Multi-physics Coupling for Nuclear Systems

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Abstract

Significant progress has been made in the past twenty years on the development of detailed first principle multi-physics numerical models for nuclear systems. These advanced numerical models allow describing the multiscale nature and the complex interactions of the phenomena taking place in nuclear reactors with a level of detail that was not possible just a few decades ago. Multiphysics numerical models open new possibilities for enhancing the actual understanding of nuclear reactors phenomena and also allow designing more accurate experiments. From an engineering perspective, multi-physics models have become a powerful tool to improve the accuracy of the nuclear safety studies and to optimize beyond the current state-of-art the design of key components of the reactor such as the fuel assemblies. These important advantages are even more evident for the next generation of nuclear reactors for which these tools are necessary to speedup the R&D work, to decrease the number of experiments and develop the prototypes. Multiphysics modeling approaches have been developed in the IN2P3/CNRS in different applications of the reactor physics domain for more than 15 years. Nevertheless, multiphysics numerical modeling for nuclear reactors involving strong coordinated numerical and experimental efforts started about 2014 in the framework of the Euratom H2020 SAMOFAR project at the FEST (Fluids Experiments and Simulations in Temperature) platform of the LPSC-Grenoble. This report is focused in these particular multiphysics activities, discusses the rationality for these efforts, the main activities and results obtained in the past seven years and the overall strategy for the next five years. Only the numerical results are reported here since the experimental activities are discussed in a separate document.

1. Introduction

1.1 Evolution of nuclear reactor designs, methods and tools over the past decades

Design trends and the methodologies used for safety assessment of nuclear reactor have considerably changed between the first generation of commercial reactors[1] connected to the grid during the fifties and the current Generation III reactors under construction. These changes have gradually integrated the lessons learned from nuclear accidents and also the operating experience gained by the utilities. The changes on the safety methods has also been driven by the dramatic improvements on the numerical tools used for these analyses. First reactor design and safety studies were actually based on experiments, analytical models and/or very rudimentary algorithms. Progressively from the sixties and later in the seventies, more sophisticate 0D or 1D numerical algorithms solving single-physics problems were developed and employed to improve the reactor analyses. These codes were based on very conservative approximations that allowed to simplified the models and also ensured that the results were conservative[2]. The first Monte Carlo codes for neutronics appeared during the sixties. First applications of Finite Element (FEM) method for structural mechanics also started at the end of the sixties. During the eighties and nineties, the numerical tools used by the nuclear industry evolved into more complex 2D/3D codes still solving a single physics (i.e. standalone core thermal-hydraulics codes, neutronics codes, fuel rod thermomechanics codes, etc.) and using equations usually based on semi-empirical laws or with important approximations (i.e. not truly first principles models). These codes could also solve the equations for other physics but with very simplified models[3]. First commercial CFD codes appear in the early 1980s. First 3D tools solving different reactor physics (neutronics, thermal-hydraulics and thermomechanics) with a similar level of precision started at the beginning of the 2000s. These first multiphysics tools were developed by coupling legacy codes (i.e. existing reactor physics codes) and thus inherit many of the conservative assumptions of the original codes. Nevertheless these codes allowed improving the accuracy of the reactor simulations since they removed some (but not all) of the conservative assumptions related to the couplings. They are now widely used for design and safety analyses in place of the standalone codes. Use of Computational Fluid Dynamics (CFD) for PWR fuel assembly calculations started approximately at the beginning of the 2000s thanks to the increase on the computing resources. Numerical simulations of reactor steady-state conditions using coupled codes based on first principles models such as Monte Carlo and CFD codes become therefore practically possible at about that time and they started shortly after. This particular coupling (Monte Carlo and CFD) was indeed among the first high fidelity multiphysics numerical models developed. One important different of the high fidelity multiphysics tools with respect to the previous generation of multiphysics codes, is that they allow calculating Best Estimates values of the reactor parameters. Large coordinate efforts initiated after 2010 between industry and academia have allowed now developing very complete multiphysics numerical platforms for nuclear reactor simulations as illustrated by the example of the CASL[4] consortium in the USA. These multiphysics numerical platforms are called to play an important role in the design and safety studies of the current and future reactor designs.

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[1] Nuclear power stations devoted to electricity generation.

[2] For example, during an accidental transient study the peak of fuel pellet temperature predicted by the models in the code was in purpose overestimated to allow for sufficient margin to the UO_2 melting point and thus accommodate all known uncertainties.

[3] For example a 3D neutronics code based on the diffusion approximation would calculate the neutron cross section of the fuel materials based on the temperatures obtained using a simplified fuel rod thermal model.

[4] https://www.ornl.gov/onramp/casl-vera

1.2 What is a Multi-Physics Model (MPM)?

A multi-physics numerical model usually refers today to an algorithm that numerically solves a set of coupled equations. The equations used in a multi-physics model represent physical laws describing a particular set of phenomena taking place in the studied system. In the case of nuclear systems, these physical laws included for example: the mass, momentum and energy conservation equations for the fluid (gas and liquid) and the solid phases existing in the system, the neutron (or gamma-ray) transport equations, the nuclear and chemical reactions equations, the equations for the exchanges of mass, momentum, energy and particles at the interfaces, etc.

In the multi-physics approaches, these equations are (more or less) simultaneously solved and thus the complex interaction between the different phenomena described by the equations can be explicitly studied. As previously discussed, simulation of coupled multiple physical phenomena is not really recent. However what it has changed in the past twenty years is the computational capability that allows now an important increase of the level of details of these models and on the number of couplings that can be explicitly modeled. Equations in current multiphysics models are thus developed from first principles, which means that they are obtained from the understanding of all the relevant phenomena (sometime also called "ab initio" phenomena) and their mutual interactions. These multiphysics models are thus supposed to involve very little assumptions and to produce high fidelity results both concerning the space (usually 3D when a flow is involved) and time scales. Multiphysics numerical tools developed from such models provide Best Estimate (BE) values of the system on the contrary to previous codes which could only provide conservative estimates. They are also able to include multiscale couplings between phenomena.

1.3 Advantages and drawbacks of MFC in reactor physics applications

From the previous discussion, it is clear that important benefits can be obtained for the study of nuclear systems by the use of multiphysics tools:

- Firstly, these models are able to provide predictions with high precision and without making significant assumptions. They are thus particularly suitable for studying novel nuclear systems where very little data exist or for systems that are difficult (or costly) to study experimentally.
- Multiphysics models can be used to obtain Best Estimates (BEs) values of the key reactor parameters on the contrary of the previous generation of reactor codes that were developed to provide only very conservative estimates.
- Multiphysics models allow accessing information on reactor parameters/properties at space (local or microcopic) and time (short or long) scales that were not otherwise possible (or very difficult/costly) from experiments or from previous numerical models.
- Multiphysics models can be used, in combination with experiments, to study the effects of the individual couplings between phenomena in the nuclear systems. This information can be used to improve the system design.
- Reactor codes based on multiphysics models allow thus to obtain a better estimation of the design and safety margins on the existing reactor plants.

On despite of these important advantages, it is not a surprise that these models also have some important drawbacks and challenges that should not be overlooked. To mention some of them:

- To obtain the expected accuracy, the multiphysics tool developer must include all the relevant phenomena and the associated interactions. This is usually made using a PIRT (Phenomena Identification and Ranking Technique) approach, which is a systematic way of gathering information from experts on the phenomena that have to be considered in the model. However, developing a PIRT for nuclear applications (or for experiments) is often not straightforward.

- The numerical resolution of the multiphysics model usually requires very refined meshes and thus important computation resources (memory and CPU time). Post-processing of the results of these numerical models can be also very challenging.
- Multiphysics model usually have to be given large amounts of very detailed data: system physical properties (thermodynamics, nuclear, mechanics, etc.), geometry characteristics, system initial conditions, system boundary conditions, etc. Even when the data is available, it can contain important systemic errors and uncertainties. Statistics studies involving propagation of input data uncertainties are thus usually necessary and also require important computing resources.
- Obtaining adequate stability, convergence and consistency of the numerical algorithms of a multiphysics model require performing numerical studies and can be very challenging.

It follows, that for safety studies, licensing of such tools is very challenging. Indeed when multiphysics models are used for performing nuclear safety studies, they often required developing a novel safety methodology which is adapted to their inherent characteristics (i.e. addresses some of the above issues). As previously noted, these safety methodologies generally involve a statistical approach, requiring input variables uncertainty propagation in order to asses the key safety parameters margins. Licensing of a numerical multiphysics model and the associated safety methodology for nuclear reactors applications is therefore complex.

2. State of art, scientific challenges and motivation

2.1 State of art in multiphysics modeling for nuclear reactors

Several initiatives have being launched in the past ten to fifteen years to develop multiphysics numerical models of nuclear reactors that can take advantage of First Principle models and the existing High Performance Computing (HPC) resources. The ultimate goal of this type advanced numerical model is to be able to create a full numeric reactor model that can be used to study phenomena at a level of detail that was not possible before. One good example of this type of initiative is the Consortium for Advanced Simulation of Light Water Reactors (CASL) project established by the US Department of Energy (DOE) in 2010. This consortium reunites several DOE national laboratories (ORNL, Idaho, Sandia, Los Alamos, etc.), American universities (University of Michigan, MIT and North Carolina State University), industrials (Westinghouse and Tennessee Valley Authority) and industrial laboratories (EPRI). The CASL project has developed the Virtual Environment for Reactor Applications (VERA) which is a multiphysics numerical platform able to model with very high resolution most of the phenomena of interest existing in normal and accidental conditions in a Pressurized Water Reactor (PWR). VERA has been built from existing numerical codes developed by the partners of the consortium (operator splitting strategy) which simplifies the licensing effort and the platform maintenance. Technical domains covered by VERA are very large and include: fuel rod thermo-mechanics, reactor thermal-hydraulics, neutron transport and reactor chemistry. VERA is indeed one of the most complete multiphysic tools that have been developed for a nuclear reactor. While it has opened novel possibilities for studying reactors and it has posed significant questions and challenges as already noted in the precedents paragraph.

