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STATUS AND PERSPECTIVE FOR A MULTISCALE APPROACH TO LIGHT WATER REACTOR THERMALHYDRAULIC SIMULATION

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Abstract

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 summarizes the state of the art of each type of code and shows how they could benefit from smaller scale simulation tools. Examples of multi-scale analyses are given and perspectives for future are drawn.

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. At the end of the nineties OECD/CSNI organized several Workshops on Transient Thermal-Hydraulic and Neutronic Codes (Aix en Provence, 1992 [1], Annapolis, 1996 [2], Barcelona, 2000 [3]). The French FASTNET project evaluated the capabilities and limitations of system codes [4], and these reflections were later extended by a community of European experts in the EUROFASTNET [5] project. These projects made a state-of-the-art of the current TH codes, along with a review of industrial needs for the medium term, which allowed experts to identify various ways of progress. One of these new ways of improvement was to develop a multi-scale analysis of thermalhydraulics. After one decade, this state of the art is here updated.

The OECD/NEA/CSNI also 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 [6] for CFD application to the field of Nuclear Reactor Safety (NRS). The second group, WG2, documented the existing assessment databases [7] 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 [8, 9]. 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 is also developed at the European level in the NURESIM (6th Framework program), and NURISP 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 [10] 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 and some guidance is given to evaluate the maturity of each of them.

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.

The multi-scale approach to reactor thermalhydraulics is illustrated in Figure 1 where four types of codes and three successive zooms are shown from the system scale to microscopic tools. The present paper will present what is the status of this approach, how mature it is and what can be expected in the future. 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, summarizes the state of the art for each type of code and shows how they could benefit from smaller scale simulation tools. Examples of multi-scale analyses are given and perspectives for future are drawn. Finally, some recommendations for future R&D are given.

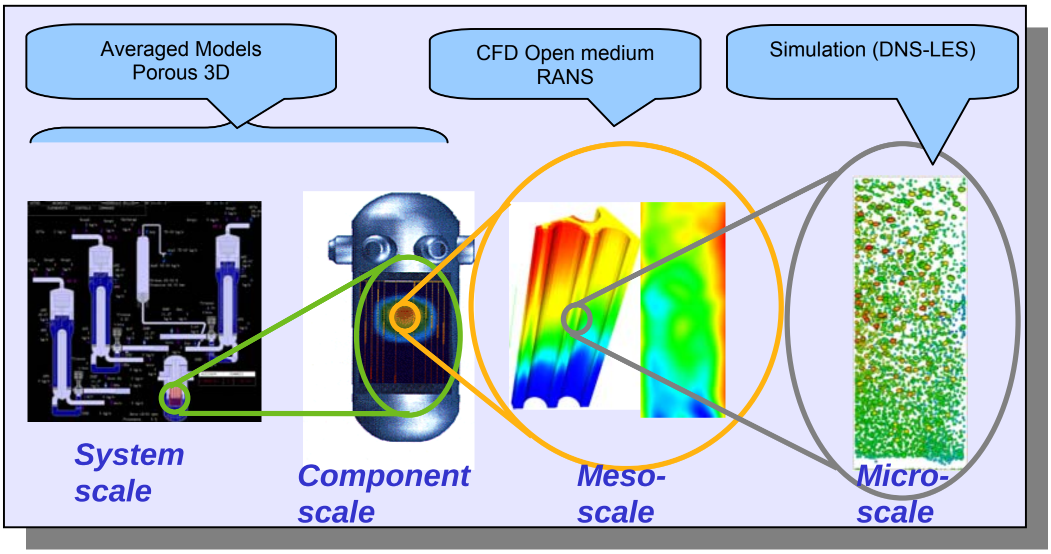

Figure 1: Illustration of the multi-scale analysis of reactor thermalhydraulics

1. The various types of Thermalhydraulic 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 main applications are accidental transient simulations for safety analysis, operation studies and real-time simulators. 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 about 10^3 3D coarse meshes. This allows simulations of all accident scenarios, including Large Break Loss of Coolant Accidents (LBLOCA), Small Break LOCAS, with a reasonable CPU time (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 by the 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 will 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.

The following Table 1 summarizes the main characteristics of the four types of codes.

	System code	**Component code**	**CFD in open medium**	**DNS & pseudo-DNS**
Type of model	0D, 1D, 2D and porous 3D	porous 3D & sub-channel analysis	RANS 3D & LES type	No model in single-phase
Nb of nodes in current applications	Few 100 nodes About 1000 nodes for 3D Pressure Vessel	10^3 to 10^5	10^6 to 10^8	10^6 to 10^8
Applications	Normal reactor operation & all accidental transients	Fuel design (CHF) HX design (steam generator) Some coupled TH-neutonics transients	Mixing problems in 1- phase flow: boron dilution, MSLB, PTS, thermal fatigue, thermal stripping,… PTS, CHF in 2-phase flow	Basic flow processes: turbulent flow in simple geometry, boiling, bubbly flow,…
Computer/run time	Few hours on single processor	Few hours to few days on single processor Few hours on multi-processor	Several days to several weeks on massively parallel computer	Several days to several weeks on massively parallel computer

Table 1: Some characteristics of the four types of codes

Most safety issues and some design issues are simulated by system codes which is by far the most used type of code for nuclear reactor thermalhydraulics by the number of applications and the number of runs per application. Applications most often require sensitivity tests or even a large number of runs to determine code uncertainty. Some design issues and safety issues are treated by component codes: CHF in core, coupled thermalhydraulic-neutronic issues including instabilities in BWR, Reactivity Insertion Accidents. A few safety issues are investigated by single phase CFD in open medium and work is in progress to apply two-phase CFD to a few issues. The trend is to increase the range of applications of the finer resolution tools but this may be a rather long process as will be shown below.

2. The various thermalhydraulic modeling approaches

The identification of the four types of codes has historical reasons although one may identify a larger number of different modeling approaches. An identification of the respective approaches was made by considering five successive choices [10]:

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 [11] by Figure 2. Four 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 2.

