QUALIFICATION OF THE CFD CODE TRIO_U FOR FULL SCALE NUCLEAR REACTOR APPLICATIONS

Ulrich Bieder[1], Estelle Graffard[2]
[1]CEA-Grenoble, DEN/DER/SSTH/LMDL, 15 rue des Martyrs, F-38054 Grenoble, France
[2]IRSN, DSR/ST3C/BATH, B.P.17, F-92262 Fontenay-aux-Roses, France

Abstract

Numerical and experimental research on nuclear safety is in the end dedicated to understand, on a plant scale, the fundamental physical phenomena which are associated to specific accident scenarios. Hence, the results derived from single effect experiments or reduced scale analysis have to be extrapolated to plant scale whereas plant scale experiments should be evaluated with respect to their applicability to the physics of the specific scenario. For several years, IRSN and CEA have used Computational Fluid Dynamics (CFD) codes for detailed nuclear safety analyses on plant scale. The paper presents a procedure which has been used to qualify the Trio_U code for the prediction of the boron concentration at the core inlet of a French Pressurized Water Reactor (PWR) in accidental conditions (inherent dilution problem)[1]. A ROCOM experiment as well as an UPTF Tram-C3 experiment has been used for this purpose.

Introduction

In PWR, boron acid is used as a neutron absorber for reactivity control. If the boron concentration in the core region is reduced (boron dilution), it might result in a power excursion with possible fuel damage. Within nuclear reactor safety analyses, one of the events that could potentially lead to such a criticality accident is a small break loss of coolant accident (LOCA) inducing a dilution in the steam generators tubes by reflux condensation phenomena then followed by the restart of the natural circulation /1/. This situation can only be mitigated by the mixing at the core inlet.

The increase of computer power allows nowadays the use of CFD for the detailed analysis of the three dimensional thermal hydraulic phenomena which occur under such accident conditions. Nevertheless, the application to full scale PWR thermal hydraulics safety issues is a challenge for CFD due to the complexity of the underlying physical phenomena and the limited field of application of the physical models which are implemented in the codes. Best Practice Guidelines (BPG) /2/, /3/ can provide CFD users with simple and practical advices on the correct application of computational methods. However, BPG can not help in the definition of the modelling hypothesis, this means to define the problem, to identify the important physical phenomena and to select an adequate solution strategy.

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For this purpose, the CFD calculations must be validated by the comparison to experimental data which represent the major physical phenomena expected in the reactor calculation. Unfortunately, for specific phenomena, full scale experimental data for the validation of CFD codes and the underlying models are rarely available. Hence, the codes have to be validated against reduced scale experimental data. The modelling hypothesis of these validation calculations are then extrapolated to plant scale simulations. CEA and IRSN have developed such a qualification procedure. This procedure is presented in here on the example of the qualification of the Trio_U code for full scale inherent boron dilution phenomena in PWR. The Trio_U calculations which are performed by the CEA serve as reference calculations for several transient CFX calculations at IRSN /1/ which are based on less CPU consuming modelling.

The CFD code Trio_U

Trio_U is the CFD reference code of the CEA which is designed for incompressible, turbulent flows in complex geometries /4/, /5/. Boussinesq's approximation is used to account for density effects. The basic idea for the conception of Trio_U was to develop a CFD tool which requires only a minimum of user attention in the mesh generation and model parameter adaptation in order to reduce the numerical restrictions of a correct application of the calculation. The code is especially designed for industrial Large Eddy Simulations (LES) on structured and non-structured grids of several tens of millions of nodes /6/. The platform independent code is based on an object oriented, intrinsically parallel approach and is coded in C++. The flexible code structure allows the user to choose a suitable discretization method and to combine various appropriate physical models. This flexibility is implemented without a reduction of the overall performance of the code.

Meshing

For unstructured grids, Trio_U uses a hybrid « Finite Volume based Finite Element » FV/FE method /7/. This method consists in determining for a continuous problem a discrete solution in the space of the finite element by maintaining the balance notation of finite volumes. The space discretization is performed with triangles in 2-D case and with tetrahedral cells in 3-D case. In Trio_U, the main unknowns (velocity, temperature and concentration) are located in the centre of the faces of an element (triangle or tetrahedron) whereas the pressure is discretized in the centre and in the vertices of the element. This staggered mesh is called VEFPreP1B. The implemented solution method is a matrix projection scheme derived from the SOLA method (Solution Algorithm for Transient Fluid Flow) originally developed by Hirt /5/, /12/. In this method, the pressure is taken implicitly in the momentum equations and the velocities are taken implicitly in the continuity equation. All other terms are taken explicitly. A Conjugated Gradient method is used to calculate this pressure field. The problem of solving a large non-linear system is thus converted into a linear problem of minimizing residuals, where a more accurate solution is obtained after any iteration. The SSOR (Symmetric Successive Over Relaxation) preconditioning technique is applied in order to improve convergence (incomplete preconditioning for parallel calculations). The user has to verify that the mass conservation is satisfied.

