURESIM as initial input as well as on development and verification of the multi-group kinetics package and nodal approach for solving the multi-group SP₃ equations were elaborated.
- The DYN3D code was implemented as the VVER reactors reference code into the NURESIM software platform SALOME.
- A pre-processor based on SALOME was developed. The visualisation of DYN3D results based on SALOME tools was implemented. A documentation of the integration was elaborated.
- Several demonstrations on the development and integration of DYN3D into the NURESIM platform were presented.
- The treatment of source and kinetics problems in the 3D advanced analytical nodal solver was implemented in the multi-group ANDES solver, and the advanced multi-scale cell-nodal COBAYA3 multi-group kinetics was developed.
- Report and sample test problems were delivered for use of the advanced analytical nodal ANDES solver multi-group kinetics package and the advanced COBAYA3 kinetics package integrated into the common NURESIM platform through links with SALOME.

4.1.4 WP 1.4: “Benchmarking of the NURESIM Core Physics Platform”

4.1.4.1: Generic strategy and guidelines for benchmarking.

A report with the definition of generic strategy and guidelines for benchmarking of the NURESIM Core Physics platform was produced from the CEA proposal and the contribution from all SP1 partners. Its scope includes the different reactor types to be considered: PWR, VVER, and square and triangular lattices in critical experimental reactor configurations.

This report defines a generic strategy for the NURESIM-CP Benchmarking which is based on a step-by-step validation process from cell geometry to core description. This process takes into account in priority only a set of “numerical” problems with references carried out by Monte-Carlo calculations and/or deterministic calculations especially for depletion cases (such as results obtained by a deterministic code with the Method Of Characteristics (MOC) and a fine energy discretization). Nevertheless, well documented experiments, accepted by the international community, are not excluded from the benchmark problems.

4.1.4.2: PWR Benchmarks.

The first phase of the work included the detailed specification of data and results to be calculated for comparison among the different codes, solvers, data libraries and model options. The benchmark problems for PWR addressed the key issues at the cell, lattice and core scales, in both clean and burnup states at stationary conditions.

The initial descriptions of the PWR benchmarks at the cell and lattice scales and at the multi-assembly and core was prepared, and already obtained the preliminary solutions with APOLLO2.7 of the PWR NURESIM Core Physics Benchmarks, in its part 1: cell and lattice scope.

To qualitatively assess the developed PSI APOLLO-2 schemes, a comparison of the obtained depletion results was made against the standard 2-D transport solver used at PSI for LWR, the OECD/NEA PWR REA (Rod Ejection Accident) benchmark for a MOX core.

The selection and actualization of the specification data for 2D and 3D mini-cores and whole core PWR steady-states at Hot Zero Power (HZP) of the NEA-OECD PWR transient benchmarks were done, for verification of the 3D multigroup nodal core solvers and lattice-core solvers, including reference and preliminary COBAYA3 solutions, which were completed with positive results.

An overview report on the specifications, reference data and results for the PWR core physics validation benchmarks and their analysis was released.

4.1.4.3: VVER Benchmark.

The first phase included the detailed specification of data and results to be calculated for comparison among the different codes, solvers, data libraries and model options. The model problems for VVER addressed the key issues at the lattice and core levels, at both clean and burnup states at stationary conditions.

A series of benchmarks was solved by using the NURESIM platform codes APOLLO2, CRONOS2 and DYN3D to validate these codes for VVER reactors calculations. Based on the general strategy of core physics code validation applied in NURESIM, a step-wise approach was chosen for benchmarking, starting from numerical problems to assess and to minimize numerical errors. The



next step was code assessment on problems, where “exact” numerical solutions with minimized numerical errors or well assessed measurement data are available. One specific objective of the analysis was to validate APOLLO2 VVER-1000 assembly calculations against Monte Carlo reference solution in accordance with the step-by-step validation procedure in NURESIM.

In the next phase of the benchmarking procedure, experimental problems were used for code validation. Measurement data gained from experiments at the zero power test facility ZR6, at the full-size VVER-1000 experimental facility V-1000, and from kinetic experiments at the LR-0 zero power reactor in NRI Řež were compared with DYN3D and APOLLO results.

The main achievements are:

- The mathematical 2D benchmarks for VVER-1000 type cores *V1000-2D-C1-C3* with reference transport solutions obtained by means of the transport codes HELIOS and MARIKO were defined.
- NEM (Nodal Expansion Method) diffusion solutions were calculated with DYN3D code. The homogenisation error was estimated by comparison of the transport and NEM diffusion.
- The DYN3D solution of the mathematical 3D benchmark *V1000-3D-C1* with fine mesh diffusion reference solution, proposed to be solved with APOLLO2 (transport reference solution) and CRONOS2 (diffusion) was provided. Other solution was obtained by the code DYN3D with HEXNEM2 nodal expansion method.
- The DYN3D solution of a kinetics benchmark *V440-AER-DYN2* with CRONOS2 reference solution was defined and provided. Both methods for the solution of the diffusion equation (HEXNEM1 and HEXNEM2) were used.
- The specifications for an extended mathematical benchmark *V1000-CT2-EXT1*, and the specifications for 5 experimental benchmarks: *ZR6 (3 lattices)*, *V1000-LR0-KIN (core)* and *V1000-VALCO-STAT (core)* were provided.
- The experimental cores *V1000-VALCO-STAT*, *V1000-LR0-KIN*, and lattice *ZR6* benchmarks were solved with DYN3D and APOLLO2.
- The multi-physics benchmark *V1000-CT2-EXT2* was defined. The benchmark comprises a VVER-1000 core calculation with MSLB TH boundary conditions, as an extension of the ongoing OECD VVER-1000 MSLB benchmark (*V1000CT-2*).

A detailed comparison of the main results from the various codes and different project partners was provided. Conclusions were drawn for each benchmark and on the general status of core physics benchmarking for VVER.

By summarising the results of the code validation, it can be concluded that the diffusion code DYN3D has proven to be an effective tool for steady-state and kinetics core calculations for VVER type reactors. The capability of the CRONOS2 diffusion solver for hexagonal fuel element geometry to provide reference solutions, at least for steady-state problems, by systematic mesh refinement was demonstrated. The APOLLO2 transport code has shown the capability to provide cell, lattice and core solutions with high accuracy and to treat burn-up problems with changing nuclide composition.



4.2 Major achievements during the project for SP2 (Thermalhydraulics)

4.2.1 WP2.1: "Pressurized Thermal Shock"

During the first year of the project (Feb. 2005 - January 2006):

- The identification of relevant PTS-scenarios was done and priorities for model improvements were established (deliverable D2.1.1)
- A data basis for the validation/verification of the common standardized NURESIM software was established, all experimental data being reviewed with respect to their relevance with the needs for model improvements (deliverable D2.1.2)

These two deliverables were loaded on the NURESIM Open Web Site.

During the second and third years of the project, the work was devoted to validation, benchmarking, development of physical models, and use of DNS-LES results for developing models.

All the tasks of WP2.1 investigate flow situations which are related to the two-phase PTS situation, i.e. Emergency Core Cooling System (ECCS) injection into a partially or totally uncovered cold leg. This also includes Direct Contact Condensation (DCC).

Most of the activities are simulations based on available or new (Poolex STB-31) experimental data. Bonetto-Lahey data and Iguchi data investigate the effects of a plunging jet with bubble entrainment below the free surface and with turbulence production, which are two basic phenomena having an influence on the PTS issue. Other simulations (Thorpe experiment, TOPFLOW horizontal air-water tests, Fabre et al. data) were devoted to the general problem of free surface modelling without condensation, focussing on momentum transfer modelling, wave prediction, and turbulence prediction close to the free surface. DCC in stratified (co-current and counter-current) flow was simulated with LAOKOON tests and COSI tests in steady or quasi-steady conditions which are also encountered during ECC injection in a PWR cold leg. KFKI data refer to condensation induced waterhammer. Poolex STB-31 test simulates steam injection in a pressure suppression pool in low flowrate condition with a quasi-steady steam-water interface.