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 2, 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 scalef 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 or ensemble 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** (largest scale fluctuations may be simulated in U-RANS & TRANS)
Requirements on dt & mesh size δ	**$\delta < \eta$** **$dt < \eta/u_\eta$**	f : length scale of filter: in inertial subrange of turbulence spectrum **$\delta < f$** **$dt < f/u_f$**	Steady algorithm possible in steady flow **δ & dt** **limited by mesh and time convergence** for mean flow resolution

Table 2: Some characteristics of the three main types of single-phase CFD for open medium

A general classification of Eulerian approaches was proposed by Bestion [10] together with a possible nomenclature.

Following the five choices above, the proposed terminology for Eulerian two-phase approaches uses a series of four groups of characters: M . T . I . n

- **M** characterizes the space averaging or filtering or integration; it can be:
  - **O:** 3D open medium (no space averaging)
  - **P:** 3D porous medium (space filtering)
  - **S2:** space averaged 2D (integrated over one space dimension resulting in a 2-D model)

  - **S1:** space averaged 1D (integrated over two space dimensions resulting in a 1-D model)
  - **S0:** Volume averaged 0D or lumped parameter model (integrated over 3 space dimensions resulting in a 0-D model)

S2 does not apply to 2D models which use some symmetry in a 3D flow to reduce the dimension to 2. It applies for example to a 2D modeling of an annular dowcomer of a reactor vessel when equations are averaged over the radial direction, keeping a 2D problem in vertical and azimuthal directions (Z, θ).

- **T** characterizes the filtering of turbulent scale:
  - **D** for Direct simulation of the whole turbulence spectrum
  - **R** for Reynolds Average approach
  - **F** for filtered turbulence like LES, DES, …
- **I** characterizes the treatment of interfaces:
  - **D** for Deterministic Interface or simulated interface using an Interface Tracking Technique
  - **S** for Statistical treatment of Interfaces
  - **F** for filtered Interfaces: an Interface Tracking or reconstruction Technique is used but it does not predict smaller scale deformations of this interface
  - **FS** for hybrid methods where the larger scale interfaces are known by an Interface Tracking or reconstruction Technique and the smaller scale interfaces are only statistically treated
- **n** is the number of fluids or fields**:**
  - **1** for the classical one-fluid approach, e.g. homogeneous model
  - **2** for the classical two-fluid approach
  - **n** for a n-field model

The application of this terminology to the six CFD approaches (for both open medium an porous medium) is shown in Table 3.

There are three filtered approaches in two-phase CFD 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 (**O.F.D.1**) all interfaces are deterministically treated (or simulated)
- In the LES with statistical interfaces (**O.F.S.i**), no interface is simulated; all interfaces are treated statistically

- In the hybrid method with filtered and statistical interfaces (**O.F.FS.i**) 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).

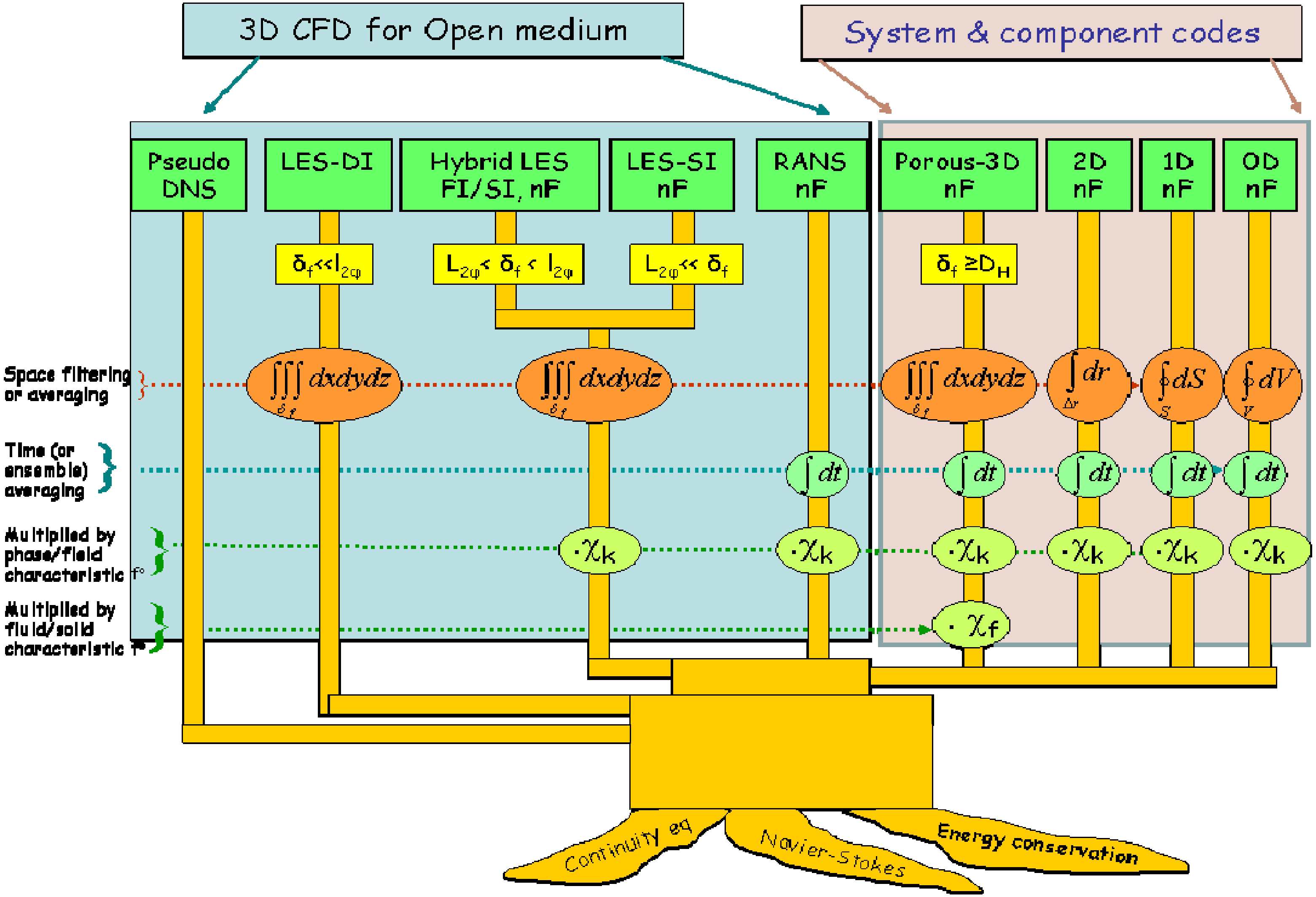

Figure 1: The tree of two-phase thermalhydraulic modeling approaches (taken from [10])

TIME AND SPACE RESOLUTION IN SINGLE-PHASE AND TWO-PHASE CFD							
		Open medium					**Porous medium**
	Time & space filtering	No filter No averaging	Space filtering			Time averaging	Time averaging Space filtering
	Turbulence	DNS	LES - VLES			RANS - URANS	RANS - URANS
Single-phase models		**DNS**	**LES - VLES**			**RANS - URANS**	**Porous medium approach**
	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-F	1-F	1-F 2-F n-F	1-F 2-F n-F	1-F 2-F n-F	1-F 2-F n-F
Two-phase models		**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
Nomenclature		**O.D.D.1**	**O.F.D.1**	**O.F.FS.i i=1,2,n**	**0.F.S.i i=1,2,n**	**O.R.FS.i i=1,2,n**	**P.R.S.i i=1,2,n**

Table 3: Time and space resolution in the various modeling approaches of single-phase and two-phase CFD

3. System codes

Best-estimate system codes play a key role in nuclear safety because of the impracticality of executing full-scale safety related experiments and of the absence of simplified scaling laws for the governing processes which would allow a direct transfer of results from small scale test facilities to the full size plant.

Early attempts in reactor safety analysis based on an “evaluation model” approach including the definition of a limited number of worst case scenarios in combination with conservative modeling assumptions have been replaced by “best-estimate” methodologies. The best-estimate approach aims at providing a detailed realistic description of postulated accident scenarios based on best-available modeling methodologies and numerical solution strategies sufficiently verified against experimental data from differently scaled separate effect test and integral effect test facilities. Best-estimate system codes are commonly used for reactor thermalhydraulic studies. The main system codes which have reached a high quality of predictions with an extensive validation are the US-NRC codes RELAP5 [12] and TRAC, followed by the TRACE code [13], the French code CATHARE-2 [14] (sponsored and developed by CEA, EDF, AREVA and IRSN) followed by CATHARE-3 [15], and the German code ATHLET [16] developed by GRS.

All of these system codes underwent an extended period of development, validation, and verification in the '70s and '80s. Despite some shortcomings and limitations, all of the system codes have attained a high level of maturity, as indicated by their principal capabilities both qualitatively and, in many cases, quantitatively, over a wide spectrum of thermalhydraulic conditions in LWR accident scenarios. However, this improvement has often been the result of a “learning” process involving how to make an optimal choice of code models, code options, and numerical and/or nodalization details. This process is acceptable as long as sufficient experimental data exist to allow the quality of the predictions to be accurately judged. After 30 years of validation and improvements, system codes can predict the main phenomena of most accidental transients of PWR & BWR with reasonable accuracy and produce reliable conclusions on safety issues.

Since the use of best-estimate codes for licensing requires the code uncertainty evaluation, uncertainty methods were developed and evaluated. BEMUSE [17, 18] was an international benchmark sponsored by CSNI in view of assessing uncertainty methods. The phase 3 of BEMUSE consisted in calculating the LOFT-L2.5 Large-Break LOCA test with a base case calculation and an uncertainty band. 8 participants out of 11 found upper and lower bands which envelop the experimental value of the maximum cladding temperature. All main system codes did the exercise and the difference between the base case calculation and the upper bound does not exceed 150K. This figure gives a good idea of the accuracy of this second generation of system codes.

Current system codes use the two-fluid model with algebraic empirical formulations of constitutive laws describing interfacial and wall-to-fluid transfer processes. The acknowledged limitations of these codes, which were identified in the late 90s [1, 2, 3, 4, 5], include a high degree of empiricism and a lack of dynamical modeling of the interfacial area and flow regime transitions. In 3D models, other limitations include the lack of adequate modeling of dispersion terms and of turbulence diffusion, and the use of idealized friction tensors in rod bundles. Both 1-D and 3-D models have limited capabilities for flow regime where a phase is present under the form of separate fields having different dynamic behaviors, such as a liquid film and a droplet field. Further progress may be obtained by additional equations (such as transport equations for interfacial area or for turbulent scales), multi-field modeling, or better spatial and temporal resolutions of 3-D calculations. It was eventually determined that a new generation of codes would be necessary to allow for the best implementation of the new models, including coupling between microscopic and macroscopic models, and coupling of thermal-hydraulics to neutron kinetics, fuel thermo-mechanics, and structure mechanics. This opened the way to the multi-scale approach of reactor thermalhydraulics. These conclusions were at the origin of the NEPTUNE multi-scale thermalhydraulic platform developed and financed by CEA, EDF, AREVA and IRSN in France [19, 20]. A similar multi-scale TH platform is being also developed in Europe in the NURESIM [21] and NURISP projects.

In the past decade some R&D work was performed in the directions defined here above. Attempts to use a dynamic interfacial area modeling instead of an algebraic model were made which still did not allow to improving system code predictions in practical applications. The main reason is that an extensive data base is necessary to obtain validated closure laws for the source and sink terms of the interfacial area transport equation to model coalescence, break up, nucleation and collapse in the whole domain of simulation. It was also found that a coupled dynamic modeling of both turbulence and interfacial area was necessary to better model non-established flow and flow regime transitions [22]. Valuable data were produced in particular by Ishii and Hibiki [23] but in a limited domain of flow regimes, flow parameters and flow geometry. Measurement of both interfacial area and turbulence in the various flow regimes is an extremely difficult task.

The development of multi-field models is more advanced with three field models for continuous gas, continuous liquid and droplets [24]. Such models were first developed in the eighties for BWR core thermalhydraulics and rather reliable closure laws exist for the case of annular-mist flow in adiabatic or heated channels. A replacement of the two-fluid model by this 3-field model could be rather soon available in system codes provided that reliable models (for deposition and entrainment of droplets) exist for other components than the core, i.e. the upper plenum, the horizontal legs...