Our multiphysics activities do not aim to develop such a large numerical platform but they are based on a similar goal: being able to predict the key phenomena of selected nuclear systems with very high fidelity. As we will discuss in the next paragraphs our efforts have been oriented toward the study of phenomena existing in smaller and geometrically simpler nuclear systems where strong couplings between the phenomena exist. These systems are often not well modeled with the standard industry tools. Good examples of them are the Molten Salt Fast Reactors (MSRs), the micro-reactors used for space power propulsion, the facilities where criticality accidents can occur and some types of targets used for neutron production. Another important difference in our activities is that for the numerical model development we rely exclusively on the use of open source codes such as Serpent[5] and OpenFOAM[6].

2.2 Scientific challenges in Multiphysics modeling

Many challenges and research opportunities exist in multiphysics modeling for nuclear systems. To mention some of them:

(i) Numerical aspects

One very important aspect regarding the multiphysics algorithms is related to the coupling strategy used between the single-physics (or uniphysics) models used by the multiphysics model. Historically, multiphysics tools employed for nuclear reactor applications, such as the VERA platform, have been developed using the operator splitting strategy in which individual existing codes (dealing with one or more physics) are coupled iteratively. This approach is often justified by the large complexity of these single physics codes (neutronics, core thermal-hydraulics, nuclear fuel thermo-mechanics, chemistry, etc.) that have been often developed over many years. Moreover, the single-physic codes have been often validated on proprietary data resulting from experiments and/or reactor operation feedback not necessary accessible to the multiphysic tool developer or the User. Finally, the significant licensing efforts required for any reactor numerical code and the associated safety methodology also justifies the use of independent codes as bricks to build a multiphysics tool. The operator splitting strategy could nevertheless introduce important limitations concerning the overall algorithm stability and robustness, the computational cost and eventually the accuracy of the multiphysics tool if the interactions between the different phenomena are not adequately implemented in the numerical coupling between the codes. For this reasons alternative methods involving truly simultaneously numerical resolution of the model equations are currently being investigated in different domains.

Other important research area is on the development of surrogate models (also called metamodels, response surface model or proxy models) from the original multiphysics models. Indeed, despite the existing HCP resources, design and optimization of nuclear systems often requires performing a large number of numerical simulations. This is in general not practical when the multiphysics model involves a CFD code and/or a Monte Carlo code. In these cases, a subrogate model which requires lower computational effort and memory storage while still reproducing the behavior of the multiphysics model in the design space should be preferred. There are different categories of surrogate models. The more often found in our applications are: (a) Data fit surrogate models such as Artificial Neural Networks and Polynomial Regressions (non-physics-based approximation) and (b) Reduce Order Models (ROM) which can model high dimensional functions.

(ii) Phenomena and coupling modeling

Development of high fidelity multiphysics models for commercial nuclear reactors started about 20 years ago. The first developments involved coupled 3D neutronics and thermal-hydraulics transient simulations that were used to study the reactor performance during accidents. These initial multiphysics models were developed from the existing industrial thermal-hydraulics and neutronics codes. In the earlier versions, the thermohydraulics codes involved subchannels and neutronics codes based on the diffusion approximation. As the computing resources increased, these codes were replaced by more detailed mechanistic codes such as CFD for thermal-hydraulics and Monte Carlo for

[5] J. Leppanen, "Serpent–a continuous-energy Monte Carlo reactor physics burnup calculation code," VTT Technical Research Centre of Finland, 4 (2013).

[6] H. Jasak, A. Jemcov, and Zeljko Tukovıc, "OpenFOAM: A C++ Library for Complex Physics Simulations," International Workshop on Coupled Methods in Numerical Dynamics, IUC, Dubrovnik, Croatia (2007).

neutronics. Based on the excellent results obtained from these initial multiphysics models, the approach has now been extended in very different domains. To mention only a few of the current working areas:

- Transient neutronics simulations based on Monte Carlo codes coupled to other core physics: one good example of these activities is McSAFER[7] project. This H2020 project develops dynamic Monte Carlo studies where a transient Monte Carlo code is coupled to a reactor thermal-hydraulics code and used to perform reactor accident analises (e.g. the Rod Ejection Accidents or REAs). Another example is the implementation of Monte Carlo Quasi-static methods coupled to CFD and/or thermomechanic codes as we have done in our activities.
- Neutronics noise of flow-induced vibration: study of the effect on neutronics noise of flow-induced vibration in reactor structures containing the nuclear fuel (for example fuel channels in CANDU reactors) is another interesting application for multiphysics models.
- Coupled fuel rod thermomechanics, thermalhydraulics and neutronics analyses: very diverse studies are being developed in this domain. For example the study of the fuel rod behavior during accidents such as the Rod Ejection Accident (REA) in PWR. Another example is the fuel assembly deformation in SFR [J1, J4].
- Reactor fluid-structure phenomena: The fluid-structure interactions involving the coupling between the reactor fluid dynamics and the structural mechanics equations describing any deformable or moving structure in the reactor. Example of this type of phenomena are the flow-induced vibration (FIV) of nuclear fuel rods that could lead in some cases to the cladding failure due to fretting-wear against the grid supports. Other example is the study of the steam generator tubes vibration.
- PWR chemistry studies: the study of crud deposition on the fuel cladding requires the use of detailed CFD fuel assembly model coupled to a coolant chemistry model, a fuel rod model and a neutronic solver since the boron deposition on the cladding surface results from coolant boiling (and thus heat flux level).
- Criticality accidents: these type of accidents could involve large range nuclear systems with a diversity of geometry, material compositions and potential phenomena. Multiphysics approaches are thus well suited for accurate modeling of the phenomena occurring during these type of accidents as we will discuss later in this document.
- Nuclear reactor using a liquid fuel: Molten Salt Reactors (MSRs) employs a molten salt that acts both a fuel carrier and coolant. In these reactors, there is a very strong coupling between neutronics and thermal-hydraulics phenomena which is not present in solid fueled reactors. Indeed, many normal operation and accidental transients can only be studied in MSRs by using multiphysics tools based on high fidelity coupled neutronics and thermal-hydraulics solvers.

(iii) Safety methods developments

Nuclear safety methods are detailed procedures that has to be followed by engineers during the numerical analyses of the reactor behavior during an accident. The final goal of these analyses is to demonstrate that the nuclear reactor fulfill all the design and safety criteria defined for the different possible plant conditions (and thus ensure that the reactor design and safety requirements are ultimately met). These safety methods are usually very closely bound to the numerical tools used for performing accidental transients. Indeed, very often the evolution of the safety methodologies is correlated to the evolution of the numerical tools used for the analyses. On the contrary to the previous generation of numerical tools which were based on conservative assumptions, multiphysics tools are used to determine Best Estimate (BE) values of the reactor key safety parameters. They can enable significantly potential gains on the design and safety margins. Nevertheless, the Best Estimate (BE) approach requires the determination of the confidence bounds of the calculated reactor

[7] https://mcsafer-h2020.eu/

parameters based on an uncertainty quantification methodology. Uncertainty quantification methodologies are quite challenging in multiphysics codes given the large amount of input data used by these models and the high complexity of the numerical algorithms. Uncertainties sources include uncertainties from the input data (properties, nuclear, geometry, etc.), uncertainties from the physical models and the numerical methods, and uncertainties from the boundary and initial conditions. Development of Best Estimate Plus Uncertainty (BEPU) methodologies for the safety methods [C19] based on multiphysics codes have been therefore an active area of research over the past twenty years but still require further progress for enabling the full implementation of these advanced multiphysics tools in reactor safety evaluations.

(iv) System design

Success simulation of complex nuclear systems with high fidelity multiphysics tools open novel possibilities related to the resolution of inverse problems and to model-constrained optimization. The last option is particularly interesting for the design of advanced reactors since only scarce experimental data is available for these systems in contrast to the actual reactor fleet. Good examples of these reactors are the Molten Fast Reactors (MSRs) or the space nuclear reactor in which we work.

2.3- Motivation and interest for performing multiphysics studies at the IN2P3/CNRS

Over the past twenty years, the IN2P3/CNRS has made important contributions to the research on advanced nuclear systems such as Accelerator Driven Systems (ADS) and Molten Salt Reactors (MSRs); and on fuel cycles. Given the current trends on nuclear engineering research, it can be concluded from the reasons stated in the previous paragraphs, that the study of advanced nuclear systems would require high fidelity simulations based on first principles multiphysics models. Therefore, continue to develop competitive research in the domain of the reactor physics will require entertaining in the institute some capability for developing and performing multiphysics simulations for nuclear systems in the coming years.

It is also worth to note that while important expertise on nuclear physics and neutronics already exist at the IN2P3/CNRS, the institute has also important numerical and experimental capabilities in fluid mechanics and heat transfer areas gained from other research domains. The IN2P3/CNRS has thus the necessary technical competences and resources for developing a meaningful research activity on multiphysics for nuclear systems.

3. Numerical and Experimental Multiphysics Program

3.1- Description

(i) Genesis of the program

First multiphysics numerical simulations at the LPSC-Grenoble can be traced back at least to 2008 with the PhD of N. Capellan[8] who developed coupled steady neutronics and thermal-hydraulics numerical simulations for PWR using the Monte Carlo code MCNP and the thermo-hydraulics code Cobra. High fidelity coupled thermal-hydraulics and neutronics simulation involving a CFD for the thermal-hydraulics started in the institute in 2012 with the PhD thesis of A. LAUREAU [J5][J8] in the framework of the Molten Salt Fast Reactor (MSFR) activities of the LPSC-Grenoble. On the experimental side, a FLiNaK forced convection loop (FFFER) was designed, built and operated at the LPSC between 2008-2017. While all these activities already involved multiphysics, the first coordinated numerical and experimental efforts for multiphysics studies started in 2015 in the framework of the SAMOFAR

[8] http://www.theses.fr/2009PA112296

project. As a result, during SAMOFAR project, the numerical model based on the code OpenFOAM was further developed to include new phenomena such as for example the possibility of studying phase change, thermal radiation heat transfer and new neutronics models. As noted, the Molten Salt Reactor (MSR) concept is an ideal nuclear system for multiphysics modeling since it has multiple strong couplings between diverse phenomena covering domains such as thermal-hydraulics, neutronics, thermo-mechanics and chemistry. It is also an ideal system for developing a multiphysics tool because the liquid fuel circuit is relatively simple and thus the mesh requirements are far smaller than other reactor concepts such as PWR or SFR.

The knowledge, either numerical and/or experimental, gained during the project SAMOFAR was later used to perform further studies on the Molten Salt Fast Reactor (through the SAMOSAFER project) and also to develop new multiphysics activities according to the research opportunities. Among these activities, the studies of criticality accidents in collaboration with the IRSN, the studies in collaboration withy EDF on the molten corium and concrete interaction during a severe accident (not reported here), the design of liquid and solid targets for neutron production and the more recent studies in nuclear space power. While these activities do not always involved the same codes and experiments, they were possible because of the knowledge gained by the team in numerical and experimental multiphysics.

(ii) Goal and overall strategy

The main goal of the Numerical and EXperimental MUltiphysicS (NEXUS) Program is to develop numerical models and the related multiphysics experiments necessary for advanced nuclear system applications. The strategy of the program is to focus the multiphysics activities (both modeling and experimental) in nuclear systems were strong couplings exist between the phenomena. Our research usually involves developing new models for the phenomena and their coupling, designing and operating experiments or using existing experimental data to compare against the models and finally contribute to the design of these advanced systems.

(iii) Coupling between the experimental and numerical activities

As discussed on the previous paragraphs, one of the strategies adopted in our multiphysics activities has been, as much as it is possible, to develop models and experiments all together. This strategy, discussed in the experimental document, has proved to be very useful in gaining a better understanding on the phenomena themselves and on the design of the components of the experiment. Successful examples are the molten salt solidification/ melting studies and the MSFR cold plug design. The use of separate water (SWATH-W) and molten salt facilities (SWATH-S) have also helped to obtain more complete dataset. For example, the velocity fields can be measured in the water model experiments (SWATH-W) while thermal data is measured from the molten salt experiments (SWATH-S). We intend to continue this approach in the remaining of the SAMOSAFER project and in the future projects.

(iv) Contribution of the multiphysics activities to education and training

One of our missions is to contribute to the education and training of the workforce needed by the nuclear sector. Moreover, multiphysics approaches are now widely used by utilities, reactor and fuel vendors, safety authority and research laboratories. The activities developed in multiphysics over the past years have contributed to this mission by either providing training opportunities (internships and PhD projects) in this area and also by improving the content of the nuclear engineering program at Grenoble. In particular, a course on molten salts for energy applications has been developed over the past two years. This course is organized in several chapters presenting: (i) Principal applications of molten salt in energy, (ii) Discussion of thermal-hydraulics, neutronics and corrosion aspects of molten salts and (iii) Lab activity where the student perform an experiment at the FEST platform (e.g. study of the working principles of a MSR bubble separator).

(v) Numerical tools

The initial multiphysics modeling efforts were focalized on the study of the Molten Salt fast Reactor (MSFR). This reactor concept provides indeed an ideal system for studies with high fidelity multiphysics models for various reasons. Firstly, the reactor uses a liquid fuel, the molten fuel salt, which acts both as fuel carrier and reactor coolant. A much stronger coupling thus exist between the neutronics and thermal-hydraulics phenomena than in solid fueled reactors. Moreover, the reactor geometry is relatively simple and the core composition more homogenous than other nuclear reactors. Mesh size for the full discretization of the core is therefore at least two orders of magnitude lower than for other reactor concepts such as PWR or SFR at same level of precision. This means that for a multiphysics model developer the efforts can be focused on the improvements of the phenomena modeling and their coupling rather than on the numeric aspects. Finally, since there is scarce information on this type of reactors, codes based on first principle models such as Monte Carlo codes for neutronics and Computational Fluid Dynamics (CFD) for thermal-hydraulics are particularity well adapted.

In order to study the Molten Salt Fast Reactor a multi-physics numerical tool was thus developed based on the numerical coupling between the codes OpenFOAM (C++ toolbox for the development of numerical solvers for continuum mechanics problems using Finite Volume Method, including Computational Fluid Dynamics) and SERPENT (multi-purpose three-dimensional continuous-energy Monte Carlo particle transport code). SERPENT and OpenFOAM codes were chosen as starting blocks because they are open source codes that can be modified in order to implement the couplings or changes the models. The resulting multiphysics tool was then employed to study various design aspects of the Molten Salt fast Reactor (MSFR). The figure 1 illustrates the coupling scheme adopted in the multi-physics tool together with the main phenomena and the relevant parameters involved in the modeling of a nuclear reactor using a molten fuel salt.

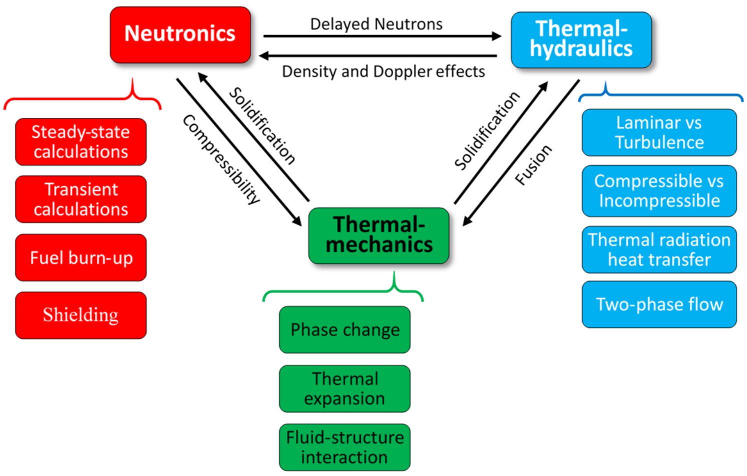


Figure 1. Multiphysics model based on a coupling between the OpenFOAM and SERPENT codes.

As it can be observed in this figure, the multi-physics tool contains three main modules: Neutronics, Thermal-hydraulics and Thermal-Mechanics. During the numerical resolution, these three modules are executed for each of the region of the reactor sequentially. A region is defined in the tool by the material properties. It can be either a solid or liquid region. The coupling between the regions is ensured by the use of appropriated boundary conditions at the interface of the regions. For example, for the case of temperature or neutron flux, the appropriate boundary conditions at the interface are the continuity of the scaler field and the continuity of the current. A brief discussion on the models implemented in these three modules is presented in the following paragraphs. A detailed discussion of these models can be found in the references of this document and in the PhD manuscripts of J. BLANCO and M. RETAMALES.

Neutronics Module

The neutronic module solves the neutron transport equation or the equivalent problem that consists in performing a balance of neutron population in the reactor according to the material composition, temperatures and densities. Two main methods are available in the tool to calculate the neutron population: (a) A deterministic approach using on a SP_N method and (b) a stochastic approach using a Monte Carlo method. The SP_N is based on a multi-group simplified spherical harmonics method (SPN). Two levels of discretization are possible in the neutronic module of the tool for the SP_N: (a) SP_1 which has a similar precision to a diffusion method and (b) SP_3 which is a high order method providing better accuracy for system where the neutron angular flux cannot be approximated as linearly anisotropic. The main advantage of the SP_N method its lower computational cost. However, the SP_1 and SP_3 approximations usually fail to accurate predict the reactivity in small nuclear systems such as the micro-reactors used for space propulsion or for example in some of the systems studied in criticality accidents. Moreover, determination of the neutronics properties required by these models is very challenging in highly heterogeneous nuclear systems (e.g. self-shielding and neutron leaks effects). In those cases, the stochastic approach should be instead used. The stochastic approach implemented in the multiphysics tool [C5][C13] is based on the Monte Carlo code SERPENT. The advantages of a Monte Carlo method are its high precision for small nuclear systems, use of first principles models and the flexibility of this method in terms of material and geometries that can be modeled. Indeed, the standard Monte Carlo codes are well suited to perform steady neutronics calculations in reactors that may have significant neutron leakage and large space heterogeneities regarding the material composition and also the neutron spectrum. In our applications, these steady calculations include fuel depletion and reactivity control studies. However, the use of a Monte Carlo method for transient calculations is more challenging due to its high computational cost. In order to overcome this difficulty, a quasi-static Monte Carlo approach was implemented in the tool to perform transient calculations. In this approach, the neutron angular flux ψ is factorized as follows:

$$\psi(\vec{r},\vec{\Omega},E,t) = n(t)\cdot\phi(\vec{r},\vec{\Omega},E,t) \qquad (1)$$

where $n(t)$ is the flux amplitude and $\phi(\vec{r},\vec{\Omega},E,t)$ is the shape function. The shape function $\phi(\vec{r},\vec{\Omega},E,t)$ is calculated by using the Serpent code at fixed times while the amplitude function $n(t)$ is determined by an Ordinary Differential Equations (ODEs) system similar to those of the point kinetics. In order to reduce the complexity of the flux shape calculations the adiabatic approximation has been used but this approximation could be removed in the future if necessary. The Monte Carlo Quasi-static method was implemented in the multiphysics tool through an internal coupling in which Serpent was integrated in OpenFOAM as an internal Class. The ODEs associated to the amplitude function $n(t)$ are solved in OpenFOAM. More details on this quasi-static Monte Carlo approach can be found in [C5][C13].

In order to fully solve the transport equation, one must also consider the presence of the delayed neutrons which are produced by the decay of fission fragments called delayed neutron precursors. In the case of a nuclear system involving a liquid fuel (such as the MSRs), the delayed neutron precursors are in addition transported in the liquid fuel and therefore their balance equation contains two more terms with respect to the case of a solid fuel: the advection and the diffusion terms. The delayed neutron precursors concentration C_g of the family *g* is thus calculated from the following equation:

$$\frac{\partial C_g}{\partial t}(\vec{r},t) = \beta_g F\psi(\vec{r},\vec{\Omega},\ E,t) - \lambda_g C_g(\vec{r},t) - \vec{u}\cdot\nabla C_g(\vec{r},t) + D_g\nabla^2 C_g(\vec{r},t) \qquad (2)$$

where F is fission operator, β_g the delayed neutron fraction for family g, $\lambda_g$the decay constant, $\vec{u}$ is the molten salt flow velocity and D_g, the diffusion coefficient. The advection term arising from the molten fuel convection is determined from the molten salt velocity field obtained by the thermo-hydraulic module together. A similar equation is also used in the tool to calculate the decay heat source in the fuel and to study for example decay heat removal after the fission chain reaction has stopped in the reactor.

Thermal-hydraulics module

This module solves the mass, momentum (Navier-Stokes equations) and energy balance equations in the fluid and solid regions. The module has been developed using the CFD (Computational Fluid Dynamics) algorithms already existing in the code OpenFOAM (with some minor modifications). In all the cases studied up to now, we have used only one fluid fuel region that is composed by the molten fuel salt. On the contrary, depending on the nuclear system studied one or two solid regions could exist. For example in the space propulsion reactor model, two solid regions are used: one for the cladding and the another one for the reflector. The molten fuel salt flow is often (but not always) approximated as an incompressible flow due to its low Mach number and the relatively small temperature gradients developed in the fluid region. In this case, the thermal-hydraulics balance equations can be therefore be simplified to:

$$\nabla \cdot \vec{u} = 0 \tag{3}$$

$$\rho \frac{\partial \vec{u}}{\partial t} + \rho \vec{u} \cdot \nabla \vec{u} = -\nabla p + \rho\, \vec{G} + \mu\, \nabla^2 \vec{u} \tag{4}$$

$$\rho c_P \frac{\partial T}{\partial t} + \rho c_P \vec{u} \cdot \nabla T = \nabla \cdot (k \nabla T) - \nabla \cdot \vec{q}_{rad} + Q_{nuc} + Q_{decay} \tag{5}$$

where $\vec{u}$ is the molten salt flow velocity, T the temperature, Q_{nuc} the nuclear power, Q_{decay} the decay heat source and $\vec{q}_{rad}$ the radiative heat transfer in the molten salt. For the study of compressible phenomena in the MSFR [C23], the above equations were replaced by the compressible Navier Stokes equations. The solid region are modeled with a similar set of equations but the velocity and pressure fields are not computed and the advection term in the energy conservation equation is set to zero. In these regions, only conduction heat transfer (eventually with thermal radiation) is solved.

Equations (3) – (5) are numerically solved in OpenFOAM using a RANS (Reynolds average Navier–Stokes) approach for turbulent flow (high Reynolds) or the Navier Stokes equations for laminar flow. In most cases, the turbulent RANS k-ε and k-ω SST model have been used to perform both steady and transient calculations. Due to the non-linearity of the advection term of these equations, the PIMPLE algorithm existing in the OpenFOAM libraries is employed to numerically solve the Eqs. (3)-(5). This algorithm uses the momentum equations to estimate the velocity fields based on an estimate of the pressure field and then use the flow mass conservation equation to correct the pressure field based on the newly found velocity fields. The PIMPLE algorithm can be used with laminar or turbulent models and for modelling a transient or stationary state. Once the velocity field is calculated, the energy conservation equation is solved by considering the advection of internal energy due to the movement of the fluid and the power source due to the nuclear fissions and the fuel decay heat (e.g. fission products).

Thermal-mechanics module

The thermo-mechanics model allows accounting for the molten salt phase change phenomena when this phenomenon is expected to occur. The model, called MASOFOAM, implements a solidification-convection coupled solver based on a standard mixture model. In this mixture model, the molten salt zone is divided in three regions: the liquid phase, the solid phase and the mushy zone. MASOFOAM solves the mass, linear momentum and energy conservation equations in each of these regions. In the liquid phase, the fluid is considered as incompressible. In the solid phase, the Duhamel-Neumann constitutive equations are used with the expansion work being neglected in the energy equation. In the mushy zone, a porous medium approach is used with approximate cloture equations for the stress tensor and the mixture enthalpy. Another solver called MUSOFOAM (MUlti-scale SOlification Foam) has also been implemented in the multiphysics tool and should be considered as a complementary solver to MASOFOAM. MUSOFOAM allows improving the accuracy of MASOFOAM by providing more accurate estimate of the macroscopic properties of the solid phase (for example the thermal conductivity tensor). To obtain these properties MUSOFOAM solves the species diffusion equation with a length adaptable phase field model and then calculate the volume average values of the properties. More details on both models are given in [J6].

(vi) Research partners

Many of the past and present multiphysics activities have been developed in the framework of international collaboration such as the SAMOFAR and SAMOSAFER Euratom H2020 projects. Within these european consortiums we have established closed research collaborations with Politecnico di Milano (POLIMI) and in a lesser degree with Delft University. We are currently developing the conjoint PhD thesis of J. NARVAEZ with POLIMI to develop a methodology and experiments for the analysis of the stability of natural convection in passive systems. Outside these European projects we have established international collaborations with the University of Texas (Texas A&M) through the NEST (Nuclear Education, Skills and Technology) program and with the Institute Balseiro (Argentine) through the ARFITEC program. Finally, since 2019 we have also been involved in the an IAEA initiative called ONCORE[9] (Open-source Nuclear Codes for Reactor Analysis) which consist in an expert group that share experiences and advocate for the development of Open-source Multi-physics Simulation tools in support of research, education and training in nuclear engineering.

At national level, two important collaborations have been developed in recent years. The first one with EDF on the modeling of the corium-concrete interactions during severe accidents and on the development of uncertainties propagation methods in multiphysics models for safety analyses. The second national collaboration was carried-out with the IRSN for the development of a multiphysics tool for the study of the criticality accidents. In the near future, a new collaboration with the CEA, ORANO and other CNRS laboratories will be developed in the framework of the ISAC project (2022-2026) concerning the modeling of fission products production, transport and removal in a Molten Salt Fast Reactor (MSFR).

3.2- Activities

The multiphysics numerical and experimental activities in the past five years have been structured about four main topics: (i) Molten Salt Fast Reactors (MSFR), (ii) Nuclear Space propulsion, (iii) Criticality and severe accidents and (iv) Targets for neutron production.

(i) Molten Salt Fast Reactor modeling

Molten salts are being considered as candidate for coolant in various Generation IV reactors concepts such as the Fluoride salt-cooled High-temperature Reactor (FHR) and the Molten Salt Reactors (MSRs) with the possible thermal or fast spectrums (MSFRs) versions. As noted, numerical models for these new reactor concepts posses unique challenges because some of the intrinsic molten salts phenomena are not found in other coolants. For example, in the case of the salt fuel-cooled MSRs the transport the delayed neutron precursors in the liquid fuel causes a reduction of the effective fraction of the delayed neutrons and therefore a coupling between the reactor thermal-hydraulics and neutronics

[9] https://www.iaea.org/topics/nuclear-power-reactors/open-source-nuclear-code-for-reactor-analysis-oncore

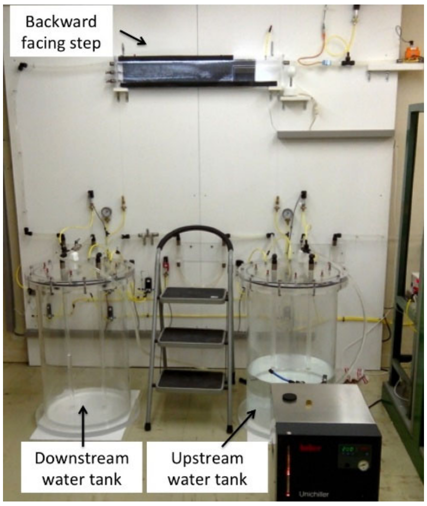
behavior not found in other types of reactors. Moreover, the fuel reactivity feedback coefficients of MSRs can also be affected by the salt compressibility, the presence of bubbles and the overall flow characteristics. Some other more convectional phenomena such as thermal heat radiation transfer or flow phase change have to be taken into account in the models and could be different with respect to those encountered in reactors using more standard coolants such as water and liquid metals. Due to their complexity, most of these phenomena require, as it has being discussed, the use of multi-scale and multidisciplinary models that can take into account the coupling these phenomena. While significant modeling progress has been made over the past ten year, further work is still required for improve the modeling of the thermal-hydraulics, thermo-mechanics and chemistry phenomena.

In the frame of the European Project SAMOFAR (2015-2019) an experimental facility called SWATH (Salt at WAll: Thermal excHanges) has been built at the CNRS (LPSC, Grenoble) as discussed in the experimental document of our activities. This facility has been used during SAMOFAR and SAMOSAFER (2019-2023) projects to study some of the thermal-hydraulics challenges found in these reactors and thus to improve the molten salt numerical models, in particular those based on Computational Fluid Dynamics (CFD) codes. In the next paragraphs, we summarize some of these multiphysics studies with the associated experiments in SWATH platform developed during these H2020 European projects and in particular in the PhD Thesis of M. TANO.

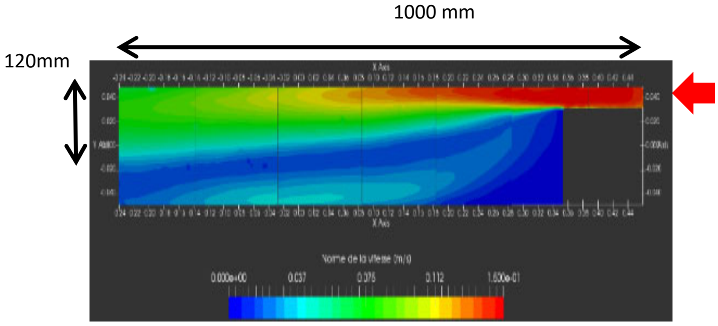
Turbulence modeling improvements using the Backward Facing Step (BFS) experiment

Performing multiphysics steady or transient studies in MSR systems usually requires the coupling of the thermalhydraulics and neutronics models. For most reactors geometries and sizes, and given the complexity of the phenomena being solved, the Reynolds Average Navier Stokes (RANS) approach provides a reasonable method for solving the Navier-Stokes equations. Other Computational Fluid Dynamics (CFD) techniques such as Large Eddy Simulations (LES) techniques can also be used (or necessary) for studies in smaller systems or for selected parts of the reactor. More accurate CFD techniques such as the Direct Numerical Simulation (DNS) are still precluded since they are practical only in very simple geometries because of their computational cost. For the current studies performed with the multiphysics tool, RANS approaches have been usually adopted and thus the modeling effort was focused on the improvement of the RANS models for molten salts.

RANS models are computationally less demanding than other CFD techniques (such as LES or DNS) but unfortunately they have an important drawback: the choice of the RANS model among the various existing for the simulations is not always straightforward. Indeed differences on the predicted velocity flow fields from similar RANS model can became relatively important (more than 10-20%) in some cases. In order to improve the accuracy of the RANS turbulence models used in modeling the MSFR a Backward Facing Step (BFS) experimental test section has been developed. The BFS geometry is particularly interesting in our applications since the flow phenomena in this geometry is representative of conditions that exist in some of the key reactor components such as the entrance region of the MSFR core cavity. The BFS geometry is particularly challenging for standard RANS models since these methods usually cannot fully predict the richness of the turbulent structures generated after the BFS. As an example of such difficulties, Table 1 presents the relative error and the computational cost for three standard RANS turbulence models: k-ε, k-ω and RSS model when used to predict the flow field measured by a PIV technique in the BFS section installed in SWATH-W. The relative error reported in Table 1 was calculated as the average weighted quadratic error between the model prediction and the experimentally measured velocity by using a PIV method (Particle Image Velocimetry). Example of a flow field measured in the BFS is shown in Figure 2.



(a) SWATH water facility with the BFS section.



(b) PIV averaged velocity field in the BFS at Reynolds equal 3900.

Figure 2. Particle image velocimetry (PIV) performed in the Backward Facing Step (BFS) section installed in SWATH-W.

Model	Relative error	CPU Time (16 core x1.2GHz)
k-ε	13.2%	721 sec
k-ω	7.2%	785 sec
RSS model	6.4 %	1921 sec
Non-linear Cubic	5.1 %	1372 sec
LES	0.7%	115869 sec

Table 1. Relative errors and computational cost for the BFS numerical simulation.

As can be seen in Table 1, it is difficult to decrease the relative error below 5-10% with the standard RANS models and in some cases such as for the k-ε model, the error is well above 10%. This could be sometime problematic in reactor design studies but especially for the analyses of the experiments that we investigate in the SWATH facility (where the studied phenomena required a good knowledge of the molten salt velocity field). It was therefore necessary to develop a methodology and a tool that allows improving the accuracy of the standard RANS model velocity field predictions. This tool was called the Genetic Evolutionary Algorithms for Turbulence modelling tool (GEATFOAM) [C27]. GEATFOAM allows constructing a mathematical expression that is used to calculate a Reynolds Shear Stress (RSS) tensor that minimizes the relative error between the model predictions and the measured experimental flow data in the BFS. GEATFOAM is a library developed in C++ that can be compiled with the OpenFOAM code. The genetic algorithm was used in the tool to perform the optimization process since it provides good robustness and decreases the computational time. GEATFOAM was then applied to improve the numerical predictions for the BFS results obtained from SWATH-W by optimizing the parameters of a standard k-ε model and a non-linear cubic model. The non-linear cubic model uses a third order tensor expression to describe the non-isotropic part of the RSS tensor and allows to better take into account the upstream flow or fluid history dependency of the turbulence in the BFS. The optimization of the parameters of this model by GEATFOAM enable decreasing the relative error to about 5.1 % without further computation cost. This level of accuracy was judged adequate for the purpose of the analyses performed in SWATH. Accuracy of hydraulics RANS models was therefore improved from SWATH-W data before use them to study thermal-hydraulics effects in SWATH-S (where velocity field cannot be practically measured).

Salt phase change modeling

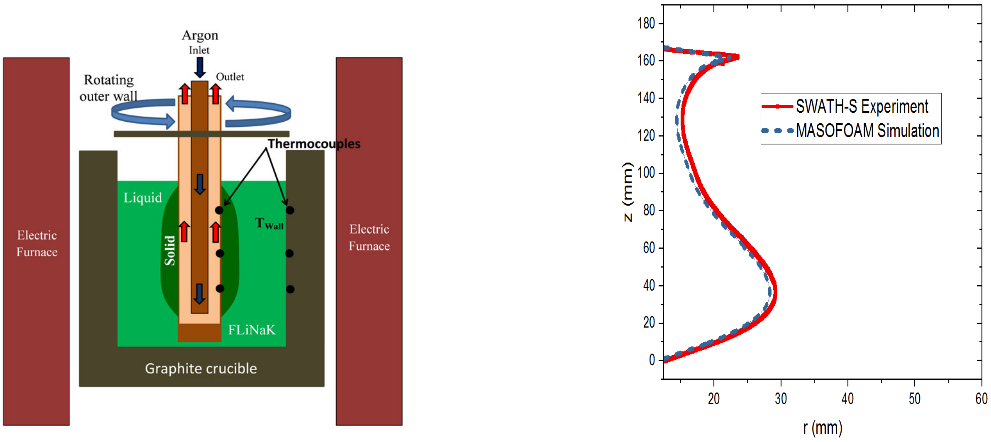
One important phenomenon in MSRs is the molten salts phase change. This can occurs at different plant operating conditions as results of accidents or abnormal operating conditions. Very little work have been done in the modeling of solidification and melting processes in molten salts. Two complementary numerical models have been developed to model the eutectic molten salt solidification and melting process: MASOFOAM and MUSOFOAM. MASOFOAM implements a solidification-convection coupled solver based on a standard mixture model. MUSOFOAM (MUlti-scale SOlification Foam) is a complementary solver at the mesoscale that provides estimate of the macroscopic properties of the solid phase (for example the thermal conductivity tensor). Both models have been implemented in the multiphysics tool.

In order to study the performance of these two models, a solidification experiment including convective effects was implemented in SWATH-S. As can be seen in Figure 3 the solidification experiment employed a rotating tube inside an annular cavity made on graphite and filled with molten salt. The rotating tube contains an inner tube that allows for the circulation of a gas coolant (argon) to decrease the temperature of the external wall of the outer tube below the FLiNaK melting point and thus initiating the solidification process. The tube rotation generates a relative simple forced convection velocity field in the fluid. The inner wall temperature of the graphite crucible was maintained at a constant temperature (above the melting point) by regulating the electric furnace power. The rotating tube and the crucible walls were instrumented with thermocouples. This experimental setup has several advantages:

- The solidification front profile could be measured at any time by extracting the rotating tube from the molten salt bath;
- Flow field established in the cavity was relatively simple although flow instabilities may appear (Taylor-Couette instability);
- Heat extracted from the tube could be estimated by performing the enthalpy balance on the argon flow;
- Boundaries conditions on the molten salt cavity were controlled or at least measured;
- Instrumentation using thermocouple was relatively simple.

The experiment design was still relatively complex and required to be installed inside a glovebox with an inert atmosphere in FEST facility. Special attention was given to the design of the thermal radiation shielding (heat screen) above the molten salt cavity to avoid excessive heating on the upper structure. In addition, a rotary tightness joint to allow for the argon gas circulation inside the tube was required on the upper part of the rotating shaft. A more detailed layout and discussion on the design of the SWATH-S solidification experiment are given in the experimental part report.

Experiments were thus carried-out by starting the tube cooling after temperatures were stabilized in the molten salt bath. More than twenty different solidification transient conditions were investigated by changing the argon rate, the rotation speed and the salt temperature at the external wall. Re-melting transients were also investigated. Once the experiment was stopped, the tube was withdrawn from the molten salt bath and the shape of the solidified salt over the tube was picture recorded and measured after cooling. The solidification profiles obtained from these experiments were then compared against the predictions from MasoFOAM (with solid phase properties calculated with MusoFOAM). An example of these comparisons is shown in Figure 3. As can be see a good agreement was found between the experimental data and the solidification model predictions. This agreement was possible but carefully accounting for all the key phenomena of the experiment.



(a) Simplified layout of the SWATH-S solidification experiment

(b) Comparison of MASOFOAM solidification front profiles against SWATH-S experimental results.

Figure 3. SWATH-S solidification experiment.

Draining transient in the MSFR

The numerical simulation of the transient associated to the draining of the molten fuel salt from the core cavity of the MSFR is a very challenging numerical simulation and thus it was an important milestone of the multiphysics modeling activities. The study [C20] was possible thanks to the development and implementation in the multiphysics tool of the models that have been discussed in the previous paragraphs. In the study presented here, it was assumed that a station blackout or total electric power failure occurs t = 0 sec and than the heat removal at the heat exchangers are stopped at the same time. As result of the station blackout, the temperature in the cold plug will increase causing its rapid melting (this is modeled by the phase change model) as thus the opening of the plug and the start of the draining process as can be seen in Figure 4. Determination of the speed of the molten salt draining from the cavity is important to avoid damage in the core structures due to excessive temperatures.

To study this transient several phenomena have to be modeled: (i) Gas-liquid flow with thermal exchanges, (ii) Gas-liquid flow mechanical interactions, (iii) Buoyancy effects, (iv) Turbulent effects, (v) Decay heat source term, (vi) Radiative heat transfer on the free molten salt surface and inside the salt and (vii) Fuel salt solidification/melting.

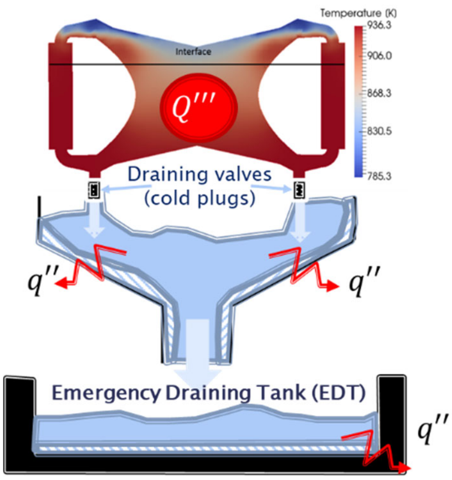


Figure 4. Sketch of the MSFR during a draining transient.

In order to study this particular transient, the following submodels were used in the multiphysisc tool: (a) Homogenized two phases model (mixture model already existing in OpenFOAM libraries),

(b) Fission power, (c) Residual heat, (d) Incompressible flow with Boussinesq approximation, (e) RSS RANS model, (f) Salt solidification/melting model, (g) Radiative heat transfer and (h) Porous medium model for the HXs. In the numerical simulations, all fuel circuit walls were considered adiabatic (except in the HXs). Results obtained for the molten fuel salt temperature field are presented in the figure 5. These simulations shown the maximal temperatures achieved in the transient do not compromise the materials.

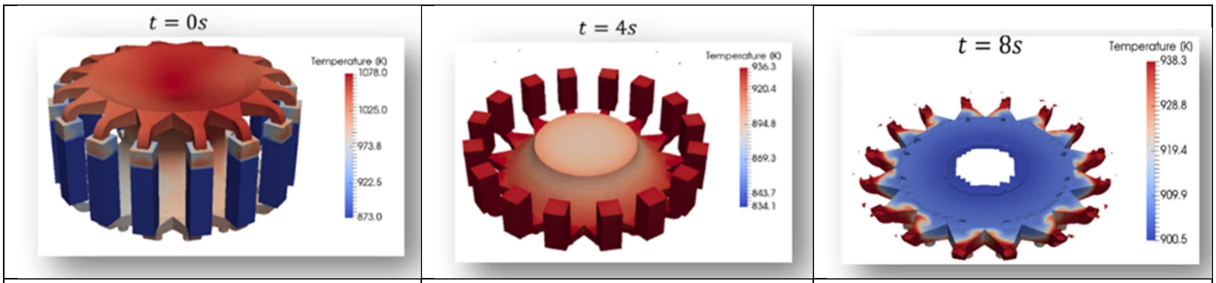
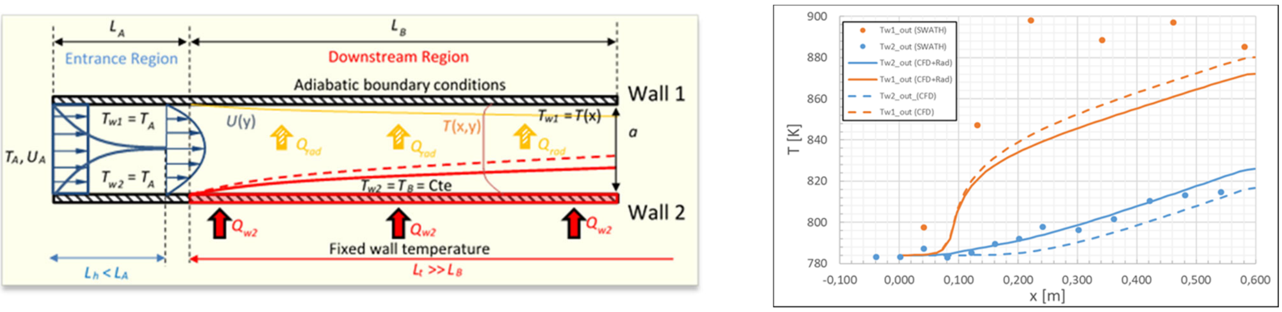


Figure 5. Molten fuel salt temperatures during the draining transient following a station blackout.

Thermal Radiation heat transfer modeling in the flat channel section

On the contrary to other coolants, molten salts can be considered as participative semitransparent media concerning thermal radiation heat transfer. While under most conditions, radiative heat transfer is not expected to be the main heat transfer mechanism in molten salts, its effects cannot be neglected at the high temperatures found during some accidental conditions or in geometries where the fluid can be considered as optically thin (e.g. in the heat exchanger). For this reason, thermal radiation heat transfer models for molten salt coolants have been developed and integrated in the multiphysics tool. In parallel to these numerical developments, an experimental study using a flat close channel has been designed and operated in the SWATH-S facility to investigate this phenomenon. The objective of this experiment is to study the effect of radiative heat transfer on a molten salt flow between two plates. Experimental study of radiative heat transfer in a molten salt is however difficult due to the high working temperatures that are required, the risk of chemical reactions and the uncertainties existing in some of the molten salt thermodynamics properties. For example, the optical properties strongly depend on the molten salt composition and on the state of the wall surfaces. Note that in the reactor both things will evolve overtime even more as results of the fission products production (in particular in a molten salt-fueled reactors) and also due to the transport and deposition of corrosion products in the molten salt.

The strategy used in the flat channel experiment in the study thermal radiation is based on the effect of radiative heat transfer on the development of a thermal boundary layer in the laminar molten salt flow inside the channel. As can be seen in Figure 6, in an optically thin flat channel a thermal boundary layer will appear at the upper wall assuming than nearly adiabatic conditions can be maintained on the wall. To design the experiment and to perform the later analyses of the experimental results, very detailed numerical studies were carried-out using CFD codes with various thermal radiation heat transfer models. These studies were key to optimize the experiment design (inlet diffuser for example) and the operating conditions (flow rate, temperatures and heat input). Preliminary results comparing the numerical model and the experiment results obtained from the first campaign in SWATH-S confirm that the effect of thermal radiation exist in the flow. They also show a reasonable agreement between the model and the results on the wall where thermal radiation would cause the development of the thermal boundary layer as can be seen in Figure 6. Novel measurements obtained from a second experimental campaign will analyzed in the next months.



(a) Flat Channel working principle: the thermal radiation effect on the boundary layer

(b) Preliminary Comparison between experimental data and model predictions.

Figure 6. Flat close channel experiment used to study thermal radiation heat transfer in a molten salt flow.

(ii) Nuclear Space propulsion

Nuclear fission power is expected to play a key role in space exploration in the coming years. Among the various reactors concepts that could be considered for such engine, Molten Salt Reactors (MSRs) offer some intrinsic advantages for Nuclear Electric Propulsion (NEP) from their unique design characteristics. In particular, a MSR allows developing core designs with relatively high power densities and temperatures while keeping lower fuel pressure and temperature gradients and using a simple reactivity control systems. These features are important since they are key to improve the operating performance and the reliability of the nuclear reactor in a space mission. Moreover, such reactor design could be easily scaled for a surface power and thus applied for other type of missions. Nevertheless, the design work of a space MSR poses significant technical challenges, which requires addressing important issues such as material, power conversion system and radiator design, nuclear tests and system integration at the early stages of the design. The IN2P3/CNRS is studying different reactors layouts for Nuclear Electric Propulsion (NEP) in space based on MSRs and also Heat Pipes Reactors (HPRs). We present here some preliminary results develop in ongoing PhD. Thesis of F. QUINTEROS [C1] for a fast neutron MSR concept to illustrate the use of the multiphysics modeling tool in these applications. The main objectives of these preliminary studies are to assess the performance of the selected reactor layout and materials. In particular, to confirm whether the design allow obtaining adequate neutron fluxes, temperatures and temperature gradients on the materials. It is important to note that these studies could not be carried-out with standard numerical tools.

The first step on the design process of a nuclear space reactor is to determine, for a given reactor layout and material composition, the minimal core mass that is required to achieve criticality and sufficient reactivity margin. The approximate core layout used in this study is shown in Figure 7. The adopted spherical core geometry is similar to one used in one of the concepts proposed in the Aircraft Nuclear Propulsion (ARE) project. This geometry allows minimizing the neutron leaks and the shielding requirements. It also helps improving the core cavity flow distribution. Two particular differences with the ARE design are that the pumps and Heat Exchangers (HX) are placed outside the core and that the flow inlet and outlet pipes are located in one side of the core cavity.

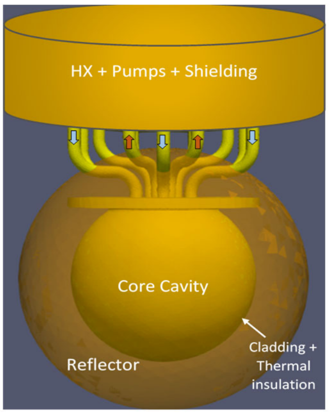
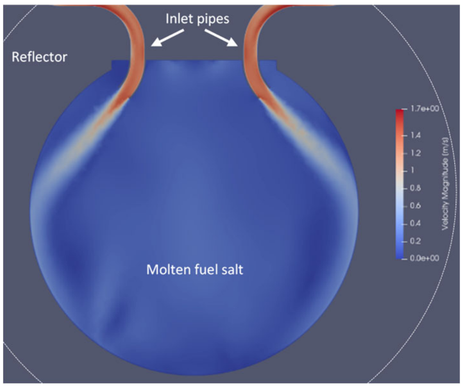
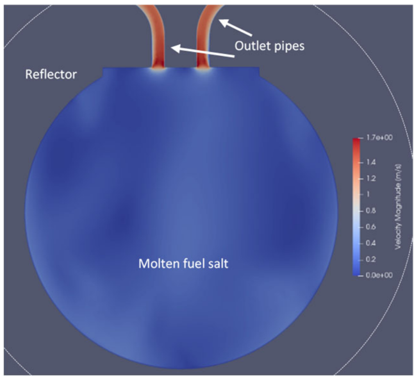


Figure 7. Approximate layout of a fast MSR for space propulsion.

In a space MSR, the selection of the material for the core reflector has to be done together with the molten salt in order to minimize the critical core mass. The critical mass studies using different materials showed that the best candidates for the reflector were Beryllium (Be) or Beryllium oxide (BeO). While BeO has a higher melting point than Be (~2550 °C versus ~1287°C respectively), Be offers a better neutronic performance and thus allows obtaining the lowest core critical mass. Once the layout and some of the material candidates were chosen, the multiphysics model was used to estimate the neutron flux and temperature distributions in the core material for a Low Enriched Uranium (LEU) and High Enriched Uranium (HEU) fuel versions of the reactor. One of the goals of these studies was to determine if some of the material limits were exceeded (for example swelling due to neutron damage). Some selected results obtained for the LEU version are presented in Figures 8 to 10.

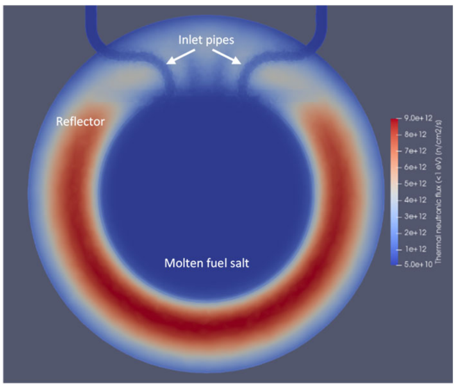


(a) Velocity magnitude across a two inlet pipes plane.

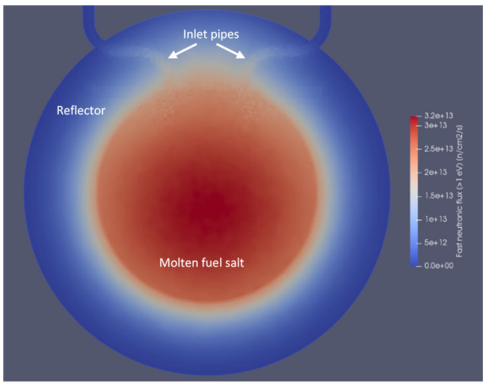


(b) Velocity magnitude across a two outlet pipes plane.

Figure 8. Molten fuel salt velocities obtained for the LEU reactor using a k-□ SST RANS models.

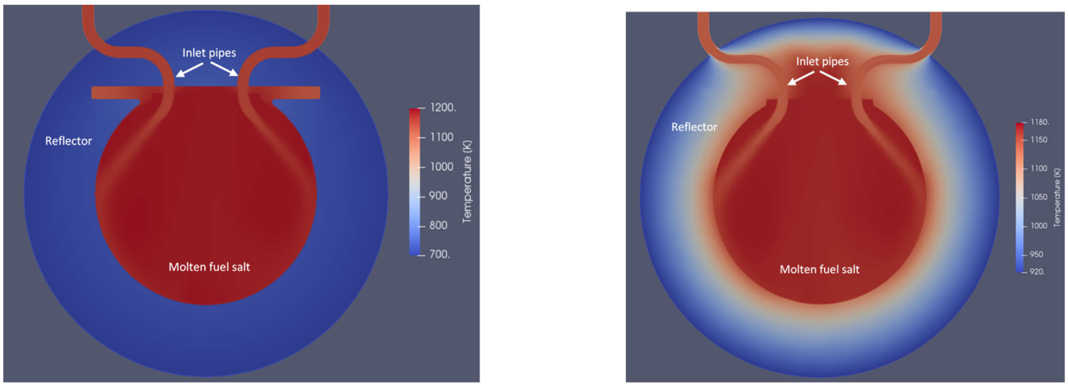


(a) Thermal flux distribution (<1 eV).



(b) Fast flux distribution (1 eV – 10 MeV).

Figure 9. Neutron fast and thermal fluxes distributions in the LEU reactor core.



(a) Temperature field with a thermal insulation. (a) Temperature field without a thermal insulation.

Figure 10. Effect of a carbon foam thermal insulation between the cladding and the reflector.

These preliminary results show that for the LEU concept show satisfactory values for temperature and power distributions in the molten fuel salt and the core structure. Moreover, the numerical simulations show that the use of a thermal insulation between the cladding and the reflector allows efficiently controlling the temperature in the reflector (this is a key point). While a HEU core version used for the purpose of a comparison would allow to obtain the lower specific mass than the LEU, the resulting higher fast fluence in the reflector would likely require the use of a different reflector material or a lower power density and thus decrease its advantages with respect to the LEU. Moreover, the use of HEU in space reactors is not judged a realistic option given the current the non-proliferation policies.

(iii) Criticality and severe accidents

Criticality accidents are accidents involving safety-criticality installations (e.g. industrial facility) containing fissile material and where criticality conditions are prohibited. The criticality accident occurs in these facilities when a persisting neutron chain is developed, eventually culminating in a critical or super-critical state as result of a design flaw or abnormal conditions. Such uncontrolled events, called criticality accidents, can result in the release of high radiation doses and cause possible dispersion of radioisotopes, while possibly exposing the workers and the public.

The modeling of the criticality accidents is challenging because of the diversity of the installations where this event could occur. Criticality accidents involved thus very diverse phenomena and configurations: (i) Time scale (from microseconds to hours), (ii) Geometry (few centimeters to many meters), (iii) Materials (metallic uranium/plutonium, uranyl nitrate, molten salts, etc.), (iv) Phases existing in the system during the accident (liquid, solid, gas) and (v) Phenomena (precursors, radiolysis, pressure waves, etc.). For these reasons, different numerical tools for specific systems have been historically developed to investigate these accidents. Today, the diversity of these numerical tools poses a challenge in term of the maintenance and also concerning the consistency on the overall modeling approach for these accidents. The multiphysics tool being developed for the MSR was actually well suited to investigate these accidents because their models are based on first principles and thus provide a large flexibility in terms of phenomena (and couplings) that can be studied. Indeed, a multi-physical and multi-scale approach aims to produce a numerical model taking into account all the important physical phenomena in nuclear systems as well as their coupling. This type of tools is therefore well suited to study criticality accidents since: (a) They can be used to numerically investigate the behavior of systems under conditions that are difficult to achieve or reproduce by experiments, (b) They provide Best Estimate (BE) values, (c) They have significant flexibility in terms of time and space scales and allow obtaining predictions on the evolution of these accidents in reasonable times.

A collaboration was the IRSN was thus developed on the used of the multiphysics tool for modeling these accidents through a conjoint PhD thesis of J. BLANCO. The objectives of this thesis were firstly to develop a new numerical scheme for the coupling between the neutronic code Serpent 2 (Monte Carlo code) and the Computational Fluid Dynamics (CFD) code OpenFOAM. Secondly, to develop the physical models that allow greater flexibility for criticality accidents studies in terms of type of transients, systems and phenomena considered. Among the various physical models developed during the work, it can be mentioned the two transient neutronic models based on a quasi-static Monte Carlo approach and on the deterministic SP_1 and SP_3 methods. A porous medium model was also developed during the work to allow performing studies on nuclear systems containing a solid nuclear fuel cooled by a fluid. The numerical implementation of the multi-physics coupling was performed in the OpenFOAM code in C++.

The performances of the coupling and the developed models were studied for different scenarios and systems as shown in the Figure 11: (1) The transient Godiva experiments (Los Alamos National National Laboratory), (2) An international benchmark for multi-physics codes for Molten Salts Reactors (in the framework of the European SAMOFAR project) and (3) The case of a hypothetical criticality accident in a Boiling Water Reactor (BWR) spent fuel pool. These diverse scenarios and systems were selected because they are characterized a multitude of highly coupled physical phenomena which required a precise modeling. Among the studied phenomena, it can be mentioned the Doppler and density effect, the thermal expansion and the thermomechanical stresses (Godiva), the laminar or turbulent flows, the mass and energy transfer phenomena in porous medium (spent fuel pool). A summary of the key phenomena in each of the studied cases is given in the Table 2.

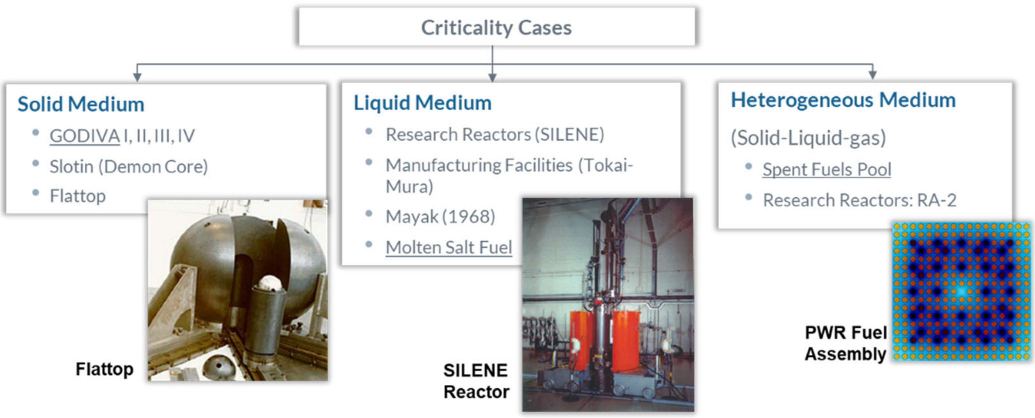


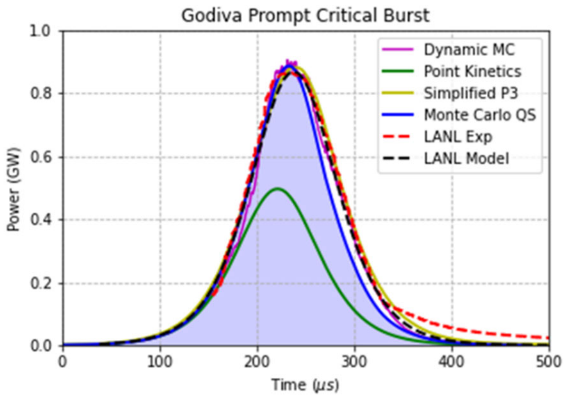
Figure 11. Nuclear systems studied in the criticality accidents collaboration with the IRSN.

Study Case	Main key phenomena
Godiva Experiment Solid Homogeneous Medium	• Prompt Supercritical Transient • Thermal Expansion and mechanical stresses • Geometry effect
CNRS Molten Salt Cavity Benchmark Liquid Homogeneous Medium	• Precursors Convection • Laminar/Turbulent Flow • Buoyancy effects • Forced Convection
Spent Fuel Pools Solid-Liquid Heterogeneous Medium	• Re-criticality • Multi-phase multi-component
Slab Reactor Solid Homogeneous Medium	• Large reactivity insertion ($\rho \cong 90\beta$) • Very rapid change on the flux shape

Table 2. Key phenomena for the various systems investigated in criticality accidents.

Selected results obtained during the PhD thesis of J. BLANCO from the multiphysics model and the comparison against the existing data for these cases are given in the next Figures. Firstly, Figure 12 compares the predictions from various the different transient neutronics models (Point kinetics, SP_n and the new Monte Carlo Quasi-static model) implemented in the multiphysics tool to the experimental data from the Godiva burst. Also results from an advanced simulations using a Dynamic Monte Carlo approach are given [C30]. Godiva experiment (the experimental setup is shown on the left of Figure 12) was built by Los Alamos National Laboratory (LANL) and has been in operation since August, 1951. The experiment uses a highly enriched uranium sphere to generate a prompt neutron burst to study very fast transients (order of microseconds). The comparison shows that the two transient neutronics models: SP_n and the Monte Carlo Quasi-Static implemented in the multiphysics tool provided very good predictions.

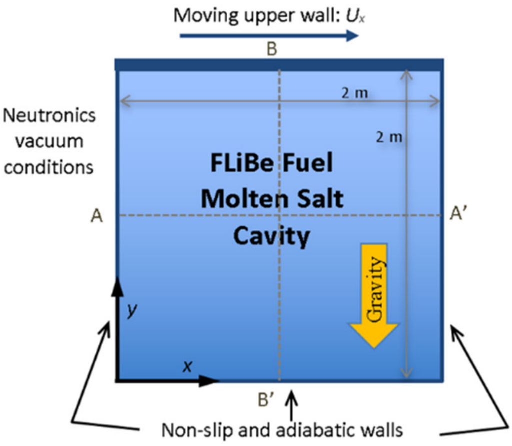
(a) The Godiva Experiment.



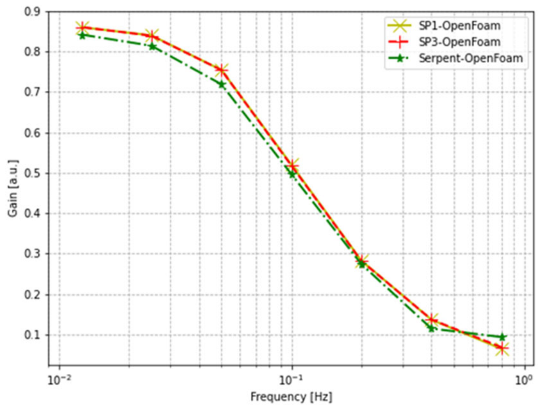
(b) Predicted Godiva prompt critical brust.

Figure 12. Numerical simulation of the Godiva reactor.

In figure 13, the multiphysics predictions for the CNRS Molten Salt Cavity Benchmark [C18] using the SP3 model (previously benchmarked with other codes [J2]) were compared against the Quasi-Static Monte Carlo model. This numerical benckmark was originally developed to evaluate the couplings in multiphysics tool and later by European Project SAMOFAR partners for multi-physics codes comparison. The benchmark uses a 2-D Square Cavity with 2 m side length and laminar flow conditions, under gravity and with a moving upper wall, filled with a U_{235} FLiBe Molten Salt, without any reactivity control external mechanisms but allowing neutronics feedback effects. The benchmark can thus be used to asses the accuracy of transient neutronics models in systems having very specific phenomena: (a) Sub- and super- critical transient ($\rho>0$), (b) Oscillatory heat sink, (c) Density Feedback, (d) Fuel Motion, (e) Forced and natural convection and (f) Precursors advection . The right side of Figure 13 display a Bode diagram for the Power Gain of this system obtained when a periodic perturbation of the system heat sink is imposed. The gain is calculated using the nuclear power of the system as the output and the perturbation in the heat sink as the input. This analysis provides thus important information on the tool response at different time scales. The results of figure 13 shows [C5] that both transient neutronics models provide similar results and they are in agreement with those of the other codes used by SAMOFAR partners.



(a) Layout of the CNRS benchmark.



(b) Predicted Power Gain.

Figure 13. Numerical simulation of the Godiva reactor.

In conclusion, comparison between the multiphysics model predictions and the available data existing from these diverse cases shows a very good agreement and confirm the pertinence and the interest of using a multiphysics tool for studying criticality accidents.

(iv) Targets for neutron production

This activity have been mainly focused on the design of liquid and solid targets exposed to a particles beam obtained from an accelerator that produces neutrons for the BNCT (Boron Neutron Capture Therapy). The liquid target being investigated in the project consists in rotating target using a lithium liquid metal where the nuclear reaction producing neutron takes place. The study of such type of targets required developing numerical models and also experiments with strongly coupled heat transfer, fluid mechanics and nuclear reactions phenomena. Further development of this activity depends upon the funding opportunities.

3.3- Program Milestones

After this overview of the main multiphysics activities developed since 2014, the following list summarizes the main milestones of the multiphysics activities both concerning experimental and numerical aspects:

- Development of a coupled thermal-hydraulics (CFD) and neutronics (TFM method) transient model for the Molten Salt Fast Reactor (PhD LAUREAU, 2015).
- Development of a numeric benchmark to evaluate multiphysics couplings (Postdoc AUFIERO, 2015).
- Use of a compressible flow solver to investigate the propagation of pressure waves in the molten salt during accidents in the MSFR (Postdoc AUFIERO, 2015)
- Design, construction and operation of the SWATH-W and SWAT-S facilities (2017).
- Perform PIV measurement in the Backward Facing Step (BFS) test section (2017).
- Development of non-linear turbulent RANS models for MSRs (PhD TANO, 2018).
- Perform the solidification experiments (2018).
- Development of a solidification/melting model for eutectics motel salts (PhD TANO, 2018).
- Perform the cold plug experiments at SWATH-S (2018).
- Perform the close circular channel experiment in SWATH-S (2018).

- Addition of thermal radiation heat transfer in the molten salt thermal-hydraulics model (PhD TANO, 2019).
- Development of thermomechanics equations and performing coupled transient neutronics and thermomechanics simulations (PhD BLANCO, 2019).
- Implementation of a SP_1 and SP_3 neutronics solvers in OpenFOAM (PhDs TANO & BLANCO 2019).
- Development of a quasi-static Monte Carlo for transient calculations based on a Serpent and OpenFOAm coupling (PhD BLANCO, 2020).
- Implementation of porous media equations with several phases to model spent fuel pool accidents (PhD BLANCO, 2020).
- Perform the square flat channel experiments in SWATH-S (2021).
- Addition of multi-region capabilities (liquid fuel, cladding and reflector), conjugate heat and decay heat modeling for the space reactor model (PhD QUINTEROS, 2021).

3.4- Education and Training (since 2015)

As discussed early, the multiphysics research carried-out at FEST have been strongly correlated to education and training activities. These activities are summarized in this section.

(i) Internship

[1] Yi DING, Mathilde SCHUCHARD, Hugo LEVICES, "*Validation of a Thermo-Electric (TE) numeric model*", UGA Master degree research project, February-May 2022.

[2] Martin MARONE, "*Development of a simplified conceptual design model for nuclear HP space reactors* », Master degree internship, February-July 2022.

[3] Tomas MOLINA, "*Thermal-hydraulics modeling of a molten salt flow in a close square channel*", Master degree internship, March-August 2021.

[4] Giulia BORTOLATO, "*Development of a numerical model for thermal-electric converters*", Master degree internship, March-July 2021.

[5] Jonas Sebastian NARVAEZ ARRUA, "*Enhancing the CNRS Multiphysics benchmark to investigate a triple coupling code for design of a Nuclear Electric Propulsion (NEP) reactor*", Master degree internship, October 2019-March 2020.

[6] Valentin RICHARD, « *Mise au point d'un modèle multi-physique pour la conception d'un réacteur de propulsion nucléaire dans l'espace* », Engineering degree internship, February - July 2019.

[7] Michel GARTNER, « *Nuclear design of space propulsion reactor concept based on a molten salt fueled reactor* », Engineering degree internship, October 2018 - March 2019.

[8] Francisco KOVACEVICH, « *Design of a close squared channel experiment to study coupled convection and thermal radiation heat transfers in a molten salt flow experiment* », Engineering degree internship, October 2018 - March 2019.

[9] Laurick HUGUET, « *Options et choix de conception pour la propulsion nucléaire dans le espace* », Engineering degree internship, March – August 2018.

[10] Ramiro FREILE, « *Determination unsteady flow patterns using noise analysis techniques and a simplified PWR core model* », Engineering degree internship, October 2017 – March 2018.

[11] Juan Antonio BLANCO, « *Thermal-hydraulic modeling of a high temperature molten-salt for the SWATH experiment* », Engineering degree internship, October 2016 – February 2017.

[12] Vincent AIT-AMMAR, « *Couplage Neutronique-Thermohydraulique pour la modélisation des accidents dans des systèmes nucléaires* », Engineering degree internship, March 2016 – August 2016.

[13] Nahuel Alejandro VILLA, « *Modélisation CFD (Computational Fluid Dynamics) d'un sel fondu à haute température* », Engineering degree internship, October 2015 – February 2016.

[14] Francisco ACOSTA, « *Étude des écoulements non-stationnaires dans les réacteurs nucléaires* », Engineering degree internship, October 2015 – February 2016.

[15] Sebastien PERRET, « *Modélisations des écoulements d'un sel fondu avec FLUENT* », Internship, June 2015 - July 2015.

[16] Mauricio TANO-RETAMALES, « *Couplage thermo-hydraulique et neutronique pour un réacteur à sel fondu* », Engineering degree internship, March 2015 - July 2015.

[17] Juan Ignacio BELIERA, « Thermal-hydraulic modeling of the Molten-Salt Fast Reactor (MSFR) Heat Exchangers (HXs)", Engineering degree internship, October 2014 - February 2015.

(ii) PhD thesis

[1] Jonás Sebastián NARVAEZ ARRUA, "*Numerical and experimental study of the dynamic behavior of natural circulation systems using molten salts for heat removal*", PhD thesis defense expected on November 2023.

[2] Franco Emanuel QUINTEROS, "*Conceptual design of a nuclear electric propulsion reactor (MSR type) for space exploration"*, PhD thesis defense expected on February 2023.

[3] Juan Antonio BLANCO, « *Neutronic, Thermohydraulic and Thermomechanical Coupling for the Modeling of Criticality Accidents in Nuclear Systems"*, December 2020.

[4] Francisco ACOSTA, "*Thermal-Hydraulics / Thermomechanics Coupling for the Simulation of the Behavior of Sodium-cooled Fast Reactors' Subassemblies under Irradiation",* October 2019.

[5] Mauricio TANO RETAMALES, "*Developement of multi-physical multiscale models for molten salts at high temperature and their experimental validation »*, November 2018.

[6] Henri GEISER, « Uncertainties propagation method for a Medium Break (MB) Loss of Coolant Accident (LOCA)", 2016 – 2018 (abandoned for personal reasons).

[7] Axel LAUREAU, "*Development of neutronic models for the thermalhydraulics coupling of the MSFR and the calculation of effective kinetic parameters"*, October 2015.

(iii) Postdoc

[1] Martin LEMES, « *Flow Induced Vibrations (FIV) due to turbulent flow and PWR fuel predict fretting-wear damage* », visiting scientist at the LPSC-Grenoble, funding from ