M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017, on USB (2017)

Multiscale simulation of Light Water reactor thermalhydraulics

D. Bestion

Commissariat à l'Energie Atomique et aux Energies Alternatives,17, Rue des Martyrs, 30054, GRENOBLE, FRANCE Email dominique.bestion@cea.fr

Abstract – Nuclear reactor thermalhydraulics is currently simulated by system codes, by component codes, and also by CFD or CMFD simulation tools. Continuous progress of computer performance allows to use more refined nodalization and to use several modeling scales in a multi-scale approach to reactor thermalhydraulic issues. This paper presents the various types of code and shows how they benefit from smaller scale simulation tools and how they can be coupled to smaller scale simulation tools. A classification of the thermalhydraulic modeling approaches is given. Two-phase CFD is still less mature than single phase CFD and will require physical model developments on the long term, but remarkable progress was made on some specific applications like the boiling flows and critical heat flux investigations, the stratified two-phase flow with condensation, or the core thermalhydraulics in some accidental transients like the loss of coolant accidents. Such examples of multi-scale analyses are presented here and perspectives for future are drawn

I. INTRODUCTION

Reactor thermalhydraulics is currently mainly simulated by system codes and component codes. CFD tools (Computational Fluid Dynamics) and CMFD tools (Computational Multi-Fluid Dynamics), which have a much finer space resolution, started to be used for some reactor issues. The OECD/NEA/CSNI promoted activities with the hope of applying Computational Fluid Dynamics (CFD) to nuclear reactor safety. Three Writing Groups were created under the auspices of the Working Group for the Analysis and Management of Accidents (WGAMA). They produced state-of-the-art reports on different aspects of the subject. The first group, WG1, established Best Practice Guidelines (Mahaffy et al, [1,2]) for CFD application to the field of Nuclear Reactor Safety (NRS). The second group, WG2, documented the existing assessment databases (Smith et al., [3,4]) for CFD application to some identified NRS issues. The third group, WG3, established some requirements for extending CFD codes to two-phase flow safety problems. The group worked for several years on these projects (2003-2009) and produced two reports (Bestion et al., [5,6]). The present paper will summarize some results of this work and will show the degree of maturity of these new simulation tools. This will be based mainly on the information gathered in French and European projects. CATHARE-2 is the current system code developed by CEA, EDF, IRSN and AREVA who also finance the future version CATHARE-3. NEPTUNE is a multi-scale thermalhydraulic platform developed by the same four French partners; it includes the system scale, the component scale, and CFD tools. A multi-physics and multi-scale reactor simulation platform was also developed at the European level in the NURESIM (6th Framework program), NURISP and NURESAFE projects (7th Framework program), which join the efforts of more than twenty partners and which is partly funded by the European Commission.

Attention will be drawn on the large variety of modeling approaches in both single-phase and two-phase CFD. A classification of the various approaches was proposed (Bestion, [7]) in order to help CFD users and those who must evaluate the reliability of code predictions. CFD includes open medium and porous medium approaches and the space and time resolution can be of three main types, the direct simulation type, the filtered approaches (such as Large Eddy Simulation) and the Reynolds Averaged (RANS) approach. Each method is associated to a set of basic equations with closure relations. While some of these methods are already operational (e.g. RANS approach in single phase turbulent flow) some other methods are still in a R&D phase.

The continuous progress of computer performance allows to use more and more refined nodalization and to use several modeling scales in a multi-scale approach to reactor thermalhydraulic issue. Examples of current multi-scale analyses will be given. There may be multi-scale coupling or more simply use of several modeling scales to analyze a reactor issue.

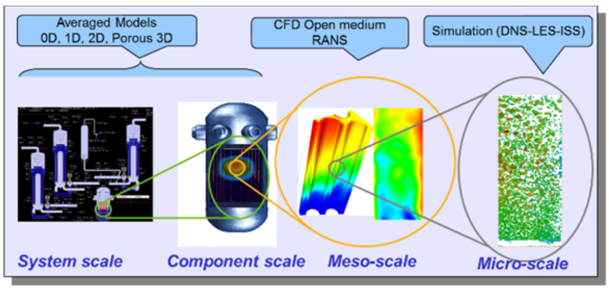

Figure 1: Illustration of the multi-scale analysis of reactor thermalhydraulics

The multi-scale approach to reactor thermalhydraulics is illustrated in Figure 1 where four types of codes and three successive possible zooms are shown from the system scale to microscopic tools. The present paper will illustrate the status of this approach. Before showing applications, it is necessary to specify the various types of codes and the various modeling approaches.

This paper first presents the various types of codes and models, and shows how they could benefit from smaller scale simulation tools. Examples of multi-scale analyses are given and perspectives for future are drawn.

II. CODES AND MODELING APPROACHES

1. The various codes

In two-phase flow thermal-hydraulics, one can distinguish four different types of codes:

- **System scale**: dedicated to the overall description of the circuits of a reactor or of a system test facility. The primary circuits – and possibly the secondary circuit and auxiliary circuits- of a reactor are modeled by coupling 0D, 1D, and 3D modules together with sub-modules for pumps, valves, breaks, safety systems, heat exchangers and control systems. The whole reactor is modeled using a few hundred 0D and 1D meshes whereas the pressure vessel uses currently 10^3 3D coarse meshes. Recent mesh refinements include several thousand meshes in the 3D pressure vessel modelling. This allows simulations of all accident scenarios with a reasonable CPU time (e.g. less than 12 hours).
- **Component codes**: this type of simulation tool is dedicated to the design, safety and operation studies for reactor components such as cores and tubular heat exchangers (steam generators, condensers, auxiliary exchangers). Rod or tube bundles may be homogenized into the control volumes using the "porosity" concept in the "porous body" approach. A particular case is the sub-channel code used for cores with rod assemblies where the spatial resolution is fixed by the sub-channel size (about 1 centimeter) in the direction perpendicular to the rod fuels.
- **CFD in open medium**: the average scale (millimeter or less) allows going beyond the limits of the component scale for a finer description of the flows. It includes turbulence modeling using either Reynolds Averaged Navier Stokes (RANS) or Large Eddy Simulation (LES). One can envisage a local analysis in some reactor components or some part of a reactor component in some particular physical situation. It is the only scale able to predict the fluid temperature field with sufficient time and space resolution for investigating thermal shocks or thermal fatigue of the reactor structures.
- **Direct Numerical Simulation** (DNS) and pseudo-DNS: the characteristic length is given smallest flow feature such as an eddy or a bubble and it may be less than the micrometer. It allows local simulations focusing on very small domains (e.g. containing a few bubbles or droplets). The use of DNS may help understanding the local flow phenomena and may be used for developing closure relations for more macroscopic models. In two-phase flow, Interface Tracking Techniques (ITM) are added to the solution of basic fluid equations to predict the position and evolution with time of every interface. The term pseudo-DNS is more adapted for the two-phase case since some sub-grid physical models are necessary to simulate some very small scale phenomena such as a film splitting during bubble coalescence.

2. Classification of modelling approaches

Beyond the four types of codes one may identify a larger number of different modeling approaches. An identification of the respective approaches was made by considering five successive choices (Bestion , 2010 [7]):

1. Selection between the CFD for open medium and the CFD for porous body by multiplying basic equations by a fluid-solid characteristic function
2. Time averaging or ensemble averaging
3. Space averaging, space integration, or space filtering

   and for two-phase flow only:

4. Choice of the number of phases or fields of the model by multiplying basic equations by phase characteristic functions or field characteristic functions
5. Treatment of interface, which can be Deterministic Interface (DI), Filtered Interface (FI) or Statistical Interface (SI)

The various modeling approaches that can be built based on the five choices mentioned here above were illustrated in (Bestion, 2010, [8]). Five different approaches are identified in the domain covered by CFD in open medium and DNS type codes and at least four different approaches are identified in the domain covered by system codes and component codes. Looking first at the simple case of single-phase flow, only three main types of CFD in open medium may be identified as shown in the Table 1.

Time or ensemble averaging of local instantaneous equations (mass momentum and energy) is used in the so-called RANS approach for steady flow. Time averaged equations are supposed to filter all turbulent eddies and to predict only a mean velocity field. The most popular RANS model (k-ε) uses a two-equation turbulence model with the Boussinesq approximation and a turbulent viscosity. Many variations of two-equation turbulence modelling exist such as k-l, k-ω, SST, RNG-k ε, k-ε -V2, non-linear k-ε. RANS was initially devoted to steady flow but may be also applied to some Unsteady or Transient flow (U-RANS or T-RANS) if the time scale of the mean flow is larger than the time scale of the largest eddies.

The Large Eddy Simulation (LES) uses a space filter to basic balance equations. This allows to simulating large eddies whereas the effects of smaller eddies have to be modelled. The Detached Eddy Simulation (DES) and Very Large Eddy Simulation (VLES) belong to the same family. Some hybrid methods between U-RANS and LES exist such as Scale Adaptive Simulation (SAS).

Direct Numerical Simulation (DNS) just solves exact local instantaneous equations without any averaging or filtering. In turbulent flow this requires that the nodalization is smaller than the smallest eddies at the Kolmogorov scale η. This approach being extremely CPU costly is limited to some investigations of simple problems.

As shown in Table 1, the requirements on the mesh size δ and time step dt depend on the method. δ and dt are only limited by mesh and time convergence of mean flow resolution in RANS type methods whereas δ must be smaller than the filter scale in LES or even smaller than the Kolmogorov space and time scales in DNS. For practical applications, these requirements generally induce increases of the number of meshes of more than an order of magnitude from RANS to LES or from LES to DNS.

Type of model	**DNS**	**LES** **(DES, VLES, SAS,…)**	**RANS** **(URANS, TRANS)**
Time averaging	No	No	Yes
Space filtering	No	Yes	No
Treatment of eddies	All eddies simulated No eddy modeled	Large eddies simulated Small eddies modelled	No eddy simulated
Requirements on dt & mesh size δ	$\delta < \eta$ $dt < \eta/u\eta$	f : filter scale $\delta < f$ $dt < f/uf$	δ & dt limited by mesh and time convergence

Table 1: Some characteristics of the three main types of single-phase CFD for open medium

A general classification of Eulerian approaches was proposed by Bestion (2010,[7]) together with a possible nomenclature.

	OPEN MEDIUM					POROUS MEDIUM
Turbulence	DNS	LES	LES - VLES	LES - VLES	RANS - URANS	RANS - URANS
Interfaces Simulated - Filtered Statistical	Simulated Interfaces	Simulated Interfaces	Filtered & Statistical Interfaces	Statistical Interfaces	Filtered & Statistical Interfaces	Statistical Interfaces
Nb of fields 1-F 2-F n-F	1-Fluid	1-Fluid	1-Fluid 2-Fluid n-Field	1-Fluid 2-Fluid n-Field	1-Fluid 2-Fluid n-Field	1-Fluid 2-Fluid n-Field
Tow-phase model	Pseudo DNS	LES with simulated interfaces	Hybrid LES with filtered & statistical interfaces	LES with statistical interfaces	RANS URANS with filtered & statistical interfaces	Porous medium approach statistical interfaces

Table 2: Classification of the five main types of two-phase CFD for open medium and the two-phase CFD in porous medium

There are three filtered approaches in two-phase CFD (Table 2) instead of only one in single-phase CFD. The three methods filter a part of the turbulence spectrum but they differ by the treatment of interfaces:

- In the LES with simulated interfaces all interfaces are deterministically treated (or simulated)
- In the LES with statistical interfaces, no interface is simulated; all interfaces are treated statistically
- In the hybrid method with filtered and statistical interfaces smaller scale interfaces (e.g. bubble or droplet interfaces) are treated statistically whereas large interfaces (free surface, film surface,…) are "filtered" which means that their shape is simplified: small scale waves or deformations are filtered (non predicted).

3. Porous 3D models and sub-channel analysis

Both the system code and the component codes use porous 3D models for the core or even the whole Pressure Vessel. In this porous medium approach, equations are multiplied by the fluid/solid characteristic function χ_f (x,t):

χ_f (x,t) = 1 when point x is in the fluid at time t

χ_f (x,t) = 0 when point x is in the solid at time t

A volume average of χ_f is the porosity factor:

$$\Phi = \langle \chi_f \rangle = \frac{\mathcal{V}_f}{\mathcal{V}}$$

After multiplication by χf, equations are averaged over time and then over a fluid volume, as follows:

$$\langle A \rangle_f = \frac{\langle \chi_f A \rangle}{\langle \chi_f \rangle} = \frac{1}{\mathcal{V}_f} \int_{\mathcal{V}} \chi_f A \ d\,v$$

Then every local fluid parameter A may be considered as an average plus a space deviation:

$$A \triangleq \langle A \rangle_f + \delta A$$

A particular case is the sub-channel analysis application where the space averaging is linked to the rods in a core. This is not exactly the porous body approach since there is no homogenization of the medium. Equations are integrated over a given space between adjacent rods to produce columns of control volumes in each sub-channel.

The space averaging in the porous body approach (or integration in the sub-channel analysis) follows a time or ensemble averaging and both averaging procedures induce additional terms coming from the nonlinear convection terms. Time averaging produces the Reynolds stress tensor and turbulent heat flux terms in momentum and energy equations and space averaging produces “dispersion terms” in momentum and energy equations as follows (in an incompressible approximation):

$$\langle \chi_f \rho \frac{\partial u_i u_j}{\partial x_j} \rangle_f = \rho \frac{\partial \Phi \langle u_i \rangle_f \langle u_j \rangle_f}{\partial x_j} + \rho \frac{\partial \Phi \langle \delta u_i \delta u_j \rangle_f}{\partial x_j}$$

$$\langle \chi_f \rho \frac{\partial u_i h}{\partial x_j} \rangle_f = \rho \frac{\partial \Phi \langle u_i \rangle_f \langle h \rangle_f}{\partial x_j} + \rho \frac{\partial \Phi \langle \delta u_i \delta h \rangle_f}{\partial x_j}$$

In the two equations above the first term on the r.h.s is a macroscopic convection term and the second is a “dispersion term”.