3.1 The need of smaller scale tools for system simulation

System simulation is necessary for many issues since all components of the LWR are interacting. The simulation of reactor transients including the whole system with a reasonable CPU time authorizes only a modeling with a coarse nodalization. This coarse nodalization is associated with geometry simplifications and also simplifications of the physical behaviour. Small scale phenomena are not predicted and large scale phenomena are predicted with some inaccuracy related to geometry and physical modeling simplifications. Smaller scale simulations may be useful to system codes for two main applications:

1. **Zooming** on some local flow details that are not predicted at system scale. 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

2. **Improving system code model accuracy** by performing small scale simulation which can take into account small scale details of the geometry and small scale flow processes in order to build more accurate system code closure laws for a given application. In this kind of application the small scale simulation may replace experiments.

Examples of the first type of application exist in both single phase and two phase conditions:

- Pressurized thermal Shock in both single phase and two-phase scenarios, which require predictions of fluid and wall temperatures with a fine space resolution
- Thermal fatigue or thermal stripping which require a fine time and space resolution of the temperature
- Local prediction of erosion, corrosion, deposition which depends on small scale flow characteristics

Applications of the second type exist for 1D and 3D models of system codes since an important limitation of the predictive capabilities and of the accuracy is related to geometrical effects. The geometry of the flow channel influences the flow structure but no general modeling of these effects exists while reactor circuits have an extreme variety and complexity of internal geometry. Flow regimes, wall transfers and interfacial transfers are geometry dependent, but flow pattern maps and closure relations were established only for some idealized geometries such as a circular pipe or a rod bundle. Extrapolation to more complex geometries in components like a downcomer, a lower plenum or an upper plenum requires prototypical validation experiments. Flows in geometrical singularities such as bends, abrupt area changes, may cause strong local flow perturbations whose effects require empirical singular pressure drops. CCFL is also likely to occur in complex geometries like a Core Upper Tie Plate, a bend, the inlet nozzle of a Steam generator tube which also requires specific validation experiments. The coarse resolution of system codes does not allow to predicting small scale geometrical effects and one may expect that CFD simulations might replace prototypical experiments for providing the necessary information to model these effects.

Also both 1D and 3D models of system codes apply rough simplifications of balance equations related to the space averaging. In many terms including advection terms and source terms the following simplifications are commonly used:

- The space average of a product is taken equal to the product of the space averaged terms : <u.v> = <u> <v>
- The space average of a non linear function of several principal variables is equal to the of the function of the space averaged variables: <F(Xj)> = F(<Xj>)

Smaller scale simulation tools, which do not use space averaging (or use an average over a smaller space domain) may evaluate the error associated to this simplification and may help to correct some formulation of the non linear terms in the system code.

It is already possible to use single-phase CFD in a RANS approach to predict pressure losses and heat transfer coefficients with an acceptable accuracy of a few percent using High Power Computing. One may expect in future that two-phase CFD will also help system codes to model and predict some two-phase small scale effects such as:

- CCFL in complex geometry
- the enhanced heat transfer due to spacer grids
- the enhanced direct contact condensation due to Safety Injection jet induced turbulence
- effects of averaging of non linear source terms (e;g. interfacial transfers) on the accuracy o the prediction

The sections below on two-phase CFD will give some information on the state of the art in two-phase CFD for such kind of applications.

4. 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: $\phi \cong <\chi_f> = \frac{V_f}{V}$

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

$$<A>_f (x,t) \cong \frac{<\chi_f A>}{<\chi_f>} = \frac{1}{V_f(x)} \int_{V(x)} A\chi_f dV$$

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

$$A \cong <A>_f + \delta A$$

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:

$$<\chi_f \rho u_i \frac{\partial u_i}{\partial x_j}>_f = \rho \frac{\partial}{\partial x_j}\left[\phi <u_i>_f <u_j>_f\right] + \rho \frac{\partial}{\partial x_j}\left[\phi <\delta u_i \delta u_j>_f\right]$$

$$<\chi_f \frac{\partial \rho u_i H}{\partial x_j}>_f = \frac{\partial}{\partial x_j}\left[\phi\rho <u_i>_f <H>_f\right] + \frac{\partial}{\partial x_j}\left[\phi\rho <\delta u_i \delta H>_f\right]$$

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.

Recent calculations of the BFBT and PSBT benchmarks in prototypical BWR and PWR rod bundles showed reasonable agreement with experiments of both component and system codes with some difficulties to predict radial transfers of void fraction.

3-D modules exist as an option in the codes TRACE, CATHARE and RELAP 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) are applied and consequently the advantage of a 3-dimensional modeling of the flow processes might be offset to a certain extent. However, large scale 3D effects can be better modeled than with 1D model [25].

4.1 The need of smaller scale simulation tools for core models and sub-channel analysis

Local measurements of flow parameters are very difficult in the complex geometry of a fuel assembly and CFD may bring information on details of the flow which may help modeling for sub-channel analysis codes:

- Model wall friction and heat transfer coefficients in the rod bundle
- Form losses and the enhanced heat transfer due to spacer grids
- Evaluation and modeling dispersion terms and turbulent diffusion terms in the rod bundle

The latter may be particularly important to predict mixing in the core in boron dilution transients and in case of Steam Line Break when investigating reactivity insertion or possible core re-criticality. It is also useful to DNB investigations and for all situations with radial transfers in a core. Evaluation and modeling of such dispersion terms and turbulent diffusion terms is in progress [26, 27, 28, 29].

4.2 The need of smaller scale tools for Pressure vessel

Pressure Vessels include various components (lower plenum, core, annular donwcomer, upper plenum, upper head), which have very different geometrical characteristics (porosity, hydraulic diameter,…). Specific closure laws may be necessary for each component to take into account the specific geometrical effects of each component and CFD may simulate flow at the required scale to provide information in complement to existing experimental data.

5. CFD in open medium

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 [6] for CFD application to the field of Nuclear Reactor Safety (NRS). The second group, WG2, documented the existing assessment databases [7] 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 third group worked for several years on these projects (2003-2009) and produced two reports [8, 9]. The content of these two reports was summarized by Bestion [30] and the whole CFD activities were summarized by Smith et al. [31].

5.1 Single phase CFD

Single phase CFD is currently used for many LWR thermalhydaulic investigations such as:

- Boron dilution transients;
- Steam Line Break with mixing of hot and cold water
- Pressurized thermal shock;
- Breaks induced by high temperature steam during a severe accident;
- Thermal fatigue in a mixing tee [32] ;
- Hydrogen distribution in a containment during a severe accident;
- Flows induced by hydrogen recombiners in containments
- Turbulent flows in various rod bundle geometries;
- Flow mixing and stratification in plant loops;
- Natural circulation in pools;
- Fluid/structure interactions
- Cooling issues associated with spent fuel storage casks

CFD codes offer many physical model options and many numerical options but a limited validation relevant for each specific application. Therefore it was necessary to elaborate Best Practice Guidelines (BPG) and to review the existing Assessment bases for application to reactor safety.

The BPG addressed the following questions:

Selecting an Appropriate Simulation Tool
Selecting Physical Models

- Selection of Turbulence Models: RANS, LES
- Buoyancy Model
- Heat Transfer

Verification of Numerical Model

- Grid Requirements
- Discretisation Schemes: Space, Time
- Convergence Control
- Target Variables
- Iteration Error
- Discretisation Error

Validation of Results

- Validation Methodology
- Target Variables and Metrics
- Sensitivity to Parameter Variations
- Treatment of Experimental Uncertainties

Looking at existing applications it is still very difficult to follow all BPG for a real reactor application. In particular the control of convergence of the space discretization scheme requires such fine nodalization that the CPU time may become prohibitive. In some cases it is possible to estimate how far is a target variable from the converged solution by extrapolation from several non-converged calculations using the old Richardson method. However this remains a difficulty but continuous progress of computer efficiency will increase the accuracy of 1-phase CFD applications and will allow to extending the domain of application.

Many International Standard Problems (ISP) were organized for system codes but only very few benchmarks addressed CFD validation such as ISP 42 on containment, ISP 43 on boron dilution UMCP tests, ISP 47 on Containment Thermal Hydraulics tests performed in TOSQAN, MISTRA, and ThAI facilities. These complex tests are necessary to evaluate the maturity of tools and of CFD users and finally to give confidence in their application to safety. More simple benchmark tests using CFD-grade experimental data such as the T-Junction Exercise [32] are also useful to validate the physical modeling in good conditions. Again the WGAMA group of OECD/NEA/CSNI intends to organize successive exercises and the next will address flow in rod bundle.

Single phase CFD have already proven its interest in some LWR issues but a continuing effort is required for extending the assessment base, for making BPG more precise and to develop uncertainty methodologies.

5.2 Evaluation of the required nodalization for CFD of a reactor core

A very rough evaluation of the number of meshes required to calculate a single-phase flow in a core with CFD for open medium may be done.

Let's consider a 3 loop 900 MWe PWR with 157 assemblies (17X17 rods) close to nominal conditions with P = 15.5 MPa and V = 5.4 m/s

One can estimate the viscous dissipation and then calculate the Kolmogorov scale $\eta \approx 12\mu m$. Then a DNS should have a maximum node size of about 12 μm.

The macroscale l of turbulence is estimated at 2mm. The filter scale f of a LES should be significantly smaller than l and greater than η. Let's say $f \approx 100$ μm.

Classical RANS simulations in a channel may be close to the converged solution with about 25 meshes in a hydraulic diameter. The average mesh will then be taken equal to $\delta \approx 500$ μm

One evaluates the approximate number of meshes required for calculating, the whole core, an assembly, a single sub-channel and a cubic centimeter. Results are given in the table 4. Evaluations are made by considering cubic meshes.

Present HPC capabilities allow simulations with 10^7 to 10^8 meshes. Even if the estimations in table 4 are not very precise on can draw some clear conclusions:

- DNS which is the only simulation without any model is restricted today to a small volume, less than a cubic centimeter of a typical single phase flow in a core.

- LES cannot be applied today to an assembly but only to a sub-channel or to part of a few sub-channels

- Even The RANS approach cannot be applied to the whole core but can already (or in near future) simulate a full assembly

Method	Mesh size	1 cm^3	1 sub-channel 310 cm^3	1 assembly 0.09 m^3	Whole core 14.1 m^3
DNS	η = 12μm	578 10^6	179 10^9	51 10^{12}	8.1 10^{15}
LES	f = 100 μm	1 10^6	310 10^6	90 10^9	14 10^{12}
RANS	δ = 500 μm	8 10^3	2.5 10^6	720 10^6	113 10^9

Table 4: Rough estimation of the required number of meshes for simulation of core or part of a core using DNS, LES or RANS in single phase flow close to nominal conditions

These estimations show that even with the rapid progress of computer power, CFD in open medium cannot replace porous 3-D approaches and demonstrate the interest of the zoom approach where the fine scale simulation is applied only to a reduced domain whereas a more macroscopic simulation covers the whole domain.

5.3 Two-phase CFD

Extending CFD codes to two-phase flow allows for safety investigations to get some access to smaller scale flow processes that are not seen by system codes. Using such tools as part of a safety demonstration may bring a better understanding of physical situations, which would result in more confidence in one's results, and a better estimation of safety margins. However, the two-phase flow models are not as mature as those in single phase CFD and a lot of work needs to be done on the physical modeling and numerical schemes in such two-phase CFD tools.

The WG3 first identified and classified the Nuclear Reactor Safety (NRS) problems [8, 9], where extending CFD to two-phase flow may bring a real benefit and also classified the different modeling approaches. A list of 26 NRS problems (see table 5) where two-phase CFD may bring real benefit has been established. These issues have been analyzed and classified with respect to the degree of maturity of present tools for solving them in a short or medium term. Then the activity was focused on a limited number of issues. Only modeling of two-phase flow configurations pertinent to NRS problems are considered.

Some NRS problems require 2-phase CFD in open medium, other require 2-phase CFD in porous medium, and for some problems investigations with a 2-phase CFD tool for open medium may be used for a better understanding of flow phenomena and for developing closure relations of a 3D model for porous medium.