Parallelism

An object oriented, parallel data structure was developed in order to hide the parallelism to the user /4/. The "Parallelization model" is data parallelism. The initial domain is split into smaller

overlapping sub-domains which are distributed among the available processors. The "Programming model" is SPMD (single program multiple data). All the processors execute the same code by using different data. The "Communication model" is message passing. The communication between processors is explicit using MPI (Message Passing Interface) libraries. Since the application is intrinsically parallel, only one problem is treated which is solved in parallel by several processors. Therefore, the calculation domain is distributed in a load-balanced way among the available processors where the initial distribution is achieved using the partitioning tool METIS. In order to optimise the communication between processors, frontier values of the sub-domains are exchanged only when needed. The parallel efficiency is in the order of 80%, tested on various clusters with a weak scaling method on up to 256 processors.

Verification, Validation Qualification

The procedure to ensure that a program solves correctly the equations is called *verification*. Numerous verification tests have been performed with Trio_U which range from

- simple conservation tests (transport of a scalar bubble in a rotational flow field) over
- the analysis of analytical solutions (laminar tube flow or Taylor Green vortices) to
- standard benchmarks (lid driven cavity, bluff body flows).

The procedure to test the extent to which a model accurately represents the reality is called *validation*. Here, Trio_U has been tested and used in a wide field of applications related to nuclear safety. The tests include small scale applications like flow in sudden pipe enlargements, fluid mixing in T-junctions /9/ or inherent boron dilution phenomena in the ROCOM model reactor pressure vessel /8/. More complex applications include in particular full scale studies of induced steam generator breaks /5/ and mixing phenomena in a full scale VVER1000 reactor /6/. The code has also been used in international benchmarks related to a new generation of high temperature gas cooled reactors /10/.

With *qualification*, we define the way to assess a modelling procedure in order to predict target quantities for a specific engineering design under well defined conditions. The procedure for the prediction of the boron concentration at the core inlet under accidental conditions is discussed in this paper in more detail.

The analysis of inherent boron dilution in a full scale reactor model

The analysis presented here is related to the comprehension of the mixing phenomena within the cold legs, the downcomer as well as the lower plenum of a French 900 MWe PWR. During loss of coolant accidents (e.g. small break LOCA), low borated water might accumulate in the steam generator and in the intermediate leg as a consequence of water steam condensation in the steam generator U-tubes /1/. After the onset of natural circulation, this low borated plug can be transported into the core region, which can lead the core to return to criticality. The fine Trio_U calculations simulate the onset of natural circulation in the reactor coolant system after a loss of coolant accident and the associated transport of low borated water within parts of the reactor pressure vessel.

The simulation concerns the onset of natural circulation in the last of the three loops of a 900 MWe reactor, and it is assumed that loop n°2 is this last loop. The localisations of the injections are

given in Figure 1. In order to show the geometrical complexity, the solid structures in the lower plenum are also given in Figure 1. They have an important effect on the boron mixing.