In addition also DNS simulations of stratified flow were done, which are devoted to the modelling of interfacial momentum transfer, turbulence modelling close to the free surface and condensation.

From all these tasks, one can draw conclusions on the modelling of Pressurized Thermal Shock and Direct Contact Condensation:

- *Basic model approach:* The most important effects of two-phase PTS can be reflected by separate flows, i.e. as two coupled single phase flows with a moving boundary. On the other hand, bubble entrainment below the free surface at the ECCS jet location creates a situation with both a free surface and a bubbly flow which can only be reflected by a two-fluid model. Bubble entrainment is of secondary importance and not well captured by presently available models. Neglecting bubble entrainment, in principle both the two-fluid model and the homogeneous model can be used. Simulations of the LAOKOON and AEKI water hammer experiments on stratified steam liquid flow with condensation were done with both methods without showing a clear advantage of one of the methods. In case of a homogeneous model with interface capturing or interface tracking any bubble entrainment by the jet or by waves has to be avoided since the entrained bubbles cannot de-entrain in the frame of this model. This cannot be guaranteed in principle. For this reason according to the present stage of development of CFD codes for two-phase flows the use of the more general two-fluid model



is recommended for near future, but it has to be considered, that it does not capture all details of the flow. In the future more sophisticated models which combine the advantages of both models should be developed to improve the simulation capabilities for PTS. One possible way is the use of so-called Large Scale Simulations (LSS).

- *Filtering or averaging procedure:* In PTS scenarios there are some rather long periods of transients with a quasi-steady flow or slowly varying flow in cold legs where a RANS approach is expected to be the most applicable approach. However, in the initial phase of ECCS injection, in condensation driven instabilities, or in case of steam injection in a pool, the transient nature of the flow makes the RANS approach inappropriate, and then URANS or LES approaches should be investigated. On the other hand, LES application in bounded flows is possible with some RANS-LES coupling. But if the presence of the walls so constricts the bulk flow region that large coherent structures cannot be sustained, RANS alone may be sufficient. If interfacial waves at the free surface are expected, it is not clear how such waves may be affected by the filtering of turbulent fluctuations and two-phase intermittency scales. Considering these uncertainties, RANS or URANS methods should be used for the near future. LES and especially scale adaptive simulation (SAS) should be tested and qualified for PTS simulations for the medium future.
- *Identification of local interface structure:* For modelling interfacial transfers it is necessary to select the adequate interfacial transfer laws and to determine the interfacial area. This requires the knowledge on interface position and structure. In case of a pure stratified flow there is a unique interfacial structure corresponding to a free surface between a continuous liquid and a continuous gas. The identification of the free surface can be done by simple criteria based on the void fraction or by using some interface recognition methods (e.g the LI3CL method proposed by Coste 2007). Interface Tracking Methods (ITM) have been benchmarked against Thorpe experiment flow conditions, in TOPFLOW horizontal tests, and in KFKI tests. As long as there are not strong surface perturbations such as breaking waves or droplet entrainment, there is not a clear advantage of using an ITM. In PTS scenarios with bubble entrainment below the free surface by the ECCS jet both a free surface and a bubbly flow are encountered and a specific identification of the local flow regime would be necessary capable of identifying both presence of bubbles and presence of the free surface. Simulations of plunging jet tests have shown that the modelling of the correct amount of entrained gas depends mainly on the identification of the specific local situation where the jet crosses the free surface. At this very location a specific interfacial friction should be used to control how much steam (or air) is entrained. In principle interface capturing seems to be sufficient if smearing of the interface is avoided. Correlations on interfacial transfers can be applied.
- *Interfacial transfer:* If bubble entrainment is considered the complete set of bubble forces has to be included in the simulation of the region of bubbly flow to reflect the interfacial momentum transfer. More problems arise for the modelling of interfacial transfers on free surfaces. Effects of the meshing have to be considered in this case. One approach which could improve the simulations regarding such effects is the so-called Large Interface Simulation, which assumes an interface modelled by 3 layers of computational cells (LI3CL method proposed by Coste 2007). However this model is not yet fully mature. Additional tests and developments are required. Other methods make use of interfacial functions similar to wall functions. They should be able to provide a good modelling without any large influence of interfacial waves. Such approaches should allow providing a converged solution with a reasonably coarse nodalization. When waves are likely to occur and to produce a strong increase of the roughness and of the friction coefficient, the main question is to be able to characterize this roughness. This remains a difficult and fully open problem.



The interfacial heat transfer in presence of condensation remains partly unresolved although some reasonable predictions were obtained for COSI and LAOKOON. The formulation of the liquid-to-interface heat transfer using a wall function approach should be able to provide a converged solution with a reasonably coarse nodalization, which is not yet achieved so far. Additional work on heat transfer is required.

- *Turbulent transfers*: Liquid turbulence plays a dominant role in PTS scenarios. It influences the mixing of the cold and hot liquids, and consequently the amount of condensation and the minimum liquid temperature at inlet of the Reactor Pressure Vessel (RPV). The jet impact being the main source of turbulence, first simulations of Iguchi jet test have shown that a k-epsilon model could predict reasonably well this turbulence but it should be complemented by measurements in a more representative geometry. Beside the choice of appropriate turbulence models discussed above also the coupling of the turbulence fields is important. In case of bubbly flows the bubble induced turbulence should be considered. For coupling of turbulence on a free surface, special measures as turbulence damping due to stratification have to be applied. The influence of condensation on the turbulent fields is still an open question. Neglecting this effect should result in conservative results regarding the thermal loads on the RPV walls.
- *Wall transfers*: Classical single-phase wall functions for momentum and heat transfer at wall are currently used in stratified flow. None of the available experiments could provide a validation of these wall functions but it is not expected that they represent a main source of uncertainty in PTS simulation.
- *DNS-LES simulations*: DNS simulation for stratified flow were used to derive some closure laws for interfacial momentum, turbulence and heat transfer, which can be used by CFD codes. Future work is still necessary to conclude, with implementation of these laws in NURESIMCFD and comparison with DNS-LES on the same flow conditions, and validation against experimental data

4.2.2 WP2.2: "Critical Heat Flux"

During the first year of the project (Feb. 2005 - January 2006), the activity started with the review of existing experimental data about CHF and the identification of new experimental needs, on existing or new facilities, in order to address knowledge gaps (deliverable D2.2.1). This deliverable was loaded on the NURESIM Open Web Site.

During the second and third years of the project, the work was devoted to validation, benchmarking, developments of physical models, and use of DNS-LES results for developing models.

4.2.2.1 –Major achievements concerning DNB

Departure from Nucleate Boiling (DNB) is the main governing Critical Heat Flux (CHF) mechanism in PWRs and the first task was to identify all basic flow processes at the various scales which play a role. Then the review of available experimental data (D2.2.1) was used and a validation matrix was defined.

The validation of NURESIM-CFD tool performed during the period up to T0+24 months includes some DEBORAH tests (boiling bubbly flow in a heated pipe), some ASU tests (boiling bubbly flow in a heated annulus), TOPFLOW vertical bubbly flow tests, DEDALE air-water bubbly flow tests, LWL tests in WWER assembly geometry, DEEN bubble column tests.