	NRS problem	**Open medium Porous medium**
1	DNB, dryout and CHF investigations	O; O $\Rightarrow$ P
2	Subcooled boiling	O; O $\Rightarrow$ P
3	Two-phase pressurized thermal shock	O
4	Thermal fatigue in stratified flows	O
5	Direct contact condensation: steam discharge in a pool	O
6	Pool heat exchangers: thermal stratification and mixing problems	O; P
7	Corrosion Erosion deposition	O
8	Containment thermal-hydraulics	O
9	Two-phase flow in valves, safety valves	O
10	ECC bypass and downcomer penetration during refill	O ; O $\Rightarrow$ P
11	Two phase flow features in BWR cores	P; O $\Rightarrow$ P
12	Atmospheric transport of aerosols outside containment	O
13	DBA reflooding	P ; O $\Rightarrow$ P
14	Reflooding of a debris bed	P; O $\Rightarrow$ P
15	Steam generator tube vibration	O $\Rightarrow$ P
16	Upper plenum injection	P
17	Local 3-D effects in singular geometries	O
18	Phase distribution in inlet and outlet headers of steam generators	O; O $\Rightarrow$ P
19	Condensation induced waterhammer	O
20	Components with complex geometry	O $\Rightarrow$ P
21	Pipe Flow with Cavitation	O
22	External reactor pressure vessel cooling	O
23	Behaviour of gas-liquid interfaces	O
24	Two-phase pump behaviour	O
25	Pipe Break-In vessel mechanical load	O; P
26	Specific features in Passive reactors	O

Table 5: Identification and classification of Two-phase NRS issues that may benefit from investigations at the CFD scale

A general multi-step methodology was proposed [8, 9], including a preliminary identification of flow processes, a model selection, and a Validation and Verification process. Then, only 6 NRS problems where two-phase CFD may bring real benefits were selected to be analyzed in more detail. These problems were the Dry-out, the Departure from Nucleate Boiling (DNB), Pressurised Thermal Shock (PTS), pool heat exchanger, steam discharge in a pool, and fire events. These are issues where some investigations are currently ongoing and their CFD investigations have a reasonable chance to be successful in a reasonable period of time. These investigations address all flow regimes so that they may, to some extent, envelop many other issues. The general multi-step methodology was applied to each issue to identify the gaps in the existing approaches. Basic processes were identified. Modeling options were discussed, including closure relations for interfacial transfers, turbulent transfers, and wall transfers. Available data for validation were reviewed and the need for additional data was identified. Verification tests were also identified.

From this analysis one could identify the range of application and the degree of maturity of each modeling approach with respect to the well known two-phase flow regimes (see table 6).

	Pseudo-DNS	**LES Simulated interfaces**	**LES Statistical & filtered interfaces**	**LES Statistical interfaces**	**RANS-URANS Statistical & filtered interfaces**
	O.D.D.1	**O.F.D.1**	**O.F.FS.i**	**O.F.S.i**	**O.R.FS.i**
Bubbly	Applied	Applied	Applied	Applied	Applied
Slug-Churn	Possible Too expensive	Possible Too expensive	Possible	Not possible	possible
Annular	Possible Expensive	Possible Expensive	Possible	Not possible	Applied
Annular-mist	Possible Too expensive	Possible Too expensive	Possible	Not possible	possible
Mist flow	Applied	Applied	Applied	Applied	Applied
Stratified	Applied	Applied	Applied	Not possible	Applied
Stratified-mist	Possible Too expensive	Possible Too expensive	Possible	Not possible	Possible
All flow regimes	**Too expensive**	**Too expensive**	**Possible**	**Not possible**	**Possible**
Degree of maturity	**Average in some flow regimes Zero for "all flow regimes"**	**Average in some flow regimes Zero for "all flow regimes"**	**Average in some flow regimes Very low for "all flow regimes"**	**Average in dispersed flow**	**Average in some flow regimes Low for "all flow regimes"**

Applied: is applicable and has been applied *Not possible: cannot be applied due to intrinsic limitations*
Possible: can be applied but not very mature *Expensive: requires a very high CPU time*
Too expensive: unaffordable with current computer power

Table 6: Applicability and degree of maturity of the various two-phase CFD approaches to every flow regime including CPU cost

The applicability of all methods is satisfactory for dispersed bubbly and droplet flows and some methods can address also separate-phase flow (annular flow, stratified flow), but the situation is not so clear for complex flow regimes such as slug-churn flows, annular-mist flow, or stratified-mist flow. Only RANS and LES with Statistical and filtered interfaces can in principle simulate two-phase flow in the whole range of flow regimes in an affordable CPU time. However the LES approach has still a very low maturity and the RANS approach, due to the time averaging, is not able to see the large scale intermittency in slug-churn flow and the large waves in separate-phase flow.

Although the two-phase CFD is still not very mature, some first Best Practice Guidelines (BPG) were created which should be complemented and updated in the future. The proposed multi-step methodology allows for a first set of Best Practice Guidelines to be implemented for two-phase CFD by inviting users to formulate and justify all their choices and by listing some necessary consistency checks. Some methods for controlling the numerical errors were also given as a part of the BPG.

Although there is an increasing activity in two-phase thermalhydraulics, one can observe that many applications suffer from three weaknesses:

1. Many 2-phase CFD applications have not a well defined modeling approach
2. Many 2-phase CFD applications use incomplete models
3. Some 2-phase CFD applications use a non-consistent modeling approach

The first weakness is the reason why we have tried to classify the various modeling approaches. All approaches use transport equations for mass momentum and energy but the formulation of source terms depends strongly on the space and time resolution, on the number of fields that are modeled and on the treatment of interfaces. Two-phase CFD tools offer many options for Interface Tracking, for Interface Recognition, for interface sharpening, and many options for wall transfers, interfacial transfers and turbulence models. The choice between all these options can only be made after having clearly identified the modeling approach. After this identification of the modeling approach one can clearly identify the list of flow processes which have to be modeled by closure relations. Many 2-phase CFD applications use incomplete models because they did not identify the modeling approach. In particular, when a Large Interface is treated by a method which filters the small scale waves and interface deformations (O.F.FS.i, or O.R.FS.i), one must develop models to evaluate the characteristics of these small scale waves and interface deformations and one must model their effects. Taking into account effects of the free surface waves which are not simulated by the model may be of prime importance to predict the interfacial transfers. Also it appears that many combinations of model options are not consistent and only a few choices are producing “consistent approaches”. Examples were given of common errors [10]. They come very often from non-consistent choices for turbulence and for interface treatment or from use of closure laws from one approach in another approach. Examples are:

- Use of a 1D closure law in 3-D CFD approaches
- Use of interfacial transfers and wall transfers of porous medium CFD in a open medium CFD
- Use a 3D two-fluid model without any turbulence modeling

- Use of RANS-Two-fluid interfacial transfer coefficients in a pseudo DNS or LES approach

In order to avoid such non-consistencies, a checklist was proposed to apply a rigorous methodology when developing a two-phase CFD application [10].

5.4 Evaluation of the required nodalization for two-phase CFD of a reactor core

Following the rough evaluation of the number of meshes required to calculate flow in a core made for single phase flow one considers now the four modeling approaches which can in principle be applied to all flow regimes that may be found in a boiling flow in a core.

The RANS approach (O.R.FS.i) should require the same type of nodalization as in single phase case. The LES with filtered and statistical interfaces (O.F.FS.i) should have similar mesh requirements as single-phase LES. Pseudo-DNS (O.D.D.1) should in principle track all interfaces including the smallest bubbles and smallest drops in an annular-mist flow. There is no lower limit for these drop and bubble size but one will consider only sizes larger than 10 μm. This is the order of magnitude of nuclei attached to the wall and most droplets in annular-mist flow are larger than 10 μm. However a special treatment should be added to simulate bubble collapse (up to diameter zero) when there is condensation and droplet collapse by vaporization. Most Interface Tracking Methods require node size not greater that 1/10 of the drop or bubble size. Therefore one will estimate the required nodalization for pseudo-DNS by using a 1 μm node size. One can also consider an LES with simulated interfaces (O.F.D.1) which considers only droplets larger than 100 μm and bubbles larger than the bubble departure diameter (which is probably > 100 μm). Therefore one will estimate the required nodalization for O.F.D.1 using a 10 μm node size.

Method	Mesh size	1 cm^3	1 sub-channel 310 cm^3	1 assembly 0.09 m^3	Whole core 14.1 m^3
Pseudo-DNS	η = 1μm	$1\ 10^{12}$	$310\ 10^{12}$	$90\ 10^{15}$	$14\ 10^{18}$
O.F.D.1	η = 10μm	$1\ 10^{9}$	$310\ 10^{9}$	$90\ 10^{12}$	$14\ 10^{15}$
0.F.FS.i	f = 100 μm	$1\ 10^{6}$	$310\ 10^{6}$	$90\ 10^{9}$	$14\ 10^{12}$
RANS	δ = 500 μm	$8\ 10^{3}$	$2.5\ 10^{6}$	$720\ 10^{6}$	$113\ 10^{9}$

Table 7: Rough estimation of the required number of meshes for simulation of core or part of a core using two-phase CFD in boiling flow conditions

One can draw some clear conclusions:

- No simulation tool using exact equations without any empirical model exist in two-phase flow
- The two microscopic approaches (Pseudo-DNS and O.F.D.1 are very far from being applicable to practical reactor simulations even for a single sub-channel
- LES (0.F.FS.i) cannot be applied today to an assembly but only to a sub-channel or to part of a few sub-channels

- Even the RANS approach cannot be applied to the whole core but can already (or in near future) simulate a full assembly

6. Multi-scale analysis and multi-scale simulation

Two main kind of multi-scale approaches 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

7. Examples of multi-scale analyses

7.1 Boiling flow and CFH analysis

Bubbly flow and boiling bubbly flow were extensively studied in the frame of the NEPTUNE-CFD project [19, 20] and in the European project NURESIM [21, 33] and NURISP [34, 35]. The general methodology defined in [8, 9, 10] was applied with a selection of modeling options and by collecting an appropriate database [36, 37].

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 Local Predictive Approach (LPA) presented by Haynes et al. [38]. 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.

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.
- **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. When a reliable local DNB criterion will be available, the Local Predictive Approach will be applicable.
- **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 “Local Predictive Approach” 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. 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 [39 to 47] 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 [48] on 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 satisfactory.
- Despite this lack of accuracy, the CFD simulations may already be used for parametric studies as a tool to help fuel design and to reduce the need of experiments.

7.2 Two-phase PTS investigations

Two-phase PTS scenarios are studied in the frame of the NEPTUNE-CFD project [19, 20] and in the European project NURESIM [21, 33] and NURISP [34, 35]. The general methodology defined in [8, 9, 10] was applied with a selection of modeling options and by collecting an appropriate database [49]. 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 3: 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.

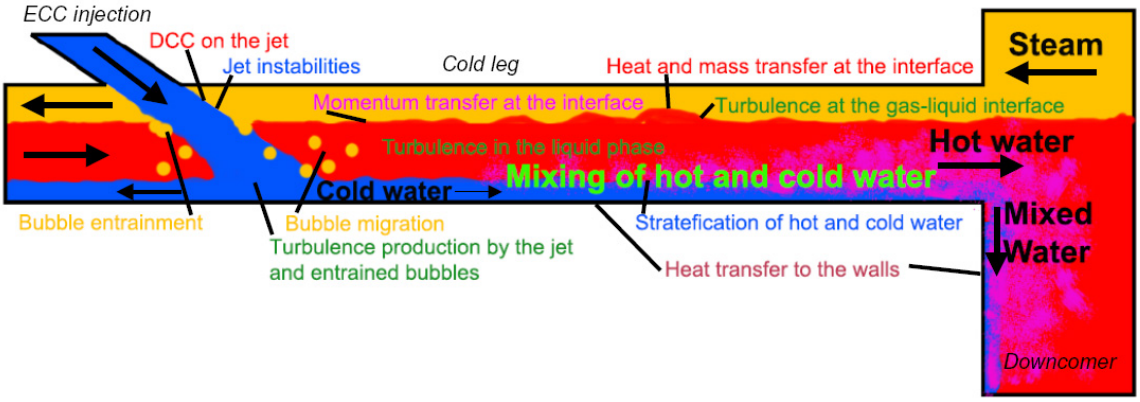

Figure 3: The two-phase PTS scenario and the associated basic phenomena

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 (O.D.D.1) and LES with simulated interface (O.F.D.1) were used for condensing stratified flow by Lakehal [50, 51]. These simulations could be used to derive interfacial transfers for the RANS approach.
- LES with filtered interface (O.F.FS.1) is validated against adiabatic and condensing stratified flow.
- URANS with filtered interface (O.R.FS.i) [52 to 57] is also validated against adiabatic and condensing stratified flow.
- URANS with a 1-fluid model (O.R.FS.1) is benchmarked against URANS with the 2-fluid model (O.R.FS.2) associated with an Interface recognition technique
- The coupling of system code and CFD is tested on the ROSA IV LSTF test [58]

Plunging jet effects are also investigated at the RANS scale [59, 60]

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

- URANS with filtered interface (O.R.FS.i) can simulate the two-phase flow in a reactor cold leg with ECCS injection and in the downcomer
- LES with filtered interface (O.F.FS.1) 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 (O.R.FS.1 and O.R.FS.2) 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.
- As was shown by simulations made at both 1-D system scale and 3-D CFD scale of COSI tests, CFD cannot yet predict averaged fluid temperature better than 1-D model and cannot yet be used as a reference tool for system codes. However CFD can predict the local temperature field which cannot be predicted at system scale.

