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CATHARE-3 V2.1: THE NEW INDUSTRIAL VERSION OF THE CATHARE CODE

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ABSTRACT

CATHARE-3 is the new version of the French thermal-hydraulic code for the safety analysis of nuclear reactors; its development has begun in 2006 as part of the NEPTUNE project launched by the CEA, EDF, AREVA-NP and IRSN in 2001. The first industrial version of the code V2.1 was delivered in December 2019, in the continuity of the reference version CATHARE-2. This article presents the main new features of the code: the 3-fields modelling capabilities, the predictive pump model; the Multi-fluid and multi-reactor modelling tools and the improved 3D modelling capabilities. The software architecture of the code, with the challenges link to code coupling and parallelism is also presented. This article shows the planned development for the next few years.

1. INTRODUCTION

In 1979, CEA, EDF and FRAMATOME launched the CATHARE project. The goal to the CATHARE project is to develop a best-estimate thermal-hydraulic code for safety analysis of nuclear reactors. In 1987, CATHARE-1 V1.3L was the first CATHARE version validated for small break Loss of Coolant Accident (LOCA). In 1996, CATHARE-2 V1.3L became the first CATHARE version qualified for safety studies (including large break LOCA). In December 2003, CATHARE-2 V2.5 was implemented in real time plant simulators.

CATHARE-3 is the new version of the CATHARE code. Its development has begun in 2006 as part of the NEPTUNE project launched by the CEA, EDF, FRAMATOME and IRSN in 2001 [1]. An initial roadmap for CATHARE-3 was presented in 2009 [2]; an evaluation version V1.0 was delivered in 2012 and a validated version V2.0 was delivered in 2016.

The first industrial version of the code validated for the Pressurized Water Reactors (PWRs), and partially validated for sodium applications, V2.1, was delivered in December 2019, in the continuity of the reference multi-concept CATHARE-2 [3]. This article first shows the current status of the CATHARE-3 code and the main new features of this industrial version. Then, the planned developments are presented.

2. CURRENT STATUS AND MAIN NEW FEATURES

In this part, the current status of the code is first presented, then, the main new features of the code are described, related to new needs for the PWR safety analysis and for reactor designs:
- The 3 fields modelling capabilities,
- The predictive pump model,
- The Multi-fluid and multi-reactor modelling tools,

- The 3D modelling capabilities

2.1. Current status: Continuity with CATHARE-2 Code

CATHARE-2 is the current industrial version of the CATHARE code; it is mainly use to safety analysis [3] and into real-time simulator of nuclear power plant [4]. The main goal of CATHARE-3 code is to be the successor of CATHARE-2 and to be a modular tool that can evolve. To perform this objective, a new language have been chosen for CATHARE-3 with a rigorous plan to ensure non-regression between CATHARE-2 and CATHARE-3.

2.1.1. A new coding language

CATHARE-2 benefits from an object-oriented conception, but its implementation is in FORTRAN so that many features of modern object-oriented languages (memory management, polymorphism, and encapsulation) are simulated. The code is therefore not as extensible, readable or maintainable as it could be with a true object-oriented language. Another important limitation of CATHARE-2 architecture relies in the fact that it is composed of two executables:
- A reader that reads the data file, do some preprocessing and writes a "memory image input file" and a FORTRAN file describing the transient to be simulated.
- A calculation executable obtained by linking the previously generated FORTRAN subroutine with CATHARE's library. This executable reads the "memory image input file" and runs the simulation.

It has been decided to develop switch language with CATHARE-3 and to have a C++ code. This C++ architecture have been obtained with the following process:
- From 2006 to April 2019, the development of CATHARE-3 was made in FORTRAN, starting with CATHARE-2 code and adding new features. In 2012, the merge of the reader and the calculation code was achieved and a 'python' translator of the input deck (needed as CATHARE-3 input decks are slightly different from CATHARE-2 due to the suppression of the reader) was written.
- From 2012 to April 2019, a FORTRAN to C++ translator was developed, including optimizations of the code, ensuring a binary non-regression between the FORTRAN and C++ results at each version of CATHARE-3.
- Since April 2019, new developments of CATHARE-3 are written in C++.

The main advantage of this progress is that it make possible to perform daily non-regression tests between the current development version of CATHARE-3 and the current industrial version of the CATHARE code: CATHARE-2 V2.5.

2.1.2. Non-Regression between CATHARE-2 and CATHARE-3

As explain in the previous part, non-regression tests are daily perform between CATHARE-3 and CATHARE-2. For the V2.1 version of CATHARE-3, more than 2000 tests are perform, including more than one hundred Integral Effect Tests (IET) and Separate Effect Tests (SET) from the CATHARE-2 validation matrix. Industrial tests are also included in non-regression tests. They confirm that the two-fluid 6-equation model of CATHARE-3 is reliable, as most of the results superimpose with those of the CATHARE-2. These tests are included in Non-Regression reports delivered with the code.
CATHARE-3 is already used for safety studies in the framework of the ASTRID project [32] [39] .

2.2. Three-Field Model

For flow conditions where both droplets and liquid film are present, the two-fluid model of CATHARE uses a correlation for the entrainment fraction, i.e. the ratio of the droplet flowrate to the total liquid flowrate, on the Steen-Wallis model. This model has some limitations, for example in annular-mist flow, because it cannot take into account the different behavior of the droplets and the liquid film on the wall, which may have very different velocities including counter-current velocities. This is also the case for stratified-mist flows encountered in hot legs, or for the estimation of the de-entrainment phenomenon in the upper plenum due to the drops impinging the structures. In such cases, a 3three-field model in which the

liquid phase is split into a continuous field (film) and a dispersed field (droplets), each having its own volume fraction, velocity and temperature seems more likely to simulate the behavior of the flows.

A three-field model is being developed in CATHARE-3, based on an extension of the two-fluid model. Three sets of mass, momentum and energy conservation equations are solved for the three fields: the gas or vapor, the continuous liquid, and the dispersed liquid flowing in the form of entrained droplets. This model has been first developed and assessed for vertical two-phase flows especially for dryout prediction. Specific correlations for the entrainment, deposition and for the estimation of the droplet size have been developed or introduced during the 2000' and validated against several experiments in tubes (e.g Wurtz, Bennett) [7] and rod-bundles (e.g. THTF, BFBT) [8]. More recently, models of entrainment and deposition due to Okawa have been developed in the code, and models of the initial entrained fraction, i.e. the entrainment at the onset of annular two-phase flow, which has a significant impact on the prediction of the dryout, have been assessed against experiments, such as pre-dryout tests performed at KTH, completing the validation matrix for this application of the three-field model [9].

The architecture of the code allows to select the three-field model in some elements of the circuit, and to keep the calculation of the flow with the 6-equation model where the droplet are not present. This is the case for example for LBLOCA application, where the calculation of the BETHSY 6.7c integral test, simulating the refilling and reflooding phases of this type of accident, has been performed using both the 3-field and the 6-equation models [10]. The three-field model is used to simulate the production of small droplets in the core at the quench front during the reflooding phase of such transients, and the liquid carryover by a strong steam flow towards the upper plenum, the hot legs and the steam generators. These phenomena, including the vaporization of the droplets in the steam generators creates the "steam binding" effect, influencing the reflooding rate. Specific models of droplet entrainment and deposition in the core, adapted to the reflooding phase conditions (namely inverted annular flow downstream the quench front, low pressure) are been developed in CATHARE-3, and validated against PERICLES and RBHT reflooding tests. ROSCO oscillating reflooding tests are also part of the validation matrix. For these tests, the three-field model better predicts, with respect to the 6-equation model, the top-down quenching where falling films and upward drop flow coexist in the upper part of the core. For the de-entrainment phenomenon in the upper plenum, SEROPS 2 experiments, devoted to study the droplets behavior in this part of the vessel, have been used to develop simple correlations in the CATHARE-3 3D module, taking into account the impact of droplets onto the upper plenum structures and the deposition of the droplets due the gravity. In the last years, one-dimensional models have been introduced in CATHARE-3 for the entrainment and deposition of the droplets in the hot legs, including both stratified and annular flow regimes. These models have been developed and validated using air-water experiments performed in large diameter horizontal pipes, including REGARD and Williams databases [11]. The deposition model takes into account the two mechanisms acting on the droplet deposition in such geometries: turbulent diffusion and gravity. For the latter mechanism, the deposition constant is related to the terminal falling velocity of the droplet, and accounts the droplet diameter, estimated using a specific correlation. MHYRESA scaled experiments, including the elbow and the inclined part of the hot leg, will be used to complete these 3-field models.

2.3. A Predictive 1D-Model for Rotodynamic Pumps

The primary circuit of nuclear reactors is composed of huge components such as primary pumps, which play a great role in reactor transients dynamics. For several years, the CEA is studying Generation IV reactors such as the Sodium cooled pool-type fast reactor concept. In this frame, hypothetic accidental transients like 'primary pump seizure' are analyzed using the CATHARE-3 code [5]. Throughout this type of transients, cavitation may occur in non-affected primary pumps and the affected (locked rotor) pump may operate in reverse conditions in terms of flow rate and rotational speed. However, neither the primary pump 4-quadrant performances nor the cavitation behavior of the pump are known at the reactor design step. Experimental constraints due to liquid sodium working fluid enhance even more these considerations concerning the measured pump performances. For this purpose, CEA and interested industrial partners (Framatome, ArianeGroup, CETIM and EDF) decided at the end of year 2015 to implement a predictive

transient, two-phase flow rotodynamic pump model in the CATHARE-3 code and to validate results at component scale (pump) and system scale (loop, reactor) with respect to available experimental data (Matteo et al. [12][13][14][15][16][17][18][19]). An attempt of a similar modelling was done earlier in the CATHARE-2V1.3L version of the code with the work of De Crecy [20] [21], Van den Hove and Geffraye [22], Coste [23] and Geffraye and Bestion [24]. Focus was mainly made on two-phase flow modelling and less on rotating machinery physics. This led to difficulties for the model to be predictive for various pump geometries (radial to mixed pumps). This model has not been maintained and is no longer available. By reconsidering the approach and developing a new rotodynamic pump model into the last version of the CATHARE code (CATHARE-3), it is intended to obtain a predictive and generic model.

The originality of the present project is to build a real 1D model -the mean streamline in the different parts of the pumps is meshed- able to predict the performance of mixed and radial flow pumps in purely liquid or gas/liquid, and four quadrant operations. The 6-equation system representing classical two-phase flows in pipes [25] is used as a basis to model each part of the centrifugal pump: suction, impeller, diffuser, volute and discharge pipe. The system is discretized according to one curvilinear direction, what allows following a mean flow path. The example of the impeller inter-blade channel is given in Fig. 1. For the suction and discharge pipes, there is no need to implement other source terms in the six-equation system. On the contrary, new source terms have to be added to correctly represent the impeller, diffuser and volute parts in order to take into account the pressure rise due to centrifugal acceleration in the moving part, the losses specific to pump geometries and the flow redress in the fixed parts.
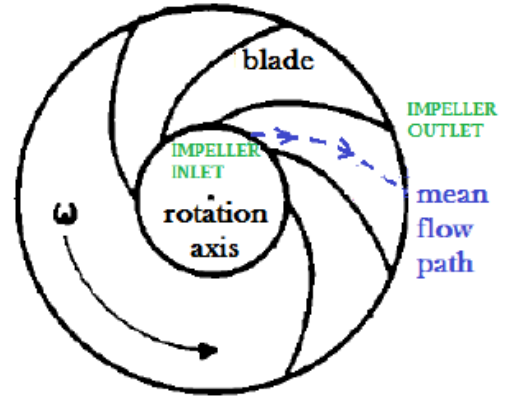
Fig. 1 : The mean flow path in the impeller inter-blade channel [14]

As the impeller is a moving part, is it solved according to the rotating frame and the associated calculated velocities are the relative ones. On the contrary, the calculated velocities are the absolute ones in the fixed parts of the pump. Consequently, a frame change has been implemented between fixed parts and the rotating one. This is operated using the velocity triangles at frame interfaces (suction-impeller and impeller-diffuser). See reference [14] for more details on the modelling (expression of governing equations and source terms in particular).

When modelling a rotodynamic pump using the new CATHARE-3 1D-pump model, the representation shown on Fig. 2 is obtained using meridian sections [14]. Each part of the pump (suction, impeller, diffuser, volute and discharge pipe) is meshed. To be able to represent pumps without diffuser or multi-stage turbomachines using the same modelling structure, the diffuser and volute parts are defined in the same CATHARE-3 one-dimensional element.


Fig. 2 : 1D-pump structure: four 1D elements (diffuser and volute belong to the same element)

A non-dimensional head curve is represented Fig. 3 with the pressure coefficient versus the flow rate coefficient for computations [14] and experimental data [26]. Two main conclusions can be drawn regarding these results : first, the similarity laws [27] are well respected by the CATHARE-3 1D pump model for the three considered rotational speeds (1000, 2000 and 3000 rpm) as the maximal relative error is 12% when considering all cases; second, off-design flow situations can be predicted (very low or very high flow rates).
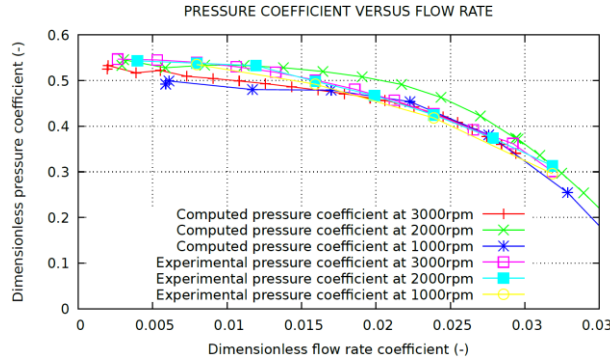
Fig. 3 : Pressure coefficient versus flow rate coefficient (experimental data from Duplaa [26])
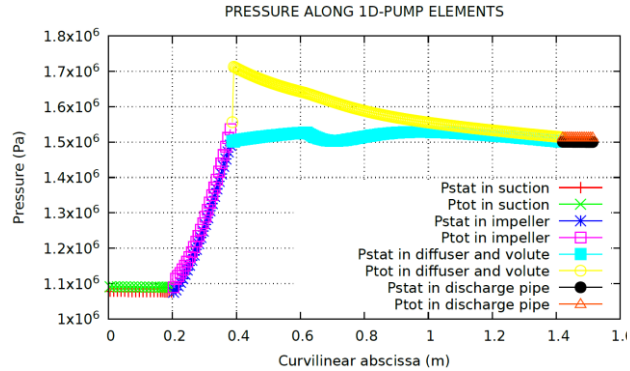
Fig. 4 : Static and total pressure profiles

On Fig. 4, static and total pressure profiles along parts of the pump are drawn at the nominal operating point of a centrifugal pump [14]. These kind of results obtained inside the pump could not be obtained using the classical non-predictive nodal pump model of the CATHARE-2 and CATHARE-3 codes. This opens new possibilities in term of pump related thermal-hydraulic studies. Qualification of this new 1D-pump model has been conducted on several cases (5 centrifugal and mixed flow pumps and one centrifugal compressor) and on single-phase or two-phase, steady or transient flow conditions. See references [2] to [9] for details on the qualification cases. It is intended to extend the model to 4-quadrant conditions and to increase the qualification in two-phase flow conditions (cavitation, air entrainment, high void fractions). The final aim being the simulation of a transient of interest for a whole primary circuit of a sodium fast reactor using this pump model which allows cavitation inception.

2.4. A Multi-Fluid and Multi-Reactor Concept Modeling Tool

The same multi-fluid and multi-reactor concept strategy as for the CATHARE-2 code [3] is being adopted for CATHARE-3 developments. This is in order to model advanced concepts such as gas-cooled fast reactors [28][29] and sodium-cooled fast reactors [5][30]. The modular structure allows the coolant circuits of any experimental facility or nuclear plant to be represented by assembling 0-D, 1-D and 3-D hydraulic modules. Thermal and hydraulic sub-modules such as thermal walls, heat exchangers, pumps, compressors, turbines, valves, fluid source or sink can be added to these main modules. Similarly, the same quality and validation procedures [31][32], as well as numerical resolution scheme and pre/post-processing tools (GUITHARE) are used for any application. All these legacy features have been reported in the new version of the code, but new ones have been developed in addition. These new developments mainly aimed to model real gas circuits used in such applications as Brayton cycle power conversion systems [33]. For high-pressure nitrogen Brayton cycles (180 bar), the CATHARE-2 calculations led to significant uncertainties due to the use of the ideal gas equation of state and models. Indeed, the way to model nitrogen in CATHARE-2 is based on the standard two-phase fluid model (residual fluid named HIGHXNC) adapted to deal with very high fraction of ideal non-condensable gas. In the operating range of the studied Brayton cycle, the maximal errors were about 10% for density, 24% for heat capacity, 28% for viscosity and 37% for thermal conductivity.

In the framework of the NEPTUNE project, the CEA built the NEPTUNE platform on a component architecture [1]. The same component can be used by different NEPTUNE thermal-hydraulics codes such as CATHARE-3 or NEPTUNE-CFD. Especially, the EOS component has been developed to compute the

thermodynamic and transport properties of the fluids from several in-house code libraries such as CATHARE-2, THETIS, FLICA-4, etc. This allowed to implement REFPROP [34] as a new library in the EOS component in order to use the nitrogen real gas equation of state in CATHARE-3. REFPROP core property routines compute thermodynamic and transport properties of many fluids using a Helmholtz energy approach mainly intended for scientific use. Moreover, new methods have been developed in the EOS component to access properties only available in the REFPROP libraries such as speed of sound and entropy.

The CATHARE-3 architecture was made in order to perform three-phase flow calculations, i.e. adding dispersed phases into the two original continuous phases (especially droplets in the continuous gas phase). It was therefore possible to choose between two-phase flow (standard CATHARE-2 model) and three-phase flow (advance model). By using this more flexible architecture, a single-phase flow model has been developed for monophasic calculations. This new feature is available for both liquid and gas single-phase flow calculations.

This single-phase flow functionality mainly contributed to the reduction of computational time and the resolution of some numerical issues due to the presence of useless residual phases. Indeed, in this single-phase case, the liquid phase properties are no longer calculated as well as some other properties such as surface tension, which is particularly expensive in terms of computing time with REFPROP. In addition, new real gas models have been implemented for the turbomachinery [35] and the sonic flow calculation [33] in order to be consistent with this new equation of state. With regard to the turbomachinery model, performance characteristics are calculated with the real speed of sound and the gas entropy that are available in REFPROP. Moreover, considering the high Reynolds number in such gas piping, specific singular [36] and regular [37] pressure drop correlations have been implemented in the CATHARE-3 code taking into account pipe roughness and abrupt flow area changes. The impact of this new CATHARE-3 models has been investigated on several case studies such as the experimental DIADEMO facility [38], a high-pressure nitrogen Brayton cycle [33] and a complete sodium-cooled fast reactor transient on a loss of power supply case [39]. New application and validation cases are already being considered such as the modeling of an organic Rankine cycle with Novec 649 used as a working fluid, a supercritical CO2 Brayton cycle, a two-phase flow ammonia cooling system or a natural gas supply system.

2.5. 3D Modelling Capabilities

This section presents the evolution of the 3D capabilities with CATHARE-3, first for the 3D modelling of the whole PWR vessel, then, for the sub-channel analysis.

2.5.1 From CATHARE-2 to CATHARE-3 for a Modular Modelling of the Vessel

The 3D module of CATHARE-2 has been validated for both whole reactor pressure vessel [40] and some subcomponents of the pressure vessel such as the core [41] or the downcomer [42] regions from the small to the large break LOCAs. A global overview of the CATHARE-2 3D module is available in [43]. One of the main goal of CATHARE-3 is to improve 3D modeling of the vessel using thin and non-conformal structured meshes [2].
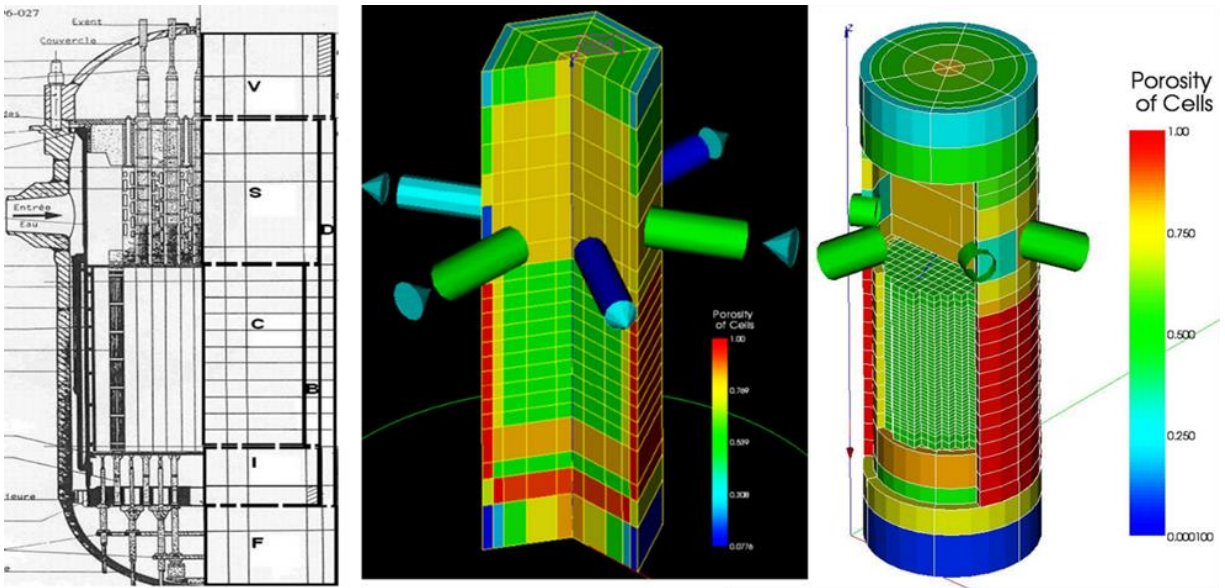
Fig. 5 : Reactor vessel modelled by CATHARE-2 (middle) and CATHARE-3 (right)

In CATHARE-2, only one cylindrical 3D grid is used for the simulation of the whole pressure vessel (see Fig. 5 – center) and it has been proved to be sufficient for simulating any kind of breaks LOCA transients. However, for a better flexibility of the modeling, for the simulation of some transients with significant transverse flow in the core, for neutronic-coupled simulations, or any other 3D flow investigations, a Cartesian 3D meshing of the core and an adapted meshing of the plena would significantly improve the simulation capabilities. In CATHARE-3, it is possible to couple different kinds of 3D modules (one for each component: core, downcomer, plena...). A typical set of grids is (see Fig. 5 – right):

- Cylindrical 3D grids for all the vessel components except the core,
- Cartesian 3D grids (one cell per assembly in a horizontal section and 40 axial meshes) for the core.

As explained in [44], new optimized resolution methods have been developed in CATHARE-3 to couple 3D modules, and the input data-deck syntax has also been adapted to these new functionalities [43].

Creating such type of modeling can be complicated for users, so the CATHARE team has improved the GUITHARE tool (based on the SALOME platform [45]) and the layout data of the 3D modules. GUITHARE stands for Graphical User Interface for caTHARE, it is a common tool for CATHARE-2 and CATHARE-3, including a syntax translator from CATHARE-2 to CATHARE-3 and now adapted to these new 3D capabilities.

Most users have a CATHARE-2 modeling of the pressure vessel, in which the 3D vessel is made up of a single 3D module. Using GUITHARE, it is possible to directly translate then split the CATHARE-3 Mono-3D dataset into multiple 3D elements. GUITHARE allows the pre- and post-processing of multiple 3D modules in the same study. Several 3D modules can be grouped together to form a macro-module that is displayed as if it was a single 3D module (see Fig. 5 – right).

GUITHARE also helps creating Cartesian-cylindrical junctions; the standard way to define the junction between two 3D modules is to let the user define the geometry and let the code compute the connectivity tables between meshes. This is well adapted when the connection is simple and does not require particular treatments. However, the case of a junction between a Cartesian-meshed core and a cylindrical-meshed plenum is much more complex and we have decided that GUITHARE would be able to calculate the characteristics of the meshing intersection between the two grids and give them to CATHARE-3 for the calculation.

Thanks to the new syntax abilities of CATHARE-3, it is possible to write a compact description of the geometry and the power distribution. Indeed, CATHARE-3 allows a multiple creation of some objects made into a loop (with the REPEAT directive). For example, it can be used for the fuel rod creation in input data

deck with a parametric distribution of the radial power. A LOCA computation using these new 3D functionalities of CATHARE-3 is available in [46].

2.5.2 Sub-channel Analysis with CATHARE-3

For core applications, the CATHARE-3 3D module includes also extended capabilities to improve the accuracy of simulations of light water reactor accidents. Both 3D modules of CATHARE 2 and CATHARE-3 are based on a porous version of the two-fluid 6-equation model, obtained from a double average process (first a time-average filtering, then a space average accounting fluid-solid interactions) of the local instantaneous two-phase balance equations. But, contrary to CATHARE-2, the 3D module in CATHARE-3 features models for turbulent dispersion and diffusion terms appearing in the 3D porous equations, which can affect the temperature map in a rod bundle, and the void dispersion phenomena is taking into account by a mixing term in the momentum balance equations [47]. These models can be activated optionally.

The 3-D validation matrix for the diffusion and dispersion terms includes two OECD/NRC benchmarks: PSBT [48] and BFBT [8] with sub-channel calculations. The latter tests are simulated using the 3-field model of the code (see paragraph 2.2). A semi-empirical relation for the turbulent diffusion-dispersion terms of the energy equation, using an algebraic model for the turbulent kinetic energy, has been established for rod bundle with PWR type geometries and calibrated from PSBT tests with mixing vane grids [48][49]. The assessment of the energy diffusion-dispersion model has also been performed against the PNNL 2×6 rod bundle single-phase tests, at low velocity [49]. Weiss experiments, consisting of two 14x14 square lattice rod bundles with unbalanced velocities at the inlet of the assemblies [49], and AGATE tests, performed in a 5x5 PWR-type rod bundle with two truncated partial grids placed at two different elevations [47], both featuring crossflows between the subchannels, are also used to assess the friction terms and/or the momentum turbulent diffusion and dispersion terms in single-phase conditions. The void dispersion effects, related to the double averaging process of the interfacial momentum term, are taken into account using a semi-empirical correlation and validated against PSBT two-phase tests series. The validation matrix at subchannel scale is completed by some rod bundle experiments, in adiabatic conditions in GRAZIELLA loop and with heated rods in OMEGA test section [47].

Sub-channel simulations require meshing with several thousands of cells, and the historical CATHARE linear solvers developed for 1D simulations or 3D modelling using a coarse mesh become inefficient in these cases. To find a more efficient resolution method, requiring less memory space, being less time consuming, and getting more flexibility in the resolution method, we have chosen to interface CATHARE-3 to the PETSC library, providing interfaces to linear solvers such as MUMPS [50]. Thanks to these numerical methods, it is now possible to perform simulations with a large number of 3D cells, up to 20,000. This capability has been used to perform sub-channel calculations with CATHARE-3, modeling some experimental facilities as PERICLES-2D [51] or LSTF core [52].

3. FUTURE DEVELOPMENTS

3.1. Physical modelling

For PWR applications, CATHARE-3 modelling is mostly based on the revision 6.1 physical models of CATHARE-2. This revision (i.e. a consistent package of closure laws validated against SETs and IETs) gives satisfactory results. However, some improvements are identify to meet the state of art, to extent the validation or to reduce the uncertainties of the models. Three main directions have been drawn to meet these requirements:

- **Improvement of the 6-equation model**. Some closure laws could be revised, aiming at reducing the uncertainties or some weaknesses of the code. Some of them have been already included into the revision 6.2, already available in option for the version 2.1 of CATHARE-3. This revision includes improvements of the flashing model at low pressure, the 2006 Loop-up table for the estimation of the critical heat flux, and minor modifications for the formulation of the interfacial

friction in the 3D module. For the next revisions of the models, one of the objectives is to better predict the critical flowrate at the break, especially in low-subcooled conditions, by the development and the assessment of mechanistic models for the flashing [53]. The formulation of the interfacial friction in the core at low pressure, typical to loss of residual heat removal conditions, is being revisited [54]. Current developments also concern the improvement of the flow map, especially for transition from and to stratified flows. Long-term researches could be the use of additional equation for the estimation of the turbulent kinetic energy for the transition and/or the use of an equation for the transport of interfacial area as suggested in [55].

- **Improvement of the 3D model**. One of the main direction concerning the physical research is relative to simulation of 3D flows, namely in the downcomer and in the core. Dedicated experiments, such as METERO-V, will provide data for the validation and development of the friction terms and turbulent-dispersion terms involved in possible crossflows in the core, occurring during the reflooding phase or the uncovering phase of LOCAs [56].
- **Improvement of the 3-field model.** The current 3-field model will be improved and extended to other parts of the circuit (e.g. near the injection system of the cold leg). The correlations developed for the 3-field could be also derived for the 6-equation model, namely for the entrainment fraction.

As far as new concepts of reactors will be study using CATHARE-3, development or extension of physical models is needed. This is case for example the passive systems for the PWRs, or the Generation IV concepts including SFRs.

3.2. Informatics Developments

In recent years, multi-scale numerical simulations are increasingly needed to provide high fidelity analysis of PWRs. These simulations often require fine multidimensional modeling to better represent physical phenomena. While it is not practical to compute the whole PWR system with a multi-dimensional resolution, a multi-scale numerical simulation of a PWR, where CATHARE-3 modules (0D, 1D and 3D) having different length scales could be used simultaneous, is useful for an accurate thermal hydraulic simulation with reasonable computing time. In order to do this, it is important to extend the numerical capabilities of CATHARE-3 3D module to perform component-scale simulations, in conjunction with physical modelling improvements (see paragraph 3.1). With this aim in mind, several point will be addressed:

- **A new architecture for 3D simulations**: the CATHARE-3 3D module would be based on the CEA's open-source software development platform – TRUST [57]. This object-oriented platform provides mesh management for parallel computation, and numerical integration methods such as PolyMAC which could be used for general meshes [58]. By using the TRUST development environment, CATHARE-3 3D code will be developed by following the same software design paradigms used for other TRUST development efforts.
- **Application Programming Interface for software coupling**: multi-scale and multi-physical calculations are one of the main targets of the NEPTUNE project. CATHARE-3 has been coupled successfully to various software by means of a common coupling interface, called **ICoCo**. This interface makes it possible to use each software as a callable library through C function calls: these calls allow a small C++ or Python program, known as the "supervisor" to perform and control a calculation. In the future, this interface will be extended for use of CATHARE-3 in the full scope and engineering simulation platforms for Operator training.
- **Improvement of the Graphical User Interface**: As presented in part 2.5, GUITHARE is the Graphical User Interface for the CATHARE code. For the component-scale approach, this tool will be complemented by the development of a preprocessor for CATHARE software, which is integrated in GUITHARE interface. This preprocessor (see Fig. 6) will be based on SALOME [45] platform capable of generating meshes on reactor core geometries defined by a set of component scale technological objects.
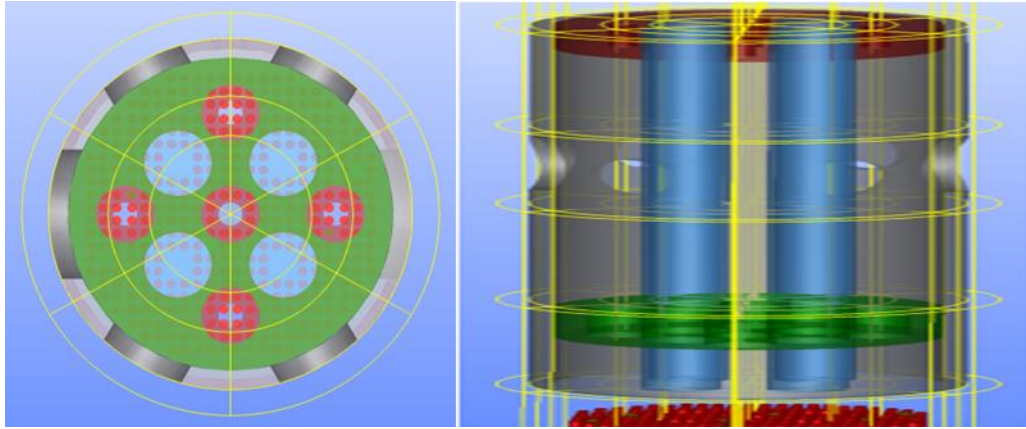
Fig. 6 : GUITHARE Pre-Processing prototype

4. CONCLUSIONS

CATHARE-3 is the new version of the French thermal-hydraulic code for the safety analysis of nuclear reactors. CATHARE 3 includes the main functionalities of the previous version CATHARE 2, with the objective to progressively succeed to it for all applications. CATHARE-3 V2.1, delivered in December 2019, is validated for the Pressurized Water Reactors (PWRs), and partially validated for sodium applications. CATHARE 3 is also developed in the objective to improve the capabilities of CATHARE 2. It already includes a 3-field model under development and partially validated for dry-out prediction and for reflooding conditions during a LBLOCA, A predictive pump model is included in the code, a well as new capabilities for multi-fluid and multi-reactor modelling. One of the major improvement concerns the 3D modelling capabilities for the simulations of the whole PWR vessel, and for the sub-channel analysis with a dedicated validation against rod bundle experiments. Future developments aim at continuing to improve or to extend the capabilities of the code. These developments will address the physical modelling (both 6-equation and multi-field models, 3D modelling), the architecture and the interface of the code for the 3D simulations and coupled simulations.

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