The following first conclusions of this work are the following ones:



- i. *Basic model approach* - As boiling bubbly flows are encountered, the two-fluid model is naturally used in this flow conditions to benefit from the possibility to model all interfacial forces acting on the bubbles such as drag, lift, turbulent dispersion, virtual mass and wall forces which control the void repartition in a boiling channel. The choice of the method to model poly-dispersion effects remains partly open.
- ii. *Filtering or averaging procedure* - Considering flow in a PWR core in conditions close to nominal, when boiling occurs, a high velocity steady flow regime takes place with time scales associated to the passage of bubbles being very small (10^{-4} , 10^{-3} s) and with bubble diameter being rather small (10^{-5} to 10^{-3} m) compared to the hydraulic diameter (about 10^{-2} m). These are perfect conditions to use a time average or ensemble average of equations as usually done in the RANS approach. All turbulent fluctuations and two-phase intermittency scales can be filtered since they are significantly smaller than scales of the mean flow. The use of a Large Eddy Simulation (LES) approach is also possible and was tested successfully in DEEN bubble column. Compared to the RANS approach, using the LES will allow to simulate bubble dispersion by liquid turbulence instead of modelling it. This LES approach has still to be evaluated and compared to the RANS approach for boiling flows.
- iii. *Identification of Local Interface structure* is necessary to select the adequate interfacial transfer laws and to determine the interfacial area. Here there is a unique interfacial structure corresponding to a dispersed gas phase in a continuous liquid. As long as bubbly flow is encountered, there is no need to develop an identification of the local flow regime and there is no need to use an ITM. Going to DNB occurrence, a gas layer appears and a criterion must be implemented for identifying this occurrence. A very simple criterion based on the local void fraction was applied to LWL tests. However, the description of the interface structure may require addition of transport equations such as IAT (interfacial area transport) or bubble number density transport. More generally the method of the statistical moments can be used to characterise the poly-dispersion of the vapour phase with a bubble size spectrum. Another approach of the poly-dispersion is to use a Multi-group model (MUSIG method) with mass (and momentum) equations written for several bubble sizes. These two methods are being used, evaluated and compared on both DEBORA and TOPFLOW tests. The MUSIG method with several mass equations for different bubble sizes and at least two momentum equations have shown good capabilities for capturing all qualitative effects in TOPFLOW vertical pipe tests. The weak part of the model is the modelling for bubble coalescence and fragmentation.
- iv. *Momentum transfer* controls the void distribution and it is necessary to model all the forces acting on the bubbles. The Virtual mass force is not expected to play a very important role, and rather reliable models exist for the drag force. More effort should be paid to the modelling and validation of both lift and turbulent dispersion forces since available models are still often tuned. In particular, since the lift force may depend on the bubble size, it is now necessary to model poly-dispersion to take this into account.
- v. *Turbulent transfers* - Liquid turbulence plays a very important role in boiling flows. It influences liquid temperature diffusion, bubble dispersion, bubble detachment, bubble coalescence and break up which affect the interfacial area. Then the liquid turbulent scales have to be predicted correctly to model all these processes and this will require additional transport equations. The k-epsilon or SST method were used with some success in DEBORA and TOPFLOW. The LES approach has been evaluated in the simulations of the DEDALE air-water bubbly flow in a vertical pipe and in the simulation of the DEEN bubble column. Apparently, the LES should be used only in situations for which the bubble size is small enough that the turbulence produced by the bubbles represents only a small fraction of the turbulent kinetic energy and can therefore be neglected, or modelled as SGS energy.



- vi. *Wall transfers* - Some improvements of wall function for momentum were obtained and validated on ASU tests. The boiling model of Kurul and Podowski implemented in the NEPTUNE-CFD code is sensitive to mesh since the near-wall properties are calculated from the state in the first wall-adjacent cell. The same problem exists with the velocity in Unal correlation for bubble detachment diameter. More generally specific wall functions have to be developed for boiling flow for both momentum and energy equations. Such wall functions should be able to provide converged solution with a reasonably coarse nodalization close to a heating wall. Further progress is still necessary for energy wall functions.
- vii. A first *demonstration test case* was performed by NRI with NEPTUNE CFD calculations of Critical Heat Flux tests in the LWL loop which is prototypical of WWER type core assemblies. Computational grid consists of 150,000 hexahedral cells. Although the simulation was not fully successful, NEPTUNE shows interesting capabilities for such a complex industrial geometry and flow conditions. Further simulations of such tests will be made in the future.

4.2.2.2 –Major achievements concerning Dry-Out

The Dry-Out - Annular flow pattern usually is the predominant flow regime in the upper core regions of BWRs. The occurrence of Dry-Out limits each assembly maximum power. There are several possible mechanisms associated to dry-out. They were first identified and a review of available experimental data to be used for modelling was made (deliverable D2.2.1).

The work performed during the first two years on dry-out focussed on the modelling of droplet deposition and on film modelling.

The conclusions about modelling of Dry-out by two-phase CFD are the following ones:

- i. *Basic model approach* - In annular flows, the gas is a continuous phase and the liquid phase is split into a film which is a continuous field and droplets as a dispersed field. The three-field model is naturally used under these flow conditions to benefit from the possibility to model separately the two liquid fields which have very different behaviours since the droplets have a high interfacial area and no wall friction whereas the film has a low interfacial area and has a friction along the wall. A simplified three-field model can be easily implemented in a two-fluid code by adding the film balance equations only in meshes along walls. These mass momentum and energy equations can be simplified by considering a unique velocity component along the vertical direction and a film thickness only depending on the vertical position.
- ii. *Filtering or averaging procedure*- Considering flow in a BWR core in conditions close to nominal, a high velocity steady flow regime takes place with times scales associated to the passage of droplets being very small (10^{-4} , 10^{-3} s) and with droplet diameter being rather small (10^{-5} to 10^{-3} m) compared to the hydraulic diameter (about 10^{-2} m). These are perfect conditions to use a time average or ensemble average of equations as usually done in the RANS approach. All turbulent fluctuations and two-phase intermittency scales can be filtered since they are significantly smaller than scales of the mean flow. There may be a difficulty if film waves have to be simulated since it is not clear how the averaging of the RANS approach may filter or damp the disturbance waves.
- iii. *Identification of Local Interface structure* is necessary to select the adequate interfacial transfer laws and to determine the interfacial area. Here there are two interfacial structures corresponding either to a dispersed liquid phase in a continuous gas in the core flow or a film surface with waves and droplet entrainment of deposition along walls. A simple way to



identify the two situations is to consider that the latter only takes place in meshes along the walls while the former takes place everywhere else. The characterization of the droplet field may require the use of additional transport equations for the droplet number density, or the interfacial area or any statistical moment of the droplet size distribution function. Another approach of the poly-dispersion is to use a Multi-group model with mass (and momentum) equations written for several droplet sizes. A more simple characterization of the droplet field by using an algebraic expression of an average drop diameter will be used and evaluated during the project.

- iv. *Interfacial transfers*: Mass transfers affect the film thickness and it is necessary to model at least the droplet deposition, the entrainment and the vaporization. A new droplet deposition model was proposed and models for entrainment and vaporization were proposed to be evaluated. Momentum transfers affect the film thickness and it is necessary to model gravity, wall friction, and interfacial friction. Models for these forces were proposed to be evaluated. Energy transfers also affect the film thickness and it is necessary to model the wall heat flux, the interfacial transfer, the evaporation and the energy transfer due to deposition and entrainment. Models for these transfers are proposed to be evaluated. Interfacial heat and mass transfer also affect the droplet field and models are necessary for the convective heat flux from steam to droplet interface and the radiation heat flux from walls to the droplets. The mechanical behaviour of the droplets is mainly controlled by gravity and interfacial friction. Again the drop size and poly-dispersion effects play an important role on these transfers. Models have still to be developed for these transfers on the droplet-vapour interface.
- v. *Turbulent transfers* - Liquid turbulence plays a very important role in annular flows in a BWR core. It influences droplet deposition, droplet coalescence and break up which affects the drop size and consequently the deposition. Then the vapour turbulent scales have to be predicted correctly to model all these processes and this will require additional transport equations to the three-field model. The k-epsilon method was used in a Eulerian-Lagrangian approach to investigate the deposition.

4.2.3 WP2.3: "development and delivery of the NURESIM TH Platform"

NEPTUNE_CFD V1.0.5 was delivered during the first year of the project and V1.0.6 during the last period. An integrated SALOME/NEPTUNE-CFD environment was delivered in July 2006.

V1.0.7 was available at the end of the project with Reynolds stress model for single phase and bubbly flow, Tchen tensorial model for gas phase turbulence in bubbly flow, addition of two types of wall-force for bubbly flows, large interface models (very useful for stratified flow), and various other new features.

The SYRTHES heat transfer module was delivered

Documentation about NEPTUNE-CFD was written and delivered to the partners including a document about theory, a User's Guide, validation and verification

Assistance to the users and maintenance were provided.

Several training sessions on NEPTUNE-CFD were organised.



4.3 Major achievements during the project for SP3 (Multiphysics)

Key achievements were the following ones:

- Successful integration of CRONOS, FLICA, COBAYA3 and DYN3D into the SALOME platform was achieved with efficient support from SP5 (integration). For each of these codes, a calculation scheme had to be developed using the SALOME tools. The examples of COBAYA3 and DYN3D are especially note-worthy as these are non-CEA code integrated into the platform.
- Mesh interpolation modules have been developed (again in collaboration with SP5) which allow for the embedding of a region with a higher level of modelling resolution (hot-channel), as the consistent interpolation of the neutronic and thermal-hydraulic solution fields is required by the coupling.
- Successful testing of the coupling schemes was achieved both for the PWR and BWR targets against known solutions from two OECD benchmarks. For PWR, the PWR Main Steam Line Break benchmark was employed, while the Peach Bottom Turbine Trip benchmark was used for BWR. For the PWR target, 2-level nested coupling scheme was successfully tested using CRONOS-FLICA. For both situation targets, coupled calculations showed reasonable agreement with the known benchmark solutions, although some deficiencies were noted during the course of the work. For the VVER situation target, first steps towards a coupled calculation were achieved. In all these cases, CRONOS-FLICA coupled through SALOME was applied.
- In light of the VVER situation target, the import and export features of the Data Exchange Model (MED) of SALOME have been extended for hexagonal geometry.



4.4 Major achievements during the project for SP4 (Sensitivity and Uncertainty analysis)

Reactor analysis and design needs experimentally validated numerical simulation tools, capable of handling the inherently time-dependent and nonlinear nature of the underlying physical phenomena.

SP4 demonstrated the applicability of a comprehensive and efficient methodology for the experimental validation and calibration of complex time-*independent* and time-*dependent* numerical simulation models, incorporating both computational and experimental uncertainties. The resulting validated and calibrated models are capable of yielding bona-fide “best-estimate” values for the quantities computed by the respective simulation tools.

This general purpose methodology for experimental validation and calibration of time-(in)dependent simulation tools has been incorporated into the software module called “BEST-EST” (for “**best estimate**”), incorporated in the dedicated platform KALIF, to be used as a general-purpose software module for validating and calibrating both time-dependent and time-independent models for numerical simulation of nonlinear systems. The BEST-EST methodology has been demonstrated both on simple (where analytical solutions exist) and complex applications:

- illustrative time - *independent* applications for simple neutron diffusion through a slab and K_{eff} for a bare, highly enriched uranium sphere – GODIVA: K_{eff} and sensitivity calculations using APOLLO2 and COBAYA3 (in cooperation with SP1)
- an illustrative time-*dependent* depletion problem (radioactive decay) and a transient thermal-hydraulic model of the BFBT benchmark (the *transient* macroscopic grade benchmark turbine trip without bypass), simulated by the FLICA4-code system, and calibrated with experimental void fraction data provided by the BFBT benchmark.

Sensitivity and uncertainty analysis procedures can be either local or global in scope.

The objective of local analysis is to analyze the behavior of the system response locally around a chosen point (for static systems) or chosen trajectory (for dynamical systems) in the combined phase space of parameters and state variables.

On the other hand, the objective of global analysis is to determine all of the system's critical points (bifurcations, turning points, response maxima, minima, and/or saddle points) in the combined phase space formed by the parameters and dependent (state) variables, and subsequently analyze these critical points by local sensitivity and uncertainty analysis.

The methods for sensitivity and uncertainty analysis are based on either statistical or deterministic procedures. In principle, both types of procedures can be used for either local or for global sensitivity and uncertainty analysis, although, in practice, deterministic methods are used mostly for local analysis while statistical methods are used for both local and global analysis. In practice, sensitivities cannot be computed exactly by using statistical methods; this can be done only by using deterministic methods.

The deterministic methods most commonly used for computing local sensitivities are: the “brute-force” method based on recalculations, the direct method (including the decoupled direct method), the Green’s function method, the forward sensitivity analysis procedure (FSAP), and the adjoint sensitivity analysis procedure (ASAP). Note there that the direct method and the FSAP require at least as many model-evaluations as there are parameters in the model, while the ASAP requires a single model-evaluation of an appropriate adjoint model, whose source term is related to the response under investigation. The ASAP is the most efficient method for computing local sensitivities of large-scale systems, when the number of parameters and/or parameter variations



exceeds the number of responses of interest. The adjoint model requires relatively modest additional resources to develop and implement if this is done simultaneously with the development of the original model. If, however, the adjoint model is constructed a posteriori, considerable skills may be required for its successful development and implementation.

Once they become available, the exact local sensitivities can be used for the following purposes:

- (i) understand the system by highlighting important data;
- (ii) eliminate unimportant data;
- (iii) determine effects of parameter variations on the system's behavior;
- (iv) design and optimize the system (e.g., maximize availability/minimize maintenance);
- (v) reduce over-design;
- (vi) prioritize the improvements to be effected in the respective system;
- (vii) prioritize introduction of data uncertainties;
- (viii) perform local uncertainty analysis by using the method of "propagation of errors" (also known as the "propagation of moments," or the "Taylor-Series"). Note that the "propagation of errors" method is used both for processing experimental data obtained from indirect measurements and also for performing uncertainty analysis of computational models. In particular, the "propagation of errors" method provides a systematic way for obtaining the uncertainties in computed results, arising not only from uncertainties in the parameters that enter the respective computational model but also from the numerical approximations themselves.

The earliest attempts at extending the region of validity of local sensitivities beyond first-order were focused on computing second- and higher-order response derivatives with respect to the system's parameters. However, the number of equations that would need to be solved for obtaining the second- (and higher-) order derivatives of the response is very large, and depends on the number of parameter variations. For this reason, none of the deterministic techniques (proposed in the literature thus far) for computing second- and higher-order response derivatives with respect to the system's parameters has proven routinely practicable for large-scale problems. In particular, the computation of the second-order derivatives of the response and system's equations is already as difficult as undertaking the complete task of computing the exact value of perturbed response. Furthermore, since the Taylor-series is a local concept, valid within some radius of convergence of the respective series around the nominal parameter values, it follows that even if the response derivatives were available to all orders, they would still merely provide local, but not global, information. Thus, they would yield little, if any, information about the important global features of the physical system, namely the critical points of the response and the bifurcation branches and/or turning points of the system's state variables.

It appears that the only genuinely global deterministic method for sensitivity analysis, published thus far, is the global adjoint sensitivity analysis procedure (GASAP) developed by Cacuci (1990). The GASAP uses both the forward and the adjoint sensitivity system to explore, exhaustively and efficiently, the entire phase-space of system parameters and dependent variables, in order to obtain complete information about the important global features of the physical system, namely the critical points of the response and the bifurcation branches and/or turning points of the system's state variables.



4.5 Major achievements during the project for SP5 (Integration)

The NURESIM-integration Sub-project activities aimed at facilitating integration of codes and solvers into the SALOME platform, assisting partners in this task, and ensuring maintenance and non regression of the products. These activities were split into four WPs: training and support on the SALOME platform (WP5.1), assistance for code integration (WP5.2), adaptation of the SALOME platform (WP5.3), and building of the NURESIM platform and ensuring non regression (WP5.4).

The main achievements of the Sub-project were:

- the development of an integration environment, including tools for automatic integration (XDATA, HXX2SALOME and MED),
- the delivery of a training session on SALOME platform, on code integration and code coupling,
- The delivery of three tutorials on Salome platform, on code integration and code coupling,
- the development of a production environment (CVS repositories, mailing lists, bugtracker, tools for building the platform, automatic testing procedure and non-regression test base
- the release of SALOME V3 and SALOME V4,
- an assistance on SALOME and code integration, the integration in coordination with SP3 of FLICA4, CRONOS2.6 and COBAYA3 into SALOME,
- the realization of an integration component and a data component,
- also in coordination with SP3, the development of the FLICA-CRONOS coupling application (PWR, BWR and VVER) and the FLICA-COBAYA coupling (PWR),
- the delivery of two versions of the NURESIM platform (V1 and V1.1), respectively running with SALOME V3 and V4, this last one includes all the developments done so far.



5 CONCLUSION

During the NURESIM project, the NURESIM platform started to become a reference instrument providing high quality software tools, physical models, generic functions and assessment results.

The NURESIM platform already provides an accurate representation of the physical phenomena in core physics, two-phase thermal-hydraulics and on some aspects of fuel modelling. It includes multi-scale and multi-physics features, especially for coupling core physics and thermal-hydraulics models for reactor safety. Easy coupling of the different codes and solvers is available through the use of a common data structure and generic functions (e.g., for interpolation between nonconforming meshes).

More generally, the platform includes generic pre-processing, post-processing and supervision functions through the open-source SALOME software, making the codes more user-friendly.

Some standards have been specified, developed and tested in order to connect different codes to the platform and make their comparison easier.

The first validation of the NURESIM platform and of the individual models, solvers and codes has been made on applications corresponding to nuclear reactor situations, and including reference calculations, experiments and plant data. Quantitative deterministic and statistical sensitivity and uncertainty analyses tools have been developed and provided through the platform.

A Users' Group of European and non-European countries, including vendors, utilities, TSO, and additional research organizations (beyond the current partners) has also been established.



6 ANNEX 1: TABLE OF ACRONYMS

ASAP	Adjoint Sensitivity Analysis Procedure
BWR	Boiling Water Reactor
CFD	Computational Fluid Dynamics
CHF	Critical Heat Flux
CIAU	Code Internal Assessment of Uncertainty
DCC	Direct Contact Condensation
DNB	Departure from Nucleate Boiling
DNS	Direct Numerical Simulation
ECCS	Emergency Core Cooling System
FSAP	Forward Sensitivity Analysis Procedure
GASAP	Global Adjoint Sensitivity Analysis Procedure
HZP	Hot Zero Power
LES	Large Eddy Simulation
MED	Data Exchange Model of SALOME
MOC	Method Of Characteristics
MOX	Mixed OXide fuel
NEA	Nuclear Energy Agency
NEM	Nodal Expansion Method
PTS	Pressurized Thermal Shock
PWR	Pressurized Water Reactor
RANS	Reynolds Averaged Navier Stokes
REA	Rod Ejection Accident
SET	Separate Effect Test
SNE-TP	Sustainable Nuclear Energy Technology Platform
SRA	Strategic Research Agenda
VVER	Russian Pressurized Water Reactor



7 ANNEX 2: LIST OF PUBLICATIONS

7.1 General Publications about NURESIM

1. D.G. Cacuci, J.M. Aragonés, D. Bestion, P. Coddington, L. Dada, C. Chauliac, “NURESIM: A European Platform for Nuclear Reactor Simulation”, in *2006 FISA Conference on the 6th Framework Euratom Research Program*, European Commission, Luxembourg, March 2006.
2. C. Chauliac, J.M. Aragonés, D. Bestion, D.G. Cacuci, P. Coddington, L. Dada, “NURESIM: A European Platform for Nuclear Reactor Simulation”, *ICONE-14 Workshop on advanced LWR*, Miami, USA, July 2006.
3. D.G. Cacuci, J.M. Aragonés, D. Bestion, C. Chauliac, P. Coddington, N. Crouzet, Towards A European Platform for Simulation of Nuclear Reactors: the NURESIM Project, *ICAPP-2007*, Nice, May 2007
4. C. Chauliac, *The NURESIM Project, presentation to OECD/NEA/NSC/DBMC*, Issy-les-Moulineaux, June 2008
5. C. Chauliac, J.M. Aragonés, D. Bestion, D.G. Cacuci, N. Crouzet, F.P. Weiss, M.A. Zimmermann, , “NURESIM – A European simulation platform for nuclear reactor safety: multi-scale and multi-physics calculations, sensitivity and uncertainty analysis”, in *FISA-2009 Conference on the Euratom Research and training Program*, European Commission, Prague, June 2009.

Furthermore, all the presentations of the NURESIM General Assemblies held in November 2006 in Paris and in November 2008 in Madrid are available on the NURESIM Open Web Site: www.nuresim.eu

7.2 List of Publications of SP1

General NURESIM-SP1 Coordination (available at NURESIM SP1 Internal Website)

1. J.M. Aragonés, “Qualification of Core Physics Codes within NURESIM”, in *Post-FISA Workshop on Qualification of Advanced Numerical Simulation Platforms*, EC, Luxembourg, March 2006.

WP1.1 Advanced Monte Carlo Methods

1. CEA Seminar on TRIPOLI 4 Code, Avignon, 11 Sept. 2005 (in NEA CDROM and MC-2005 web site).
2. J. Dufek, W. Gudowski, “Stochastic Approximation for Monte Carlo Calculation of the Steady-State Conditions in Thermal Reactors”, *Nuclear Science Engineering*, March 2006.
3. S. Christoforou, E. Hoogenboom, “A Zero-Variance Scheme for Variance Reduction in Monte Carlo Criticality”, *Physor-2006*, B094, Vancouver, Sept. 2006.
4. S. Christoforou, E. Hoogenboom, E. Dumonteil, O. Petit, “Implementation of an Approximate Zero-Variance Scheme in the Monte Carlo code TRIPOLI4”, *Physor-2006*, C2138, Vancouver, Sept. 2006.
5. Eric Dumonteil, Aurélien Le Peillet, Yi-Kang Lee, Odile Petit, Cédric Jouanne, and Alain Mazzolo, “Source convergence diagnostics using Boltzmann entropy criterion Application to



different OECD/NEA criticality benchmarks with the 3D Monte Carlo code Tripoli-4”, Physor 2006, Vancouver, September 2006.

6. *J. Dufek, W. Gudowski*, “Parallelization of Monte Carlo Calculations by Stabilized Fission Matrix Method”, submitted to Nuclear Science and Engineering, January 2007.
7. *S. Christoforou, J.E. Hoogenboom*, “Transition and Collision Biasing in a Variance Reduction Scheme for Criticality Calculations”, Proceedings M&C2007, Monterey, USA, April 2007.
8. *E. Dumonteil, F.-X. Hugot, C. Jouanne, Y.K. Lee, F. Malgavi, A. Mazzolo, O. Petit, J.C. Trama*, “An Overview of the Monte Carlo Particle Transport Code TRIPOLI-4”, in Advanced Methods, Codes and Benchmarking of the NURESIM Core Physics European Simulation Platform, American Nuclear Society and the European Nuclear Society International Conference on Making the Nuclear Renaissance Real, Washington D.C., Nov. 2007, Trans. TANSO 97, 694-695, ISSN: 0003-018X (2007).
9. *J.E. Hoogenboom*, “Zero-Variance Monte Carlo Schemes Revisited”, Nucl. Sc. Eng. **160**, 1-22 (2008).
10. *J.E. Hoogenboom*, “The Two-Direction Neutral-Particle Transport Model: A Useful Tool for Research and Education”, Transp. Theory & Stat. Physics, **37**, 65-108 (2008).
11. *S. Christoforou, J.E. Hoogenboom*, “Investigating the minimum achievable variance in a Monte Carlo criticality calculations”, Proceedings Physor2008, Interlaken, Switzerland, September 2008.
12. *J.E. Hoogenboom*, “Improved estimation of the variance in Monte Carlo criticality calculations”, Proceedings Physor2008, Interlaken, Switzerland, September 2008.
13. *F. X. Hugot, Y. K. Lee, F. Malvagi*, “Recent R&D around the Monte-Carlo code Tripoli-4 for criticality calculation”, PHYSOR’2008 conference, Interlaken, Switzerland, September 14-19, 2008.
14. *N.P. Koley, N. Petrov, G. Todorova, P. Bellier*, “APOLLO2 and TRIPOLI4 solutions of the OECD VVER-1000 LEU and MOX assembly benchmark”, submitted to ANE, Elsevier, 2008
15. *N. Petrov, N.P. Koley, G. Todorova, F.-X. Hugot, T. Visonneau*, “TRIPOLI4 Solutions to VVER-1000 Assembly and Core Benchmarks”, accepted at the International Conference on Mathematics, Computational Methods & Reactor Physics M&C-2009, Saratoga Springs, New York, May 3-7, 2009.
16. *S. Christoforou, J.E. Hoogenboom*, “Using a Zero-Variance Scheme to Accelerate the Fission Source Convergence in a Monte Carlo Calculation”, accepted at the International Conference on Mathematics, Computational Methods & Reactor Physics M&C-2009, Saratoga Springs, New York, May 3-7, 2009.

WP1.2 Advanced Deterministic Transport and Diffusion Methods

1. CEA Seminar on APOLLO 2 Code, Avignon, 11 Sept. 2005 (in MC-2005 web site).
2. *M. Coste et al.* (CEA), “New Developments in Resonance Mixture Self-shielding Treatment with Apollo2 Code”; MC-2005, Avignon, Sept. 2005.
3. *C. Calvin* (CEA), “DESCARTES: A New Generation System for Neutronic Calculations”; MC-2005, Avignon, Sept. 2005.
4. *AM. Baudron, JJ. Lautard* (CEA), “MINOS: A SPN Solver for Core Calculations in the DESCARTES System”; MC-2005, Avignon, Sept. 2005.
5. *JM. Aragonés, C. Ahnert, N. García-Herranz* (UPM), “The Analytic Coarse-Mesh Finite-Difference Method for Multigroup and Multidimensional Diffusion Calculations”, in *Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications (MC-2005)*, Am. Nucl. Soc., Avignon, p. 194, Sept. 2005.



6. *J.A. Lozano, J.M. Aragonés, N. García-Herranz*, “Development and Performance of the Analytic Nodal Diffusion Solver ANDES in Multigroups for 3D Rectangular Geometry”, in *Mathematics & Computations and Supercomputing in Nuclear Applications, M&C/SNA-2007* Monterey CA, T. Rubia, J. Vujic (Eds.), Vol. 4A5, 1-13, American Nuclear Society Ed., La Grange Park, IL-USA, ISBN: 0-89448-059-6 (2007).
7. *J.J. Herrero, C. Ahnert, J.M. Aragonés*, “3D Whole Core Fine Mesh Multigroup Diffusion Calculations by Domain Decomposition through Alternate Dissections”, in *Mathematics & Computations and Supercomputing in Nuclear Applications, M&C/SNA-2007* Monterey CA, T. Rubia, J. Vujic (Eds.), Vol. 8D9, 1-13, American Nuclear Society Ed., La Grange Park, IL-USA, ISBN: 0-89448-059-6 (2007).
8. *J. Jiménez, D. Cuervo, J.M. Aragonés*, “Multiscale and Multiphysics Coupling in COBAYA3”, in *Nuclear Reactor Thermal-hydraulics, NURETH-12* Pittsburgh PA, 12 pp., Am. Nuc. Soc. Ed., La Grange Park, IL-USA, ISBN: 0-89448-058-8 (2007). Accepted for publication in *Nucl. Eng. and Design* (2008).
9. *J.M. Aragonés, C. Ahnert, N. García-Herranz*, “The Analytic Coarse-Mesh Finite Difference Method for Multigroup and Multidimensional Diffusion Calculations”, *Nucl. Sci. Eng.* **157**, 1-15 (2007).
10. *C. Calvin, C. Fédon-Magnaud*, “DESCARTES: An advanced code system for neutronics calculations”, in *Advanced Methods, Codes and Benchmarking of the NURESIM Core Physics European Simulation Platform*, American Nuclear Society and the European Nuclear Society International Conference on Making the Nuclear Renaissance Real, Washington D.C., Nov. 2007, Trans. TANSO 97, 691-693, ISSN: 0003-018X (2007).
11. *J.A. Lozano, J.M. Aragonés, N. García-Herranz*, “Development and performance of the analytic nodal diffusion solver ANDES in multigroups for 3D rectangular geometry”, in *Advanced Methods, Codes and Benchmarking of the NURESIM Core Physics European Simulation Platform*, American Nuclear Society and the European Nuclear Society International Conference on Making the Nuclear Renaissance Real, Washington D.C., Nov. 2007, Trans. TANSO 97, 696-697, ISSN: 0003-018X (2007).
12. *J.J. Herrero, C. Ahnert, J.M. Aragonés*, “Spatial Domain Decomposition for LWR Cores at the Fuel Pin Scale”, in *Advanced Methods, Codes and Benchmarking of the NURESIM Core Physics European Simulation Platform*, American Nuclear Society and the European Nuclear Society International Conference on Making the Nuclear Renaissance Real, Washington D.C., Nov. 2007, Trans. TANSO 97, 698-700, ISSN: 0003-018X (2007).
13. *D. Cuervo, C. Ahnert, J.M. Aragonés, N. García-Herranz, J. J. Herrero, J. Jiménez, J.A. Lozano*, “Participación española en el desarrollo de la Plataforma Europea para Simulación de Reactores Nucleares (NURESIM)”, *Nuclear España*, January 2008.
14. *J.A. Lozano, J.M. Aragonés, N. García-Herranz*, “Transient analysis in the 3D nodal kinetics and thermal-hydraulics ANDES/COBRA coupled system”, in *PHYSOR’08 International Conference on the Physics of Reactors*, Vol. 16C3, 1-8, Interlaken, Switzerland, September 14-19, 2008.
15. *J.J. Herrero, A. F. Badea, D. G. Cacuci*, “Sensitivity analysis and cross sections data adjustment for multigroup transport and diffusion”, in *PHYSOR’08 International Conference on the Physics of Reactors*, Interlaken, Switzerland, September 14-19, 2008.
16. *J. Jiménez, J. J. Herrero, J. A. Lozano, D. Cuervo, N. García, C. Ahnert, J.M. Aragonés*, “Descomposición espacial en subdominios para reactores de agua ligera a la escala de la barra de combustible”, *Sociedad Nuclear Española Anual Meeting*, Murcia, October 2008.



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18. *J.J. Herrero, J. Jiménez, J.M. Aragonés and C. Ahnert*, “Performance of whole core pin-by-pin calculations by domain decomposition through alternate dissections in steady state and transient calculations”, accepted at the International Conference on Mathematics, Computational Methods & Reactor Physics M&C-2009, Saratoga Springs, New York, May 3-7, 2009
19. *J. A. Lozano, J. Jimenez, N. García-Herranz and J.M. Aragonés*, “Development and performance of the ANDES/COBRA-III coupled system in hexagonal-z geometry”, accepted at the International Conference on Mathematics, Computational Methods & Reactor Physics M&C-2009, Saratoga Springs, New York, May 3-7, 2009.

WP1.3 Advanced Kinetics Methods

1. *U. Rohde et al. (FZD)*, “Comparative Assessment of Coupled DYN3D Code against the Kozloduy-6 Pump Trip Test”; MC-2005, Avignon, Sept. 2005.
2. *Grundmann, U.*, “Calculations of a steady state of the OECD/NRC PWR MOX/UO₂ transient benchmark with DYN3D”, Annual Meeting of German Nuclear Society, Aachen, May 2006.
3. *Petkov P., Mittag S.*, “Evaluation of homogenisation error in two-group nodal diffusion calculation for VVER-1000 core”, Annual Meeting of German Nuclear Society, Aachen, May 2006.
4. *Beckert, C.; Grundmann, U.; Mittag, S.*: “Multigroup Diffusion and SP3 Solutions for a PWR MOX/UO₂ Benchmark with the Code DYN3D”, in Advanced Methods, Codes and Benchmarking of the NURESIM Core Physics European Simulation Platform, American Nuclear Society and the European Nuclear Society International Conference on Making the Nuclear Renaissance Real, Washington D.C., Nov. 2007, Trans. TANSO 97, 701-702, ISSN: 0003-018X (2007).
5. *Beckert, C.; Grundmann, U.*: A nodal expansion method for solving the multigroup SP3 equations in the reactor code DYN3D, M&C+SNA 2007 - Joint International Topical Meeting on Mathematics & Computations and Supercomputing in Nuclear Applications, 15.-19.04.2007, Monterey, United States
6. *Beckert, C.; Grundmann, U.*: Development and verification of a multigroup SP3 method for reactor calculations, Annual meeting on nuclear technology 2007, 22.-24.05.2007, Karlsruhe, Germany
7. *C. Beckert, U. Grundmann*, “Development and verification of nodal approach for solving the multi-group SP3 equations in the code DYN3D”, *Annals of Nuclear Energy*, 35, 75-86 (2008).

WP1.4 Benchmarking of the NURESIM Core Physics Platform

1. *Gy. Hegyi*, “Some new experience with ZR-6 measurements using different code systems”, AER-17 Annual VVER Conference, Yalta, 2007.
2. *N.P. Kolev, G. Todorova, N. Petrov, P. Bellier*, “OECD VVER-1000 LEU and MOX Assembly Benchmark Solutions with APOLLO2”, in Advanced Methods, Codes and Benchmarking of the NURESIM Core Physics European Simulation Platform, American Nuclear Society and the European Nuclear Society International Conference on Making the Nuclear Renaissance Real, Washington D.C., Nov. 2007, Trans. TANSO 97, 705-706, ISSN: 0003-018X (2007).
3. *H. Ferroukhi (PSI), J.M. Hollard (PSI), O. Zerkak (PSI), P. Coddington (PSI)*, “PWR Cell Calculations using APOLLO-2 within the NURESIM Benchmark Framework”, in Advanced Methods, Codes and Benchmarking of the NURESIM Core Physics European Simulation



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5. *J. Hádek (NRI), S. Mittag (FZD)*, “Validation of DYN3D Pin-Power Calculation against Experimental VVER-Full-Core Benchmark”, International Conference on Mathematics, Computational Methods & Reactor Physics M&C-2009, Saratoga Springs (NY), May 3-7, 2009.
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7.3 List of Publications of SP2

Papers published in conferences

1. Y. Bartosiewicz and J.-M. Seynhaeve “Numerical investigation on the Kelvin-Helmholtz instability in the case of immiscible fluids” The 13th International Conference on Fluid Flow Technologies Budapest, Hungary, September 6-9, 2006
2. Y. Bartosiewicz and J.-M. Seynhaeve “Assessment of the NEPTUNE_CFD code to model the occurrence of instabilities in a stratified flow” 10TH International Conference Multiphase Flow in Industrial Plant, Tropea (Italy), 20-22 September 2006
3. Y. Bartosiewicz, J. Laviéville, J.M. Seynhaeve, A Validation Case for the NEPTUNE_CFD Platform: Instabilities in a Stratified Flow. Experimental, Theoretical and Code to Code Comparisons, NURETH-12, Sheraton Station Square, Pittsburgh, Pennsylvania USA, 30 Septembre-4 Octobre 2007
4. Y. Bartosiewicz, J.-M. Seynhaeve, C. Vallée, T. Höhne, J.-M. Laviéville, Modelling free surface flows relevant to a PTS scenario: comparison between experimental data and three RANS based CFD-codes, XCFD4NRS, Experiments and CFD Code Applications to Nuclear Reactor Safety OECD/NEA & IAEA, Grenoble, France, 10 - 12 September 2008
5. Bestion, D., Anglart, H., Pétureaud, P., Smith, B., Krepper, E., Moretti, F., Macek J.: « Review of available data for validation of NURESIM two-phase CFD software applied to CHF investigations » [043], NURETH-12, Sheraton Station Square, Pittsburgh, Pennsylvania USA, 30 Septembre-4 Octobre 2007
6. P. Coste, J. Pouvreau, J. Laviéville, M. Boucker, “Status of a two-phase CFD approach to the PTS issue”, XCFD4NRS, Experiments and CFD Code Applications to Nuclear Reactor Safety OECD/NEA & IAEA, Grenoble, France, 10 - 12 September 2008
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9. M. T. Dhotre, B. Smith, B. Niceno, CFD Simulation of Bubbly Flows: Random Dispersion Model, Gas-Liquid-Solid-8 Conference, Delhi, India, 9-13 Dec. 2007
10. M. T. Dhotre, B. Niceno, B. Smith, M. Simiano, In-depth analysis of bubbly flows: CFD simulations and experiments, ICMF Paper No. 86
11. M.C. Galassi, C. Morel, D. Bestion, J. Pouvreau, F. D’Auria, Validation of NEPTUNE CFD Module with Data of a Plunging Water Jet Entering a Free Surface, NURETH-12, Sheraton Station Square, Pittsburgh, Pennsylvania USA, 30 Septembre-4 Octobre 2007
12. M. C. Galassi, F. Moretti, F. D’Auria, CFD Code Validation and Benchmarking Against BFBT Boiling Flow Experiment, XCFD4NRS, Experiments and CFD Code Applications to Nuclear Reactor Safety OECD/NEA & IAEA, Grenoble, France, 10 - 12 September 2008
13. B. Koncar, E. Krepper, CFD simulation of forced convective boiling in heated channels. V: Benchmarking of CFD codes for application to nuclear reactor safety, (CFD4NRS), Garching, Munich, Germany, 5-7 September 2006.



14. B. Koncar, K. Mramor,. Simulation of boiling flow experiments close to CHF with the NEPTUNE-CFD code. International Conference Nuclear Energy for New Europe 2007, Portorož, Slovenia, September 10-13. Conference proceedings. Ljubljana: Nuclear Society of Slovenia, 2007, 11 pp.
15. B. Koncar, Use of two-phase wall functions for simulations of boiling flows , NURETH-12, Sheraton Station Square, Pittsburgh, Pennsylvania USA, 30 Septembre-4 Octobre 2007
16. B. Končar, B. Mavko, Wall-to-fluid transfer modeling in boiling flows, XCFD4NRS, Experiments and CFD Code Applications to Nuclear Reactor Safety OECD/NEA & IAEA, Grenoble, France, 10 - 12 September
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18. Lakehal D.: DNS of Turbulent Transport at Deformable sheared Interfaces: Statistics and Modelling Parameterization. VKI Lecture Series 2007-05, CFD of Multi-fluid Flow, J-M. Buchlin (Ed.), Von Karman Institute for Fluid Mechanics, Rhodes-St-Genese, Belgium, 28 pages, 2007.
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20. Lakehal D.: Advances in Computational Heat Transfer & Two-Phase Flow based on Direct Interface Tracking. In Proc. of 5th Int. Conf. Transport Phenomena in Multiphase Systems - HEAT5, Keynote Lecture, June 30 - July 3, 2008, Bialystok, Poland.
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22. D. Lucas, D. Bestion, E. Bodèle, M. Scheuerer, F. D'Auria, D. Mazzini, B. Smith, I. Tiselj, A. Martin, D. Lakehal, J.-M. Seynhaeve, R. Kyrki-Rajamäki, M. Ilvonen, J. Macek, On the simulation of two-phase flow Pressurized Thermal Shock , NURETH-12, Sheraton Station Square, Pittsburgh, Pennsylvania USA, 30 Septembre-4 Octobre 2007
23. J. Laviéville, P. Coste, "Numerical modelling of liquid-gas stratified flows using two-phase Eulerian approach", 5th International Symposium on Finite Volumes for Complex Applications, Aussois, France, June 08-13, 2008.
24. J. Macek, L. Vyskocil, Simulation of Critical Heat Flux Experiments in NEPTUNE_CFD Code XCFD4NRS, Experiments and CFD Code Applications to Nuclear Reactor Safety OECD/NEA & IAEA, Grenoble, France, 10 - 12 September 2008
25. Martin, F. Lestang, S. Bellet, A. Barbier, S. Cornille, C. Vit, CFD use in PTS safety analysis State of art and challenges for industrial applications, submitted to NURETH13
26. Niceno, B. Smith, M. T. Dhotre, Euler-Euler Large eddy Simulation (EELES) of a square cross section bubble column using the NURESIM CFD platform, NURETH-12, Sheraton Station Square, Pittsburgh, Pennsylvania USA, 30 Septembre-4 Octobre 2007
27. Petruzzi A., Bousbia Salah A., D'Auria F., Sub-channel analysis by Relap5 system code of Boil-off experiment (test 5002) with Neptun facility, Canadian Nuclear Society (CNS) Sixth Int. Conf. on Simulation Methods in Nuclear Engineering, Montreal (Quebec, Canada), Oct. 12-15, 2004, ISBN 0-919781-80-1 © 2004 CNS-SNC



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29. M. Schmidtke, D. Lucas, On the modelling of bubble entrainment by impinging jets in CFD-simulations, XCFD4NRS, Experiments and CFD Code Applications to Nuclear Reactor Safety OECD/NEA & IAEA, Grenoble, France, 10 - 12 September 2008
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35. F. Terzuoli, M. C. Galassi, D. Mazzini, F. D'Auria, CFD code validation against stratified air-water flow experimental data, International Conference on Nuclear Energy for New Europe (NENE), Portoroz (SLO), September 10-13, 2007
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- 5 M. T. Dhotre, B. Smith, CFD simulations of large scale bubble plumes-comparison to experiment Che. Eng. Sci., 62, 6615-6630 (2007).
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- 7 M. C. Galassi, D. Bestion, C. Morel, J. Pouvreau, F. D'Auria, Validation of NEPTUNE-CFD with data of a plunging jet entering a free surface, accepted for publication in Nuclear Technology
- 8 M.C. Galassi, P. Coste, C. Morel and F. Moretti, "Two-Phase Flow Simulations for PTS Investigations by Means of NEPTUNE_CFD Code", to be published in Science and Technology of Nuclear Installations.
- 9 Hazi G., Mayer G., Markus A., "Drag force acting on bubbles in a subchannel of triangular array of rods", Int. J. Heat and Mass Transfer, in press
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- 11 B. Koncar, E. Krepper, CFD simulation of convective flow boiling of refrigerant in a vertical annulus. Nucl. Eng. Des. Volume 238, Issue 3, 2008, pp. 693-706.
- 12 B. Koncar, I.Tiselj, Influence of near wall modelling on boiling flow simulation, Nuclear Engineering and Design (In Press)
- 13 B Koncar, B.Mavko, Simulation of boiling flow experiment close to CHF with the NEPTUNE code. Science and Technology of Nuclear Installations (In Press)
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- 17 vapor-liquid flow, Phys. Fluids, 20, 065101, 2008.
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- 25 Martin Schmidtke and Dirk Lucas, CFD Approaches for Modelling Bubble Entrainment by an Impinging Jet, , Science and Technology of Nuclear Installations, Volume 2009 (2009), Article ID 148436
- 26 L. Strubelj, G. Ezsol, I Tiselj, Numerical modelling of direct contact condensation in transition from stratified to slug flow, submitted to Nuclear Engineering and Design
- 27 F. Terzuoli, M. C. Galassi, D. Mazzini, F. D'Auria, CFD Code Validation and Benchmarking Against Stratified Air-Water Flow Experimental Data, accepted for publication in Science and Technology of Nuclear Installations



7.4 List of Publications of SP3

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2. *C. Debergé, E. Royer, A. Geay, N. Crouzet*, Simulation of a Main Steam Line Break on VVER-1000 reactor with CRONOS2 and FLICA4 codes, PHYSOR'08, International Conference on Physics of Reactors, Interlaken, Switzerland, September 14-19,2008.
3. *J. Jiménez, M. Avramova, D. Cuervo, K. Ivanov*, Comparative analysis of neutronics/thermal-hydraulics multi-scale coupling for LWR analysis, PHYSOR'08, International Conference on Physics of Reactors, Interlaken, Switzerland, September 14-19,2008



7.5 List of Publications of SP4

- 1 A. Petruzzi, F. D'Auria, W. Giannotti, K. Ivanov, "Methodology of Internal Assessment of Uncertainty and Extension to Neutron-Kinetics/Thermal-Hydraulics Coupled Codes", Nuclear Science and Engineering, 149, pp 1-26, 2005.
- 2 A. Petruzzi, F. D'Auria, "Relap5/Mod3.2 Post-Test Analysis and CIAU Uncertainty Evaluation of LOFT Experiment L2-5", 11th International Topical Meeting on Nuclear Reactor Thermal-Hydraulics (NURETH-11), Avignon, France, October 2-6, 2005.
- 3 D. G. Cacuci, "On the Use of Adjoint Operators for Global Optimization and Data Assimilation", Lectures Notes; Workshop on "Predictability, Observations, and Uncertainties in Geosciences", Florida State University, Tallahassee, Florida, USA, March 13-15, 2006.
- 4 A. de Crecy, P. Bazin, A. Petruzzi, F. D'Auria, Y-H. Ryu, "The BEMUSE Programme: Results on the First Part Concerning the LOFT L2-5 Test", 14th International Conference on Nuclear Engineering (ICONE 14), Miami, Florida, USA, July 17-20, 2006
- 5 A. Petruzzi, F. D'Auria (Editors), A. de Crecy, P. Bazin, S. Borisov, T. Skorek, H. Glaeser, J.P. Benoit, E. Chojnacki, K. Fujioka, S. Inoue, B.D. Chung, I. Trosztel, I. Toth, D.Y. OH, R. Pernica, M. Kyncl, J. Macek, R. Marcian, E. Tanker, A.E. Soyer, O. Ozdere, M. Perez, F. Reventos, "BEMUSE Programme. Phase 2 report <Re-Analysis of the ISP-13 Exercise, post test analysis of the LOFT L2-5 experiment>", OECD/CSNI Report NEA/CSNI/R(2006), JT03210882, Paris, France, OECD 2006, pp 1-625, 2006.
- 6 F. D'Auria, D.G. Cacuci, A. Petruzzi, "Approaches for Computing Uncertainties in Predictions of Complex-Codes", Int. Nuclear Atlantic Conference INAC 2007, September 30 – October 5, 2007, Sao Paulo, Brazil.
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- 9 D.G. Cacuci, I. Balan, M. Ionescu-Bujor, "Adjoint Sensitivity Analysis Procedure for Reliability Analysis: Application to a Model of the International Fusion Materials Irradiation Facility", Nucl. Sci. Eng., 2008.
- 10 J.J. Herrero, A.F. Badea, D.G. Cacuci, "Sensitivity Analysis and Cross Section Data Adjustment for Multigroup Transport and Diffusion", PHYSOR-08 Int. Conf. on the Physics of Reactors "Nuclear Power: A Sustainable Resource", Interlaken, Switzerland, September 14-19, 2008.
- 11 A.F. Badea, D.G. Cacuci, M. Badea, "Time-Dependent Model Calibration through Consistent Data Assimilation", PHYSOR-08 Int. Conf. on the Physics of Reactors "Nuclear Power: A Sustainable Resource", Interlaken, Switzerland, September 14-19, 2008.
- 12 A. Petruzzi, "Development and Application of Methodologies for Sensitivity Analysis and Uncertainty Evaluation of the Results of the Best Estimate System Codes Applied in Nuclear Technology", Universita di Pisa, Scuola di Dottorato in Ingegneria "Leonardo da Vinci", Tesi di Dottorato di Ricerca, 2008



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- 15 A. Petruzzi, F. D’Auria, “Thermal-Hydraulic System Codes in Nuclear Reactor Safety and Qualification Procedures”, Hindawi Publishing Corporation Science and Technology of Nuclear Installations, Volume 2008, Article ID 460795, 2008.



7.6 List of Publications of SP5

- 1 *Vincent Bergeaud, Samuel Kortas, Bernard Sécher*, A data exchange model for code coupling, Seminar ESA “Interfaces and Data Exchange for Integrated Open CAD/CAE Platforms”, Netherlands, October 12, 2006
- 2 *A.-M. Baudron, N. Crouzet, C. Döderlein, A. Geay, J.-J. Lautard, E. Richebois, E. Royer, P. Siréta*, *Unstructured 3D MINOS/FLICA4 coupling in SALOME Application to JHR transient analysis*, International Conference on the Physics of Reactors, Interlaken, Switzerland, September 14-19, 2008