7.3 Revisiting some LOCA issues with a multi-scale approach

In the NURISP project [35], some LOCA issues such as Reflooding, core radial power profile effects, or Condensation induced waterhammer, and flashing in choked flow are 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.
- An **Eulerian-Eulerian two-phase CFD-RANS** approach (**O.R.S.2**) 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 (P.R.S.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 (S1.R.S.2) and 1-D 3-field models (S1.R.S.3) of CATHARE-3
- The porous 3-D model of CATHARE-3 (P.R.S.2 and P.R.S.3)
- The CFD RANS in open medium (O.R.S.2)

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

Condensation induced waterhammer may occur during a safety injection in a horizontal leg and this is a very unstable process which is a difficult challenge for codes. Within NURESIM and NURISP both the CFD-URANS and the 1D approaches were used and are still being used [61, 62, 63, 64].

Flashing in choked flow controls critical flow and the prediction of break flow by system codes depends on the modeling of flashing. Flashing was first modeled in 1D 2-fluid models of CATHARE-2. It is now revisited with a new model [65]. Then CFD modeling of flashing flow may help in understanding how 3D or 2D effects can taken into account in 1D to improve break flow prediction.

8. Perspectives for future multi-scale thermalhydraulics

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.

The computer power increases approximately by a factor 100 per decade. This is true for single processor computers as well as for massively parallel High Power Computing (HPC). Considering the solution methods of 3-D thermalhydraulic equations, an increase by a factor 100 of the computer power allows an increase by about a factor 15 on the number of meshes and a decrease of the mesh size by about a factor 2.5 only per decade.

As shown in section 5.4, a rough estimation of the required number of meshes to simulate a single core sub-channel thermalhydraulics in a typical boiling situation with a pseudo-DNS approach is about 10^{14}. This corresponds to approximately 10^{19} meshes for the whole core.

A similar estimation for a two-phase CFD for open medium approach using a RANS model gives approximately 10^{6} meshes for a single core sub-channel and 10^{11} meshes for the whole core. This shows that 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.

A system code user who simulates a typical accidental transient using a coarse 3-D Pressure Vessel modeling (e.g. 1000 meshes) with a single processor computer needs a few CPU hours in 2010. This coarse nodalization corresponds to an average mesh size of about 0.4 m. The same simulation in 2030 with a single processor computer using the same CPU time would allow a mesh refinement to about 6 cm. This simple estimation shows that the impressive progress of computer power will not allow to skip from a porous body approach to a CFD for open medium for current applications in the coming few decades. Moreover, the use of system codes for safety requires a Best-Estimate Plus Uncertainty (BEPU) approach. In the most widely used BEPU method, a Monte-Carlo type technique requires a rather large number of calculations of the same transient with every uncertain parameter being randomly changed according to predetermined probability density functions. Therefore the increasing computer power may be first used to multiply the number of calculations before reducing the mesh size.

A typical current application of a component code uses 10^{4} to 10^{6} meshes for a core with a porous body approach or in the context of a sub-channel analysis. In case of a sub-channel analysis, only a few sub-channels or a single fuel assembly is modeled. A modeling of the whole core with a porous body approach does not allow a converged meshing. Most applications combine a rather coarse nodalization of the core with a finer nodalization in a part of the core where attention is focused. The evolution in the next two decades will allow a better space resolution of the porous body approach or a more extended use of the sub-channel modeling.

Single phase CFD application to some reactor issues is in progress mainly with RANS and URANS approaches which require a more reasonable CPU time than LES or VLES approaches. However, looking at the past international benchmarks, it is clear that the high CPU cost remains the main difficulty to obtain a reliable simulation with a converged meshing. The strict application of Best Practice Guidelines is difficult when Validation experiments are simulated and is even more critical for any reactor application. Therefore, one may expect that the increasing computer power of the next decades will be used first to get converged meshing before extending the domain of application of CFD. The same conclusion applies to the few two-phase CFD applications.

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.

9. Conclusion and Recommendations

Reactor thermalhydraulics will use several simulation tools from system codes to several kinds of CFD models to solve all design and safety issues. Although computer power increases rapidly the market share of CFD application in reactor thermalhydraulics 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.

BPG and assessment bases already exist for some single phase reactor issues that require CFD and they should be complemented in future.

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.

In two-phase conditions, no "pure numerical experiment" is possible since all modeling approaches need some validation and specific experimental programs with advanced measurement techniques will be necessary. The effort to further develop new local measurements techniques is mandatory to obtain reliable and validated physical models for the various CFD approaches.

Two-phase CFD is much 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.

In the present state of the art, two-phase CFD is not yet accurate enough to make better predictions of macroscopic quantities than system codes but it can already predict small scale phenomena that system codes will never predict.

More effort should be spent in future to develop and apply the methods to derive averaged information from microscopic simulations (DNS, pseudo-DNS, LES) in view of developing closure laws for averaged models.

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.

Although the reduction of system code uncertainty will be also a slow process, the use of CFD tools in multi-scale analyses is a good way to attract new people to reactor thermalhydraulics and to keep the necessary expertise in reactor safety.

The multi-scale approach requires high level experts in each domain from DNS tools to system codes. Its success also depends on the links between all these experts and on the emergence of a new expertise in "multi-scale analysis" able to create the required synergy. R&D at the micro-scale and meso-scale should be directed to the end users which are very often system and component codes.

The credibility of the CFD seen by the safety evaluators has to be reinforced by giving even more precise BPGs, by developing even more specific Validation and Verification plans, and by organizing international benchmarks.

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