No general modeling of these dispersion and turbulent diffusion terms exist for the core geometry or the Pressure Vessel in general. In the case of sub-channel codes, transfer terms between sub-channels are developed and validated to predict mainly the enthalpy mixing between sub-channels for CHF prediction. These terms model together dispersion and turbulent diffusion. Dispersion terms are expected to have more effects than turbulent diffusion.

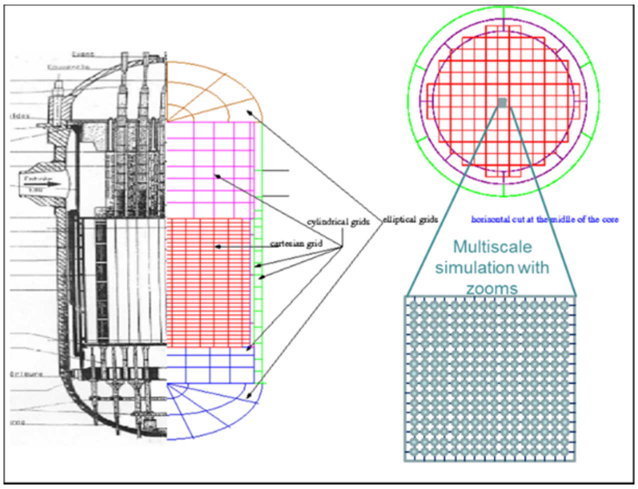

Figure 2: Perspective for future modelling of a reactor pressure vessel.

3-D modules exist as an option in the system codes for the reactor pressure vessel. The main objective of such 3D modules is the modeling of large scale 3D effects in a pressure vessel during LBLOCA and SBLOCA such as downcomer penetration of ECCS water, transverse core power profile effects in Reflooding or in core uncovery. In most applications, rather coarse nodalization schemes (about 1000 nodes for a CATHARE Pressure Vessel 3D nodalization) were first applied and consequently the advantage of a 3-dimensional modeling of the flow processes might be offset to a certain extent. However computer power now allows a mesh refinement and prospectives for future pressure vessel modelling include local refinements and various zones of the vessel modeled by various types of meshing. Figure 2 shows a nodalization of a PWR pressure vessel using a 3D module. One can see a cylindrical system of coordinates in all parts except the core which is modelled in a cartersian frame of reference and one column of meshes per assembly. In the radial direction, there is a radial mesh in the downcomer, a radial mesh for the core baffle, and 5 radial meshes in lower plenum, upper plenum and upper head. This nodalization is clearly much finer in the core with about 6000 meshes. The continuous progress of computer power will allow in future a nodalization with the possibility to combining various sub-components using either cartesian, cylindrical or elliptical frames of reference depending on the local geometry as in Figure 2. One may also imagine local mesh refinements in one or a few fuels assemblies which would be treated by sub-channel analysis model, i.e. with one raw of meshes for each sub-channel.

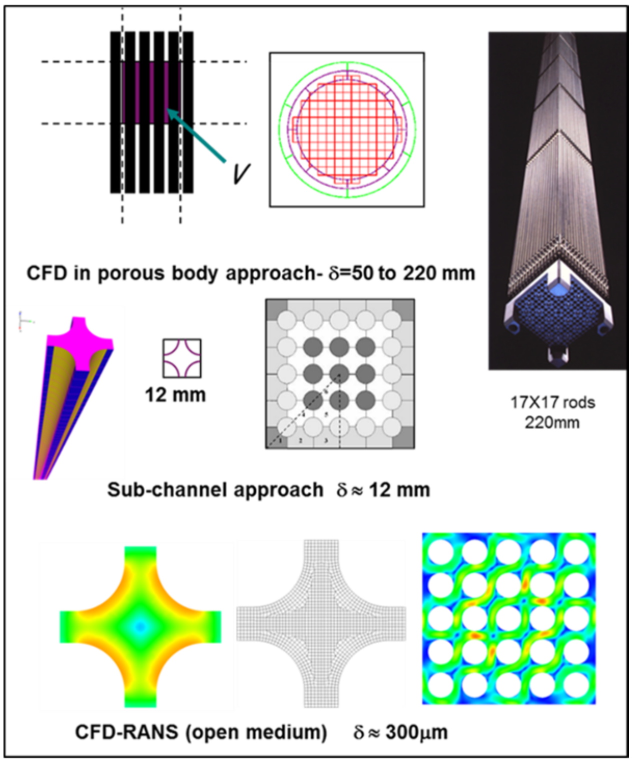

Figure 3: The various modeling scales of reactor core therlhydraulics

III. MULTI-SCALE ANALYSIS AND MULTI-SCALE SIMULATION

Two main kind of multi-scale approaches (Bestion, 2012) are identified:

1. **The multi-scale simulation with zooming**: a finer scale tool is used in a part of the domain simulated by more macroscopic tool. The objective is to predict local flow details that are not predicted at the macroscopic scale when there is a specific interest on small scale phenomena only for a limited part of the domain. The local zoom can be coupled to the system calculation or it can simply be done in parallel using some results of the system calculation as boundary condition. There may be several scales in series: one may imagine a system code to predict the whole behavior of the primary circuit which gives boundary conditions to a component code for the core thermalhydraulics. Within the core, a few sub-channels could be simulated with a CFD for open medium using the component code results as boundary conditions. Finally a DNS of a very small part of a sub-channel may be used to predict a very local phenomenon such as a Departure from Nucleate Boiling (DNB) occurrence. This is an extreme case which is not the current practice. A more common case is the coupling of a system code with a single-phase or two-phase CFD tool for a few safety issues:
    - Boron dilution transients
    - Steam Line Break
    - Pressurized Thermal Shock

2. **The multi-scale analysis:** it consists in using the smaller scale simulation without coupling to macroscopic scales. The small scale simulation is used to understand the basic phenomena and to develop more physically based models or closure laws for a more macroscopic model. In the example of the DNB occurrence in a reactor core, the role of the various scales is the following:
    - Pseudo-DNS simulations may be used to identify the physics of the DNB process and to derive a physically based local DNB criterion for a two-phase CFD for open medium using a RANS approach.
    - The CFD for open medium using a RANS approach may simulate the few sub-channels which are likely to create conditions for a DNB occurrence (see for example in section 7 below how this approach is developed in the NEPTUNE, NURESIM and NURISP projects)
    - A sub-channel analysis code may be used to give boundary conditions to the CFD code

IV. BOILING FLOW AND CFH ANALYSIS

Bubbly flow and boiling bubbly flow were extensively studied in the frame of the NEPTUNE-CFD project (Bestion & Guelfi, 2005 [9], Guelfi et al., 2007 [10]) and in the European project NURESIM (www.nuresim.com) and NURISP [7] (see also www.nurisp;com). The general methodology defined in (Bestion et al, 2006 [6]) was applied with a selection of modeling options and by collecting an appropriate database (Bestion et al., 2009 [11], see also www.nuresim;com). The multiscale approach for CHF investigations is presented in Figure 3.