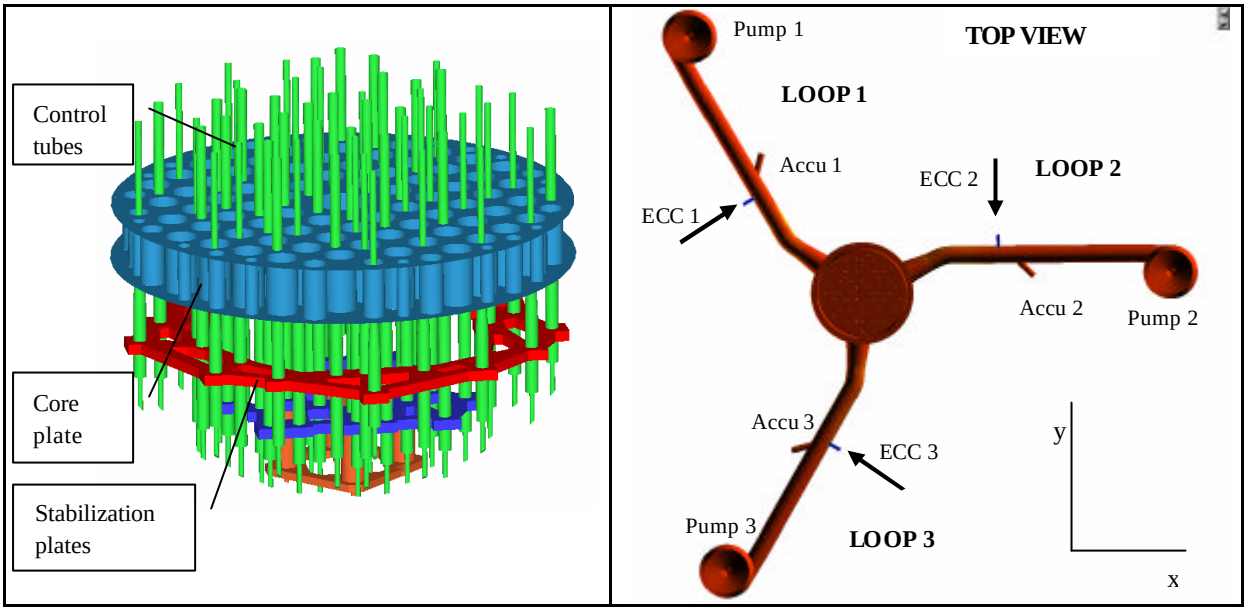

Figure 1: Full scale reactor calculation: lower plenum internal structures and boundary conditions

The low borated plug is situated in the U-form intermediate leg and the steam generator outlet plenum. The plug is thus composed by 2.7 t of low borated water of 320 ppm (intermediate leg) and 5.6 t of almost unborated water of 50 ppm (steam generator). The conditions of the scenario which have been established by IRSN are summarized in Table 1.

Table 1: Thermal-hydraulic conditions of the analyzed scenario

	Loop 1	**Loop 2**	**Loop 3**
Mass flow rate of the natural convection flow (Pump)	135 $kg.s^{-1}$	135 $kg.s^{-1}$	135 $kg.s^{-1}$
Mass flow rate of safety injection (ECC)	15 $kg.s^{-1}$	15 $kg.s^{-1}$	15 $kg.s^{-1}$
Temperature of the natural convection flow	179°C	179°C	179°C
Temperature of safety injection	7°C	7°C	7°C
Boron Concentration before the plug	2425 ppm	2425 ppm	2425 ppm
Boron Concentration of the plug	2425 ppm	2,7 t of 320 ppm 5,6 t of 50 ppm	2425 ppm
Boron Concentration after the plug	2425 ppm	2425 ppm	2425 ppm
Boron concentration of safety injection	2425 ppm	2425 ppm	2425 ppm

The Trio_U qualification procedure for inherent boron dilution

Two test cases have been selected in order to qualify Trio_U for inherent boron dilution; the full scale UPTF test TRAM C3 10b /11/ and a buoyancy driven 1/5 scale ROCOM experiment /8/, /13/. Both experiments represent the major physical phenomena expected in the PWR scenario. Qualifying Trio_U for inherent dilution phenomena means that the PWR model and the models of the qualification calculations UPTF and ROCOM rely on the same modelling hypothesis. BPG are followed for all calculations. They concern:

- the consistent physical modelling of the test cases,
- a reliable discretisation of the convection and diffusion terms as well as of the pressure gradient, the temporal derivative and the source terms,
- a homogeneous meshing and here in particular a coherent discretization of boundary layers (y+=50),
- a mesh independent result for the qualification calculations UPTF and ROCOM and
- sufficiently severe convergence criteria in all simulations.

The flow sheet which ensures the consistent modelling is given in Figure 2. The resulting model is discussed later for the "reactor case".