Current industrial methods investigate CHF by performing prototypical experiments in full height full power full pressure rod assembly and by developing CHF correlations to be used by a sub-channel analysis code. A step forward is anticipated from the use of two-phase CFD and the associated development of a DNB prediction method based on CMFD. The DNB (Departure from Nucleate Boiling) is a privileged application for multi-scale approach since all scales have important flow processes which may influence its occurrence.

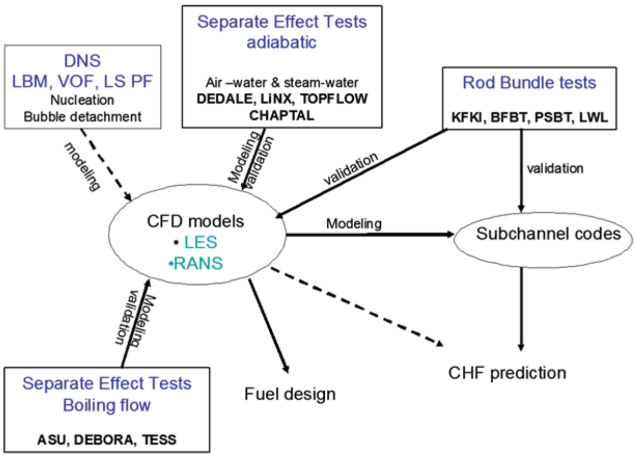

Figure 4: The multiscale approach for CHF investigations

Any modification of core boundary conditions may be predicted by a system code. A component code applied with the sub-channel analysis may model the mixing between sub-channels, cross-flows, turbulent effects of grid spacers. However two-phase boundary layers appear along fuel rods in the sub-channels and many small scale phenomena control the dynamics of these two-phase layers: bubble transport and dispersion, bubble growing and collapse due to vaporization and condensation, coalescence and break up, turbulent transfers of heat and momentum, local grid spacer effects. Two-phase CFD can predict these phenomena. The DNB process itself occurs at the very vicinity of the heating wall and all small scale phenomena occurring at the finest scale may influence the process: activation of nucleation sites, growing of attached bubbles, sliding of attached bubbles along the wall, coalescence of attached bubbles, bubble detachment, wall rewetting after detachment. Pseudo-DNS including Interface Tracking Methods (ITM) may in principle predict such small scale phenomena since detached bubbles have a diameter of a few tens of micrometers. In NEPTUNE, NURESIM and NURISP projects the following approach is used:

- **Pseudo-DNS** (Lattice Boltzman Method, Level Set, Front Tracking) is used and will be used to investigate forces acting on bubbles, detachment frequency and size of bubble at detachment,…On may expect that in future, the mechanism of DNB, which is not yet clearly identified, could be discovered by such pseudo-DNS tools. G. Bois (2016) [12] simulated high pressure bubbly flow in a vertical channel and Y Sato (2016, [13]) already simulated the transition from pool boiling to DNB with a pseudo-DNS method. Extensions to convective boiling are in progress.
- **CFD-RANS** approach is used and will be used to predict local flow parameters. A local DNB criterion is necessary to predict DNB occurrence as function of these local flow parameters. Several successive local DNB criteria were used (Macek & Vyskocil, 2008 [14], Mimouni et al., 2016 [15]).
- **Sub-channel analysis** may benefit from CFD-RANS simulations by better understanding the flow processes and to develop better closure laws for mixing between sub-channels, spacer grid effects and better CHF correlations. In particular the well-known "non-uniform heat flux effect" could be understood at the CFD scale and physically based models could be developed for the sub-channel scale.

Even if the CHF predictive by CMFD is a rather long term objective, Pseudo-DNS and CFD-RANS investigations may help nuclear industry in the design/optimization of fuel assemblies and for optimizing CHF test procedures, reducing the number of tests. Also sub-channel models may be improved based on CMFD simulations. Finally a decrease of conservatisms through more general and accurate CHF correlations will result in additional operation margins.

A RANS modeling of boiling flow up to DNB occurrence was developed and validated (Morel et al., 2003 [16] Mimouni et al., [17]2008, Macek & Vyskocil, 2008 [14], Morel & Laviéville, [18] 2009, Koncar & Krepper, 2008 [19], Koncar & Matkovic, 2011 [20], Perez et al., 2011 [21], Mimouni et al. [22 , 23], Merigoux et al., 2016 [24]) with particular attention to some phenomena:

- Forces acting on bubbles including, drag, virtual mass, lubrication, lift and turbulent dispersion forces
- Wall friction and wall heat transfers
- Bubble size and poly-dispersion effects
- Turbulence modeling
- Bubble condensation
- DNB criterion

From what has been obtained so far one can draw the flowing preliminary conclusions:

- Boiling Bubbly flow can be simulated at the CFD-RANS approach with an accuracy which is limited by some difficulties in the modeling of wall transfers, poly-dispersion effects and also turbulence.
- As was shown by simulations made at both sub-channel and CFD scales of OECD-NRC benchmark tests BFBT and PSBT, CFD cannot yet predict averaged flow parameters better than sub-channel codes and cannot yet be used as a reference tool for component codes. However they can already predict some small scale phenomena such as geometrical effects (spacer grids) which can only be fitted on experimental data at sub-channel scale.

- Using a very simple DNB criterion, CHF may be predicted at CFD scale with an accuracy of 10 % in a rather large domain of parameters, which is not yet fully satisfactory.
- Pseudo-DNS made remarkable progress in bubbly flow and boiling flow but its application as a support for RANS-CFD is still limited by the CPU cost. G Bois (2016) performed bubbly flow simulations with pseudo-DNS which could provide interesting information for two-phase RANS turbulence models which lacks validation data and Y Sato (2016) simulated DNB with a pseudo-DNS method. Future computer power increase will open a huge domain of investigations to Pseudo-DNS.
- Despite the present limitations, the CFD simulations may already be used for parametric studies as a tool to help fuel design and to reduce the need of experiments. It can also provide useful information to improve sub-channel models.

V. TWO-PHASE PTS INVESTIGATIONS

Two-phase PTS scenarios have been studied in the frame of the NEPTUNE-CFD project [9,10], and in the NURESIM, NURISP [7] and NURESAFE European projects. The general methodology defined in Bestion et al. [6,7] and was applied with a selection of modeling options and by collecting an appropriate database (Lucas et al., 2009 [25]). There may be High Pressure Injection (HPI) and accumulator injection into the cold leg with single-phase flow conditions in the cold leg for some scenarios, but also two-phase flow situations in other scenarios. In these two-phase flow scenarios the cold leg is either partially uncovered, or totally uncovered. Both situations have to be covered by simulations on two-phase PTS.

Resulting from the identified scenarios, the two-phase flow PTS simulations should cover the many single effect phenomena shown in figure 5: behaviour of the cold water jet (including jet stability and condensation on the jet), jet impingement (including turbulence production by the jet, bubble entrainment and migration of the entrained bubbles), stratified flow including mass, momentum and heat transfer on the free surface and their interaction with interfacial waves, temperature stratification, turbulence production, and flow separation in the downcomer at the cold leg nozzle. The most important process is the condensation on the free surface which is affected by the turbulence and which is the main heat source for the water going to the Pressure Vessel.
Several experimental data sources were identified which can be used for the development and a partial validation of physical models. Experiments provide information on plunging jets, with entrainment of air bubbles and production of turbulence below the free surface. Free surface flow experiments without mass transfer were used to investigate mechanical interfacial transfers in stratified flow. Condensation at a free surface of a stratified steam-water flow in rectangular channel was used to validate condensation. COSI tests and TOPFLOW-PTS tests are combined effect tests with several phenomena representative of the PTS scenarios and a UPTF-TRAM test could simulate at reactor scale many phenomena but without condensation whereas ROSA IV LSTF tests can simulate system effects in PTS scenarios.

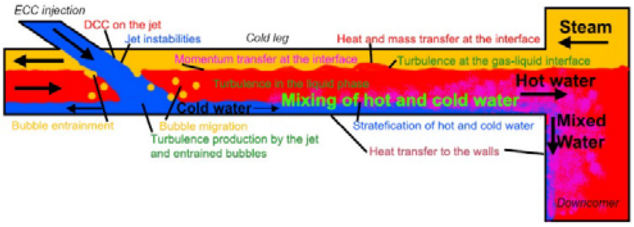

Figure 5: The two-phase PTS scenario and the associated basic phenomena

The multiscale method applied for PTS investigation is presented in Figure 6. System codes cannot predict the fluid and wall temperature field at a sufficient fine resolution to solve the issue and the objective here is to simulate the whole transient with the system code and to couple the system code with a CFD calculation of the cold legs and the downcomer. In the NURESIM and NURISP projects the following multi-scale approach is applied:

- Pseudo DNS and LES with simulated interface were used for condensing stratified flow by Lakehal (2008, [26,27]). These simulations could be used to derive interfacial transfers for the RANS approach.
- LES with filtered interface is validated against adiabatic and condensing stratified flow.
- URANS with filtered interface (Bartosiewicz et al, [28]2008, Coste et al., 2008 [29], Scheuerer et al. 2007 [30], Strubelj & Tiselj, 2008 [31], Coste et al., 2010 [32], Apanasevich et al., 2011 [33]) is also validated against adiabatic and condensing stratified flow.
- URANS with a 1-fluid model is benchmarked against URANS with the 2-fluid model associated with an interface recognition technique
- The coupling of system code and CFD is tested on the ROSA IV LSTF test (Scheuerer et al., 2010 [34])

Plunging jet effects are also investigated at the RANS scale (Galassi et al., 2007 [35], Schmidtke & Lucas, 2008 [36]).

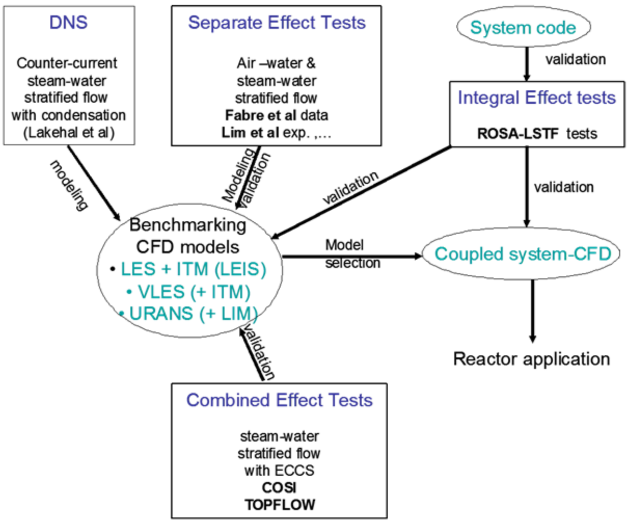

Figure 6: The multiscale approach for PTS investigations

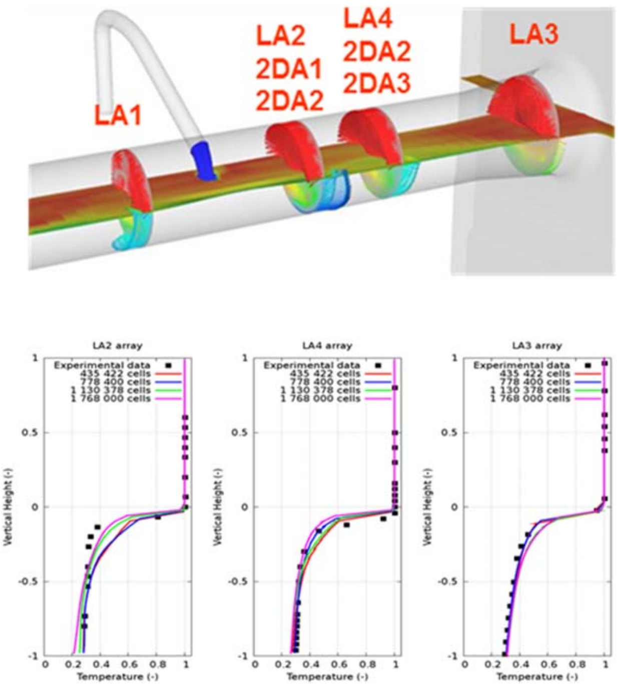

Figure 7: NEPTUNE-CFD simulation of TOPFOW-PTS test SSSW 3-17 with mesh sensitivity (From Coste & Merigoux, 2014)

From what has been obtained so far one can draw the flowing conclusions:

- URANS with filtered interface can simulate the two-phase flow in a reactor cold leg with ECCS injection and in the downcomer
- LES with filtered interface may also be able to simulate the reactor transient but CPU time requirements may be more difficult to satisfy.
- 2 RANS methods are benchmarked for free surface flow either with a two-fluid model or a single-fluid model. In both case the modeling of interfacial transfers require the knowledge of the interface position in order to model transfers with "wall function like" method.
- CFD could predict the fluid temperature field in TOPFLOW-PTS test with a very good agreement with data (See Figure 7). A benchmark of methods was organized on a TOPFLOW test showing a good maturity of simulation tools (Coste and Mérigoux, 2014 [37], Mérigoux et al., 2016 [38])
- The NEPTUNE_CFD code has followed an exhaustive validation program with satisfactory results on all dominant phenomena (Merigoux et al., 2017 [39])

VI. A MULTI-SCALE APPROACH OF CORE THERMALHYDRAULICS

In the NURISP and NURESAFE projects, some LOCA issues such as Reflooding, core radial power profile effects, were revisited with state of the art tools including a multi-scale approach. The multi-scale approach for Reflooding will use three types of models:

- A **Lagrangian Particle Tracking** (LPT) method is used to investigate droplet flow in the dry zone of the core during Reflooding. The steam flow is simulated with CFD-RANS (Badillo and Andreani, 2016 [40]).
- An **Eulerian-Eulerian two-phase CFD-RANS** approach is used to simulate the mist flow in a core rod bundle with particular interest for a ballooned zone. The results of the LPT treatment of droplets may help in modeling interfacial transfers in Eulerian-Eulerian CFD method.
- At the end better models for the system scale **3-field model of CATHARE-3** will be developed based on CFD simulations

Steam to droplet heat transfer $q_{vi}(Xj)$plays a very important role in dispersed flow film boiling. As explained in section 3.1 due to the space averaging of a nonlinear source term:

$$<q_{vi}(Xj)> \neq q_{vi}(<Xj>)$$

The two CFD methods may give the estimation of the profile effects on this transfer.

Core radial power profile effects can be investigated by analyzing the OECD-NRC benchmarks based on BFBT and PSBT bundle tests. Radial transfers of enthalpy and of void fraction are measured in these tests. The tests are simulated at three scales:

- The 1D 2-fluid and 1D 3-field models of CATHARE-3
- The porous 3-D model of CATHARE-3
- The CFD RANS in open medium

Here again the finer scale simulations may be used to improve macro-scale models.

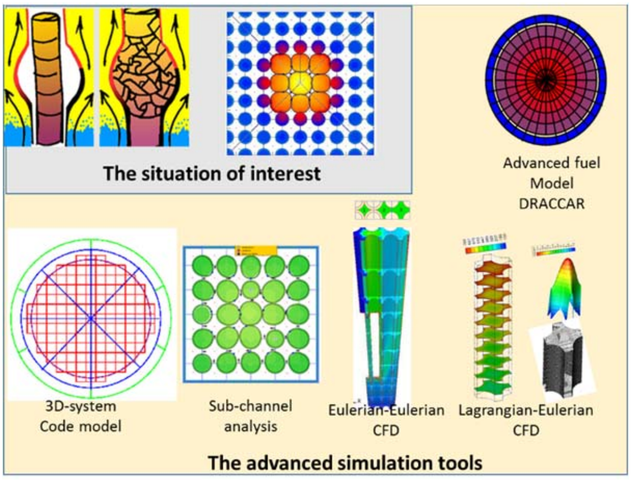

Figure 8: The situation of interest with a ballooned zone and the various simulations tools

More recently a new interest in SBLOCA, IBLOCA came from the requirement to take a possible fuel relocation into account in case of fuel ballooning (Ricaud et al., 2013 [41]). This makes the safety analysis more difficult and more accurate description of the single phase and two-phase flow is needed. The Figure 8 shows the situation of interest and the set of simulation tools that are being used. The Figure 9 shows the global multiscale methodology. 1-Phase CFD can provide the flow repartition in the deformed zone and the heat transfer coefficients. The CFD results may be used to improve the modelling of the same zone with sub-channel analysis code coupled to an advanced 3D fuel thermos-mechanics code. Then System code modelling may be improved from results of the sub-channel code simulations. In two-phase steam-droplet flow the Lagrangian-Eulerian approach is first used as explained above. Then Eulerian CFD, sub-channel analysis and system modeling are progressively improved. Such a multi-scale analysis needs some validation: available data and new experimental programs are being planned for a more complete validation.

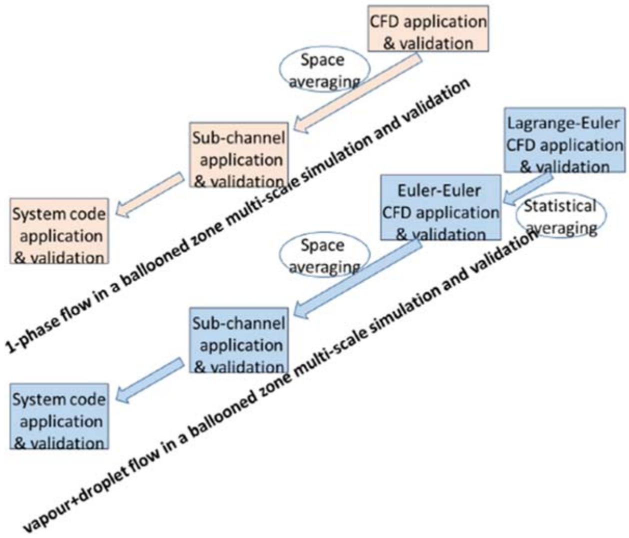

Figure 9: Multiscale analysis of core flow in single-phase and two-phase flow

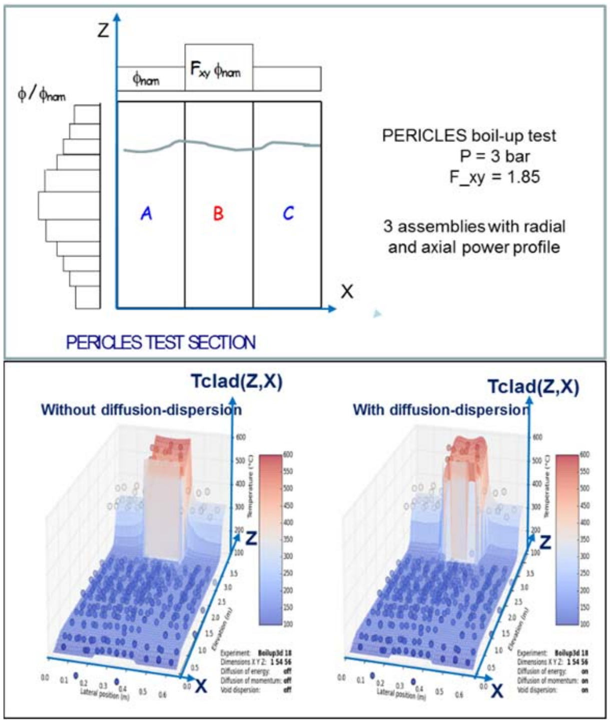

Figure 10: CATHARE-2D simulations of a PERICLES boil-up test using sub-channel modeling with and without diffusion-dispersion

An example of up-scaling method application was already successfully applied during the NURESAFE project. T Alku (2017) [42] simulated a core reflooding test in presence of axial and radial power profiles with bot a sub-channel modelling and a system-type modelling using one mesh per assembly. The objective was to demonstrate that the diffusion and dispersion effects did not play a significant role on peak clad temperature in such situations. Since validated model for diffusion and dispersion exist at sub-channelm scale they were used and showed a rather low effect on clat temperature as shown in Figure 10. This confirms that the systems scale modelling which does not model diffusion and dispersion cannot degrade significantly the results.

VII. CONCLUSIONS

The continuous progress of computer power will progressively increase the market share of CFD application in reactor thermalhydraulics. However this process will remain rather slow and the macroscopic approaches using system codes and component codes will still play a dominant role during a few decades for solving most LWR thermalhydraulic issues. Two-phase CFD for open medium will not replace component and system TH codes in the short and medium term (the next two decades). However two-phase CFD for open medium may be used for a local zooming of for improving models of macroscopic tools and for reducing the need of the most expensive experiments. The impressive progress of computer power will not allow to skip from a porous body approach to a CFD for open medium but it will first allow a finer nodalization in porous body approach and a more extended use of the sub-channel modeling.