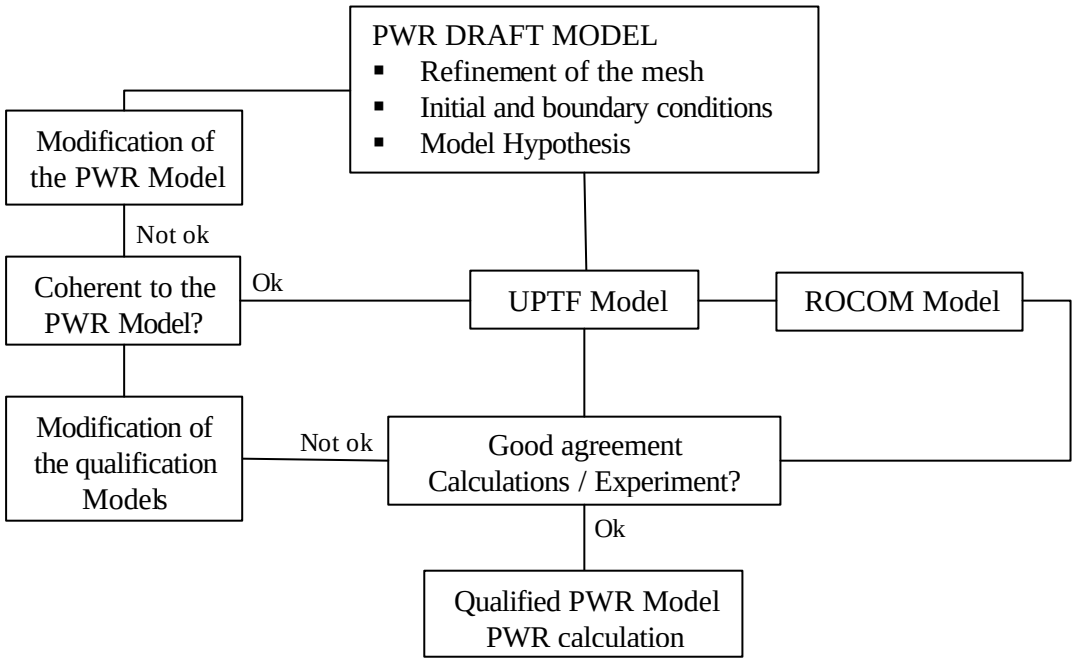

Figure 2 Flow sheet to insure a consistent modelling of the reactor application as well as of the qualification calculations.

From a draft PWR model, a UPTF calculation is done by using the same hypothesis as in the PWR model. If the UPTF calculation is not satisfying compared to the experimental findings, the UPTF model must be modified and the consistency with the PWR model is checked. In this context, modification does not mean *adaptation* of model parameters but *addition of important physical phenomena* into the modelling. In order to ensure the consistency of the models, the PWR model has to be made coherent if necessary before the UPTF calculation is performed. This process is performed until the UPTF calculation shows a good agreement with the experiment.

Then, the ROCOM experiment is analysed. The numerical ROCOM model is based on the hypothesis of the updated PWR model. If the agreement to the experimental findings is not satisfying, the ROCOM model must be improved and the consistency with the PWR model (and with the UPTF

model) has to be verified. After the necessary modification of the models, both the UPTF as well as the ROCOM model are tested and the procedure is performed until both calculations show satisfying agreement between experiment and calculation. The resulting final PWR model represents the qualified model which must not be modified further more when PWR calculations are performed.

The simulation of the UPTF experiment

The UPTF experiments /11/ have been performed by SIEMENS/KWU in order to conduct full scale separate effect studies on multi-dimensional thermal hydraulic phenomena in the primary system. The TRAM-C3 test series analyze the single-phase mixing of hot and cold water in the Reactor Pressure Vessel (RPV) under accidental conditions. The test 10b of these series, which is presented here, is dedicated to the formation of a thermal stratification in the RPV when the natural circulation restarts after the successful reflood of the primary circuit. Figure 3 shows the important physical phenomena which are present in the experiment. The inflow boundary conditions of the test (see also Figure 3) present the following situation:

- Natural convection (simulated by hot water injection) is reestablished in three of the four primary loops.
- The condensate slug (low borated water) is characterized by hot water injected in these three loops
- Highly borated water is characterized by the cold Emergency Core Cooling water injected in one loop
- One loop has no injection flow (dead branch)

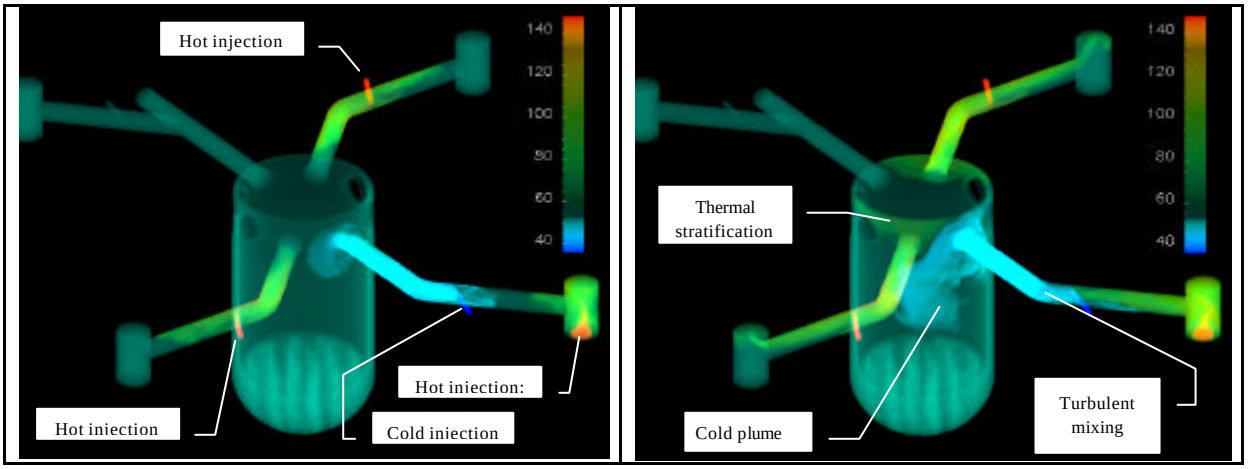

Figure 3: Inflow boundary conditions and important physical phenomena

These phenomena as well as possible synergetic effects must be accurately calculated in order to correctly predict the stratification in the RPV, which is shown in Figure 4. For the end of the test, the comparison of the calculated and measured temperature distribution in the unwrapped downcomer is also given in Figure 4, where the azimuthal temperature distribution at 8 elevations is shown. It is clear that the measured thermal stratification is well represented in the calculation.

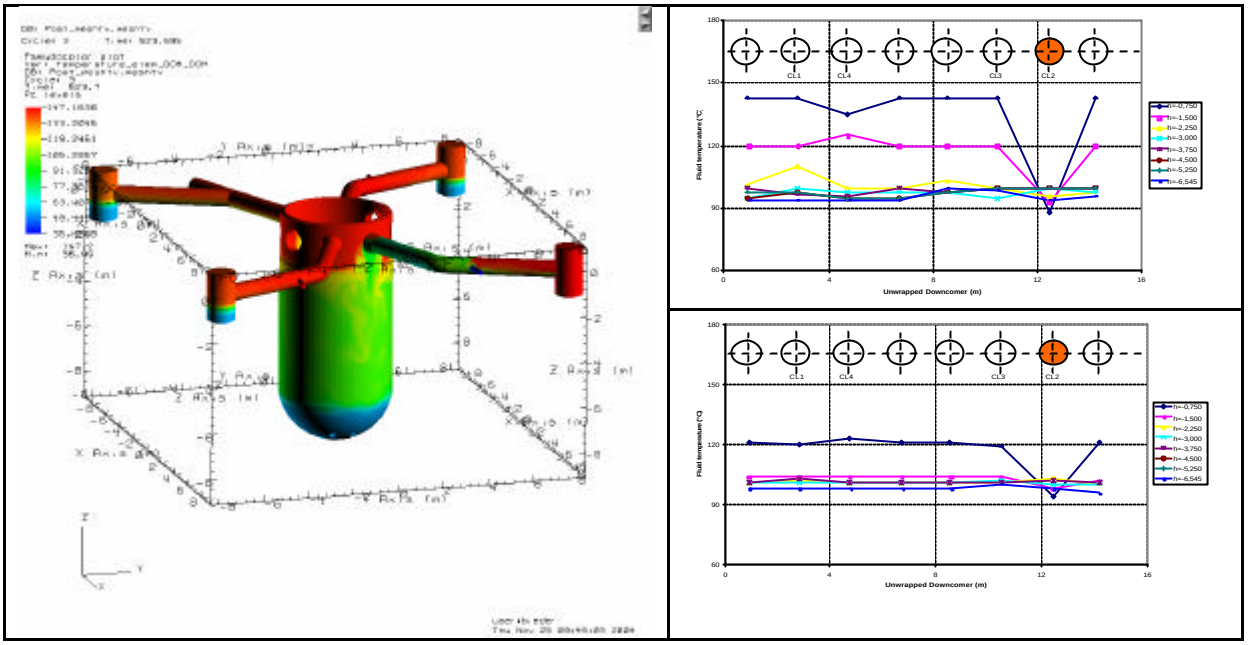

Figure 4: Temperature distribution in the RPV at the end of the UPTF Tram-C3 10b experiment and comparison of the fluid temperature in the downcomer: top calculation, bottom experiment

The simulation of the ROCOM experiment

A generic investigation of the influence of density differences between the primary loop inventory and the ECC water on the mixing in the downcomer was made at the ROCOM mixing test facility at Forschungszentrum Rossendorf /8/, /13/. ROCOM consists of a RPV model with four inlet and four outlet nozzles.

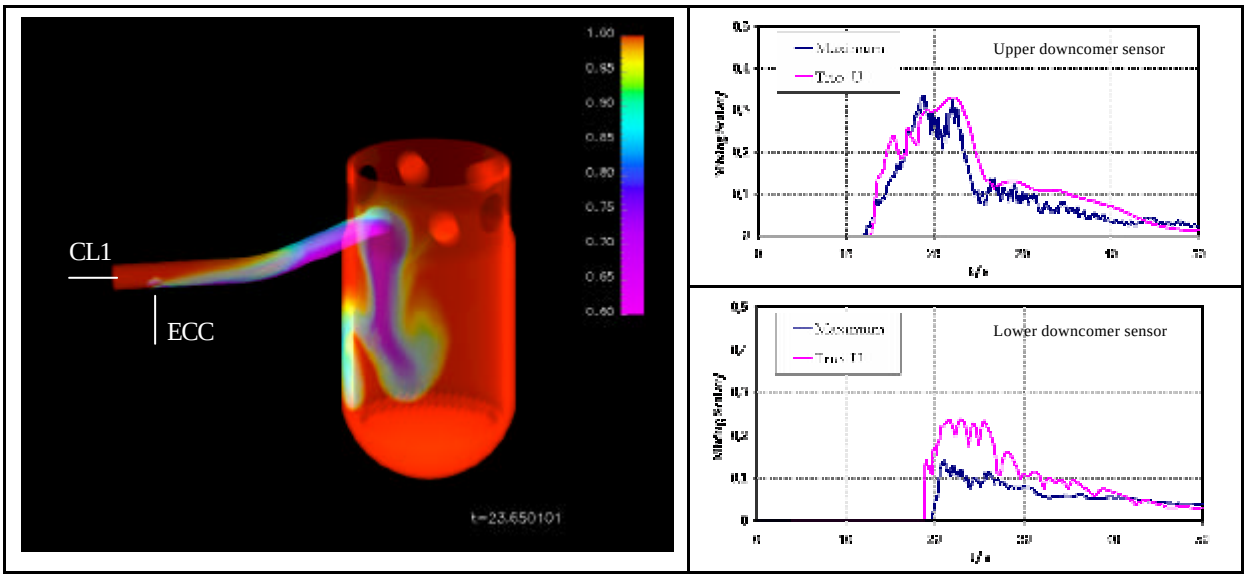

Figure 5: Concentration distribution in the RPV in the ROCOM experiment. Comparison of the maximum concentration at the downcomer sensors: top upper sensor, bottom lower sensor

The test facility is equipped with advanced instrumentation, which delivers high-resolution tracer information characterizing either temperature or boron concentration fields in the investigated pressurized water reactor.

The calculated concentration field in the RPV 3.6 s after the end of tracer injection is shown in Figure 5. The calculated concentration field in the downcomer is compared in Figure 5 to data measured in the middle of the upper and lower downcomer sensor plane. The maximum of the concentration which was measured at the 32 circumferential sensor positions is compared to the corresponding calculated value. The scalar concentration in the calculation (CL1=1, ECC=0) was inverted for comparison. The comparison shows a very good agreement at the upper downcomer position. The calculated concentration at the lower downcomer position is too high, which can be interpreted as an underestimation of the mixing in the downcomer.

The Trio_U model for a full scale reactor simulation experiment

In accordance to the UPTF and ROCOM analysis, the calculation domain covers the fluid part of a French 900 MWe PWR. The domain goes from the main coolant pumps inlet plenum to the lower core plate with all the internal structures in the downcomer and the lower plenum. Dirichlet boundary conditions are imposed at all inflow faces (imposed velocity, temperature and Boron concentration) whereas a von Neumann boundary condition (imposed pressure) is used to simulate the free outflow at the lower core plate. Adiabatic walls and logarithmic wall functions are applied at all solid structures bounding the flow domain. The fluid is assumed to be incompressible (constant density). Thermal effects in the Navier-Stokes equations are considered by the Boussinesq approximation. The highly diluted Boron is transported with the flow as passive scalar without any feedback on the momentum equations. The Euler explicit time scheme is used to integrate the conservation equation in time. In the case of three-dimensional convection/diffusion problems the stability conditions are expressed as the Courant Friedrich Levy criteria for convection and the Fourier criteria for diffusion /12/. Both criteria are evaluated for each cell and each time step. The overall time step is imposed by the overall flow stability criteria which is calculated in analogy to parallel resistances in an electrical network. A Conjugated Gradient method with SSOR preconditioning is used to calculate at each time step the pressure field in order to satisfy very precisely the mass conservation. Further particular user attention is not needed to assure numerical stability. A summary of the numerical scheme is found on Table 2.

Table 2: Numerical Scheme for the reactor calculation

Geometry model	**Physical Data**	**Time scheme**	**Navier_Stokes equations**					**scalar transport equations**		
			Pressure solver	**Diffusion term**	**Convection term**	**Sources**	**Turbulence model**	**Diffusion term**	**Convection term**	**Turbulence model**
tetra mesh	values at 175 °C 9 MPa	1st order Expl.	Conjug. Grad. SSOR	2nd order central	2rd order upwind	Bouss. approx.	Smago. Logarithic wall law	2nd order central	2nd order upwind	Prandtl Adiabatic wall

Special attention has been taken on turbulence modelling. It is well known, that the standard k-ε model shows important weaknesses in the prediction of /3/:

- Flow impingement and reattachment,
- Swirling and re-circulation flow,
- Flow with strong buoyancy effects and high streamline curvature.
- Turbulence driven secondary flows as well as laminar or transitional regions can not be predicted at all.

In order to overcome these limitations, non-linear eddy viscosity models as the k-ω based SST model or Reynolds Stress Model can be used. On the one hand, these models require the solution of various transport equations what can be very CPU-time consuming in instationary flows. On the other hand, model parameters often do not signify a general character but require the adaptation to local flow phenomena. This is not always possible in complex geometry.

The CEA has developed the Trio_U code to apply Large Eddy Simulations (LES) not only to small scale problems but also to reactor scale simulations. The basic idea of the LES approach is to compute explicitly the large turbulent structures and to model the small scale turbulence which is more isotropic and has more universal characteristics. The large, non-isotropic flow structures are directly affected by the boundary conditions as well as by the geometry of the flow domain.

In the reactor case, the filter size of the meshing might not be placed in the inertial sub-range of the turbulent energy spectrum, as postulated by the LES modelling. Nevertheless, under-resolved LES modelling keeps the general character of the modelling approach and extended test on LES modelling have shown that in complex geometries, even under-resolved LES calculations represent turbulent flow as good as well resolved RANS modelling /13/. This is especially true for flow situations where the structure of the geometry influences the mixing process and not the boundary layer formation /6/.

The meshing of the flow domain must be fine enough to capture all important flow features. This is achieved by local mesh refinement. Unstructured meshes are perfectly suited for this purpose. In particular, fine and complex geometrical structures can be very well represented by tetrahedral meshes. The advantage of hexahedral meshes compared to tetrahedral meshes is that one dimensional flow stays one dimensional, as long as the flow direction is orthogonal to the mesh. However, numerical diffusion is high when hexagonal meshes are non orthogonal to the flow direction. In complex flow situations, it is impossible to align the hexa meshes to the flow direction. Therefore, the convection schemes and pressure discretization are optimized in Trio_U in order to minimize numerical diffusion even in the case of non orthogonal tetra meshes with high aspect ratios as e.g. in boundary layers.

For Trio_U calculations, the total meshes number of a certain discretized geometry is only limited by the available computer power. The reactor case simulations have been limited to a runtime of about 45 days for a calculation on 16 nodes of 1.8GHz AMD OPTERON quadri-processors (64 processors), i.e. 70.000 hours CPU. The total meshes number is than defined by:

- the simulation domain which represents the fluid from the main coolant pump inlet plenum to the lower core plate ;
- the duration of the transient which is performed until the lowest boron concentration has traversed the lower core plate (180s).

Due to the vast simulation domain, a grid between 15 to 25 million nodes is anticipated. The time step of the explicit time marching scheme is calculated due to the overall stability criteria and is directly

dependent on mesh size. In 45 days runtime, about 250.000 time steps can be calculated with such a mesh by respecting very strict criteria for the mass conservation. Thus, the final time step should be greater than 0.0007s! Since the smallest mesh size directly affects the time step, the smallest mesh size must be controlled in the mesh generation process with respect to:

- the local refinement of the meshing in the boundary layers and the resolution of the turbulent flow field far from walls, as well as
- the need to represent small geometrical structures as well as the associated flow in the wake.

A grid of 20 millions nodes has finally been created with the commercial mesh generator ICEM. As shown in Figure 6, the grid is locally refined in the boundary layers of the cold leg, the downcomer and near the control tubes in the lower plenum. In the cold leg, the first calculation point is located in the logarithmic zone at about y+=60. Due to the expected long runtime, the resulting mesh is defined a priori without the possibility to make intense sensitivity analyses on the mesh size as required by the BPG. The sensitivity analyses were done in the framework of the qualification calculations.

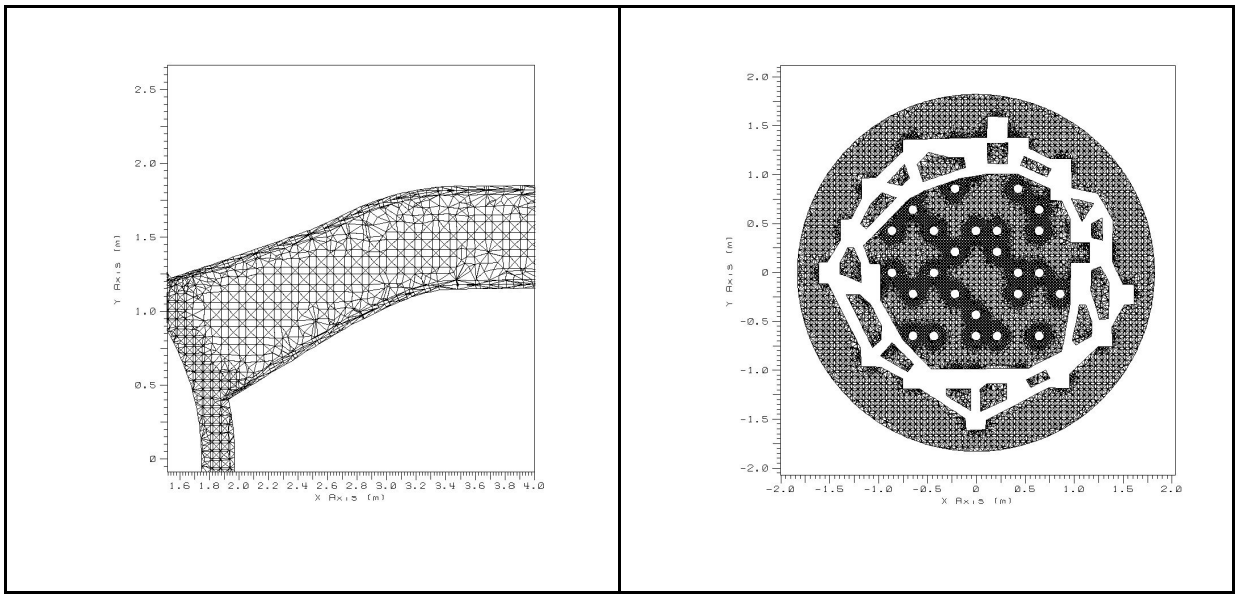

Figure 6: Local refinement of the meshing in the cold leg and the lower plenum

The boron concentration 80 seconds after the onset of natural convection in the loop n°2 is given on Figure 7. The tail of the plug has already traversed the main coolant pump while the head of the plug is situated in the lower plenum and approaches the core support plate. The lowest boron concentration can still be found in the cold leg and a complex zone of weak mixing is formed in the downcomer and lower plenum. An example of the boron concentration at the core inlet at 130 seconds is also added to Figure 7.

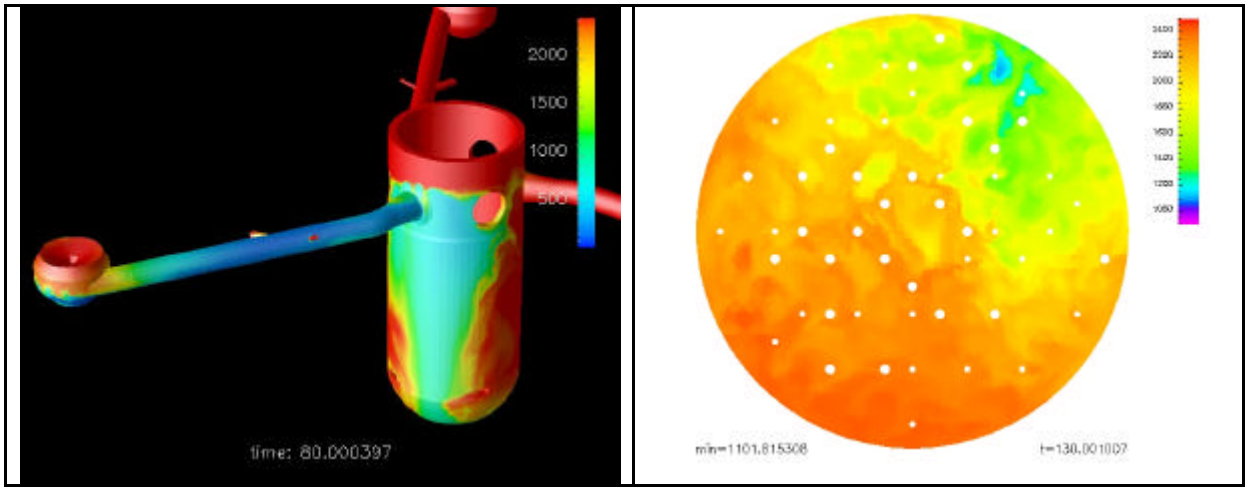

Figure 7: Calculated Boron concentration in the RPV and at the core inlet

The minimum boron concentration at the core inlet shows that the potential return to criticality might not be excluded on the basis of these calculations in the case of a Small Break LOCA : some neutronic evaluations are needed.

Conclusion

A qualification procedure is presented to analyse inherent boron dilution on reactor scale. The objective of this procedure is to ensure that the validation calculations are performed with the same modelling hypothesis as the reactor analysis, for which no experimental data are available. For Trio_U, two test cases, a UPTF and a buoyancy driven ROCOM test, have been selected as validation test cases. Both test cases are correctly represented by Trio_U when using BPG for the setup of the calculations and introducing a stepwise improvement of the description of the main physical phenomena.

The simulation of the transport of a slug of low boron concentration in the primary circuit of a French PWR has been performed which was based on the presented qualification procedure. The predicted boron concentration at the core inlet shows that the potential return to criticality might not be excluded in the case of a Small Break LOCA. Further neutronic calculations are necessary to confirm this result.

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