The cost and the availability of HPC for nuclear engineering and for the R&D community will probably restrict the use of this technology to a few selected reactor issues for which it is necessary or brings a real added value. One may expect the following types of application of HPC in the next two decades:

- Optimizing the design of core, evaluate pressure losses and heat transfer efficiency
- Safety issues with single phase turbulent flow such as boron mixing, cold water mixing with hot water in steam line Break accident, containment mixing of air steam and hydrogen, Pressurized Thermal Shock (PTS), thermal stripping,…
- A more limited number of safety issues with two-phase flow such as some PTS scenarios
- Coupled problems: TH-core physics, fluid-structure interaction…

In addition to this direct application of HPC to reactor issues, one may also expect some limited use for the basic research by providing “numerical experiments” or reference calculations in a multi-scale analysis approach. Examples are:

- DNS or LES reference simulations of single phase situations to evaluate the capability of RANS and URANS models to adequately capture the phenomena and to measure the accuracy of RANS-URANS predictions. This may be used either in the context of basic research or as a support to CFD application to safety demonstrations.
- RANS simulation in open medium to improve porous 3D models
- Two-phase pseudo-DNS of boiling flow used as “numerical experiments” to investigate micro-scale flow processes which are not clearly visible by available experimental techniques such as the DNB.
- Two-phase pseudo-DNS “numerical experiments” of prototypical flow configuration to derive averaged models for CFD in porous medium, CFD in open medium, or even 1D model of system codes.

Reactor thermalhydraulics will use several simulation tools from system codes to several kinds of CFD models to solve all design and safety issues. Single phase CFD used in a multi-scale approach is able or will soon be able to solve some issues and to allow improvement of system and component codes.

Two-phase CFD is less mature than single phase CFD and will require physical model developments on the long term. Due to the large variety of model options in two-phase CFD one should take care to clearly define the selected modeling approach, in order to select the appropriate closure models and to obtain a consistent approach. The use of a multi-scale approach for improving the modeling of 3D Pressure Vessel models and component codes should be a priority since it is a way to reduce uncertainty in safety analyses.

NOMENCLATURE

BPG	Best Practice Guidelines
CFD	Computational Fluid Dynamics
CHF	Critical Heat Flux
CMFD	Computational Multi-Fluid Dynamics
DNS	Direct Numerical Simulation
HX	Heat Exchanger
IBLOCA	Intermediate break LOCA
ITM	Interface Tracking Method
LBLOCA	Large break LOCA
LOCA	Loss of coolant accident
LES	Large Eddy Simulation
PTS	Pressurized Thermal Shock
RANS	Reynolds Averaged Navier Stokes
RNG-k-ε	Re-Normalisation Group k-ε model
SBLOCA	Small break LOCA
SST	k-omega two-equation turbulence model of F. Menter
URANS	Unsteady RANS

VLES Very Large Eddy Simulation

ACKNOWLEDGMENTS

The author is grateful to the members of the NEPTUNE project for a multi-scale thermalhydraulic platform and to CEA, AREVA, EDF and IRSN, who finance the project. The thanks are extended to the members of the CSNI working groups on CFD application to safety, to the members of the NURESIM, NURISP, and NURESAFE European projects, who contributed to the multi-scale analyses, and to the European Commission who funded these projects.

REFERENCES

1. MAHAFFY, J. (ed.), 2007, "Best Practice Guidelines for the Use of CFD in Nuclear Reactor Safety Applications", OECD, Nuclear Energy Agency, Technical Report, CSNI/R(2007)5, April 2007
2. J.H. MAHAFFY (ed.), "Best Practice Guidelines for the use of CFD in nuclear reactor safety applications – Revision", OECD Nuclear Energy Agency, NEA/CSNI/R(2014)11, February 2015
3. SMITH, B.L. (ed.), 2008, "Assessment of Computational Fluid Dynamics (CFD) for Nuclear Reactor Safety Problems", OECD Nuclear Energy Agency, Technical Report, NEA/CSNI/R(2007)13, Jan. 2008.
4. B.L. SMITH (ed.), "Assessment of CFD codes for nuclear reactor safety problems", OECD Nuclear Energy Agency, NEA/CSNI/R(2014)12, Jan. 2015 (Revision 2)
5. D. BESTION (ed.), "Extension of CFD codes to two-phase flow safety problems", OECD Nuclear Energy Agency, NEA/SEN/SIN/AMA(2006)2, August 2006
6. D. BESTION (ed.), "Extension of CFD codes application to two-phase flow safety problems – Phase 2", OECD Nuclear Energy Agency, NEA/CSNI/R(2010)2, July 2010a

7 D. Bestion, 2010b, Applicability of two-phase CFD to nuclear reactor thermalhydraulics and elaboration of Best Practice Guidelines, Nuclear Engineering and Design, Volume 253, Pages 311-321, December 2012

8. D. BESTION, Status and perspective for a multiscale approach to Light Water reactor thermalhydraulic simulation, NURETH 14 topical Issue of Nuclear Engineering and Design, 2012
8. D. BESTION, 2010c, From the Direct Numerical Simulation to system codes – Perspective for the Multi-scale analysis of LWR Thermalhydraulics, Nuclear Engineering and Technology, VOL.42 NO.6 December 2010
9. D. BESTION, A. GUELFI, 2005, « Status and perspective of two-phase flow modelling in the NEPTUNE Multiscale thermal-hydraulic platform for nuclear reactor simulation », Nuclear Engineering and Technology, Vol. 16, Nos 1-3, pp 1-5, 2005
10. A.GUELFI, D. BESTION, M. BOUCKER, P. BOUDIER, P. FILLION, M. GRANDOTTO, J.M. HERRARD, E. HERVIEU, P. PETURAUD, 2007, NEPTUNE A new Software Platform for advanced Reactor Thermalhydraulics, Nuclear Science and Engineering, 156, 282-324, 2007
11. D. BESTION, H. ANGLART, D. CARAGHIAUR, P. PÉTURAUD, B. SMITH, M. ANDREANI, B. NICENO, E. KREPPER, D. LUCAS, F. MORETTI, M. C. GALASSI, J. MACEK, L. VYSKOCIL, B. KONCAR, AND G. HAZI, 2009, Review of Available Data for Validation of Nuresim Two-Phase CFD Software Applied to CHF Investigations, Science and Technology of Nuclear Installations, Volume 2009 (2009), Article ID 214512
12. G. BOIS, Direct numerical simulation of a turbulent bubbly flow in a vertical channel: Towards an improved second-order reynolds stress model, Nuclear Engineering and Design, In Press, Corrected Proof, Available online 2 March 2017
13. Y. SATO, B. NICENO, "Pool boiling simulation up to critical heat flux using an Interface tracking method", *NUTHOS-11*, Gyeongju, Korea, October 9-13, 2016.
14. J. MACEK, L. VYSKOCIL, 2008, Simulation of Critical Heat Flux Experiments in NEPTUNE_CFD Code XCFD4NRS, Grenoble, France, 10 - 12 September 2008
15. S. MIMOUNI, C. BAUDRY, M. GUINGO, J. LAVIEVILLE, N. MERIGOUX, N. MECHITOUA, Computational multi-fluid dynamics predictions of critical heat flux in boiling flow, Nuclear Engineering and Design, Volume 299 , Pages 28-36, April 2016
16. C. MOREL, WEI YAO, D. BESTION, 2003, Three Dimensional modelling of boiling flow, The 10th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-10), Seoul, Korea, October 5-9, 2003
17. S. Mimouni, F. Archambeau, M. Boucker, J. Laviéville, 2008, CFD Modelling of subcooled boiling in the NEPTUNE_CFD code and application to fuel assembly analysis , XCFD4NRS, GRENOBLE, FRANCE, Sept10-12, 2008
18. C. Morel and J. M. Laviéville, 2009, Modeling of Multisize Bubbly Flow and Application to the Simulation of Boiling Flows with the Neptune CFD Code, Science and Technology of Nuclear Installations, Volume 2009, Article ID 953527
19. B. Koncar, E. Krepper, 2008, CFD simulation of convective flow boiling of refrigerant in a vertical annulus, Nucl. Eng. Des. ,Volume 238, Issue 3, 2008, pp. 693-706
20. B. KONČAR, M. MATKOVIČ, 2011, Modelling and validation of turbulent boiling flow in a rectangular channel, The 14th International Topical Meeting on Nuclear Reactor Thermalhydraulics, NURETH-14, Toronto, Ontario, Canada, September 25-30, 2011

21. J. PÉREZ M, M. BÖTTCHER, V. SÁNCHEZ, 2011, Validation of NEPTUNE_CFD Two-phase flow models using the OECD/NRC BFBT benchmark database, The 14th International Topical Meeting on Nuclear Reactor Thermalhydraulics, NURETH-14 , Toronto, Ontario, Canada, September 25-30, 2011
22. S. MIMOUNI, F. ARCHAMBEAU, M. BOUCKER, J. LAVIEVILLE, C. MOREL, A second order turbulence model based on a Reynolds stress approach for two-phase boiling flow and application to fuel assembly analysis, Nuclear Engineering and Design, Volume 240, Issue 9, September 2010, Pages 2225-2232
23. S. MIMOUNI, J. LAVIÉVILLE, N. SEILER, P. RUYER, Combined evaluation of second order turbulence model and polydispersion model for two-phase boiling flow and application to fuel assembly analysis, Nuclear Engineering and Design, Volume 241, Issue 11, November 2011, Pages 4523-4536
24. N. MÉRIGOUX, J. LAVIÉVILLE, S. MIMOUNI, M. GUINGO, C. BAUDRY, Reynolds stress turbulence model applied to two-phase pressurized thermal shocks in nuclear power plant, Nuclear Engineering and Design, Volume 299, 1 April 2016, Pages 201-213
25. D. LUCAS, D. BESTION, E. BODÈLE, P. COSTE, M. SCHEUERER, F. D'AURIA, D. MAZZINI, B. SMITH, I. TISELJ, A. MARTIN, D. LAKEHAL, J.-M. SEYNHAEVE, R. KYRKI-RAJAMÄKI, M. ILVONEN, AND J. MACEK, 2009, An Overview of the Pressurized Thermal Shock Issue in the Context of the NURESIM Project, Science and Technology of Nuclear Installations, Volume 2009 (2009), Article ID 583259
26. D. LAKEHAL, 2008a, 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.
27. D. LAKEHAL, 2008b, LEIS for the Prediction of Turbulent Multifluid Flows Applied to Thermal Hydraulics Applications. XFD4NRS, Grenoble, Sep. 10-12, 2008.
28. Y. BARTOSIEWICZ, J.-M LAVIÉVILLE AND J.-M SEYNHAEVE, 2008, "A first Assessment of the NEPTUNE_CFD code: Instabilities in a Stratified Flow, Comparison between the VOF Method and a Two-Field Approach", International Journal of Heat and Fluid Flow, vol. 29, pp. 460-478, 2008.
29. P. COSTE, J. POUVREAU, J. LAVIÉVILLE, M. BOUCKER, 2008 “Status of a two-phase CFD approach to the PTS issue”. XCFD4NRS, Grenoble, France, 10 - 12 September 2008
30. M. SCHEUERER, M.C. GALASSI, P. COSTE, F. D’AURIA, 2007, Numerical simulation of free surface flow with heat and mass transfer, NURETH-12, Pittsburgh, Pennsylvania USA, 30 September-4 October 2007
31. L. ŠTRUBELJ, I. TISELJ, 2008, Numerical simulation of vapour condensation on highly subcooled liquid surface, XCFD4NRS, Experiments and CFD Code Applications to Nuclear Reactor Safety OECD/NEA & IAEA, Grenoble, France, 10 - 12 September 2008
32. P. COSTE, J. LAVIÉVILLE, J. POUVREAU, C. BAUDRY, M. GUINGO, A. DOUCE, 2010, Validation of the large interface method OF NEPTUNE_CFD 1.0.8 for PTS applications, CFD4NRS-3, Washington-DC, sept 2010, to be edited in Nuclear Engineering and Design
33. P. APANASEVICH, D. LUCAS, T. HÖHNE, M. BEYER, 2011, Numerical investigations of thermalhydraulic phenomena during ECC injection, Proceedings of ICONE19, 19th International Conference on Nuclear Engineering, May 16-19, 2011, Chiba, Japan
34. M. SCHEUERER AND J. WEIS, 2010, Transient computational fluid dynamics analysis of Emergency Core Cooling injection at natural circuulation conditions, CFD4NRS-3, Washington-DC, sept 2010
35. M.C. GALASSI, C. MOREL, D. BESTION, J. POUVREAU, F. D’AURIA, 2007, Validation of NEPTUNE CFD Module with Data of a Plunging Water Jet Entering a Free Surface, NURETH-12, Pittsburgh, Pennsylvania USA, 30 September-4 October 2007
36. M. SCHMIDKTE, D. LUCAS, 2008, Simulation of the air entrainment caused by an impinging jet, XCFD4NRS, Grenoble, Sep. 10-12, 2008
37. P. COSTE AND N. MÉRIGOUX, “Two-phase CFD validation: TOPFLOW-PTS steady-state steam-water tests 3-16, 3-17, 3-18, 3-19”, CFD4NRS-5, September 9-11, 2014, Zurich, Switzerland
38. N. MÉRIGOUX, P. APANASEVICH, J.-P. MEHLHOOP, D. LUCAS, C. RAYNAUD, A. BADILLO, CFD codes benchmark on TOPFLOW-PTS experiment, Nuclear Engineering and Design, In Press, Corrected Proof, Available online 5 November 2016
39. N. MÉRIGOUX, J. LAVIÉVILLE, S. MIMOUNI, M. GUINGO, C. BAUDRY, S. BELLET, Verification, validation and application of NEPTUNE_CFD to two-phase Pressurized Thermal Shocks, Nuclear Engineering and Design, Volume 312, February 2017, Pages 74-85
40. A. BADILLO, M. Andreani, An exploratory work on the use of a Lagrangian-Eulerian model for simulating heat transfer of subchannels under reflooding conditions, Nuclear Engineering and Design, In Press, Corrected Proof, Available online 16 December 2016
41. J.M. RICAUD, N. SEILER, G. GUILLARD, Multi-pin ballooning during LOCA transient: A three-dimensional analysis, Nuclear Engineering and Design, Volume 256, March 2013, Pages 45-55
42. TORSTI ALKU, Modelling of turbulent effects in LOCA conditions with CATHARE-3, Nuclear Engineering and Design (2016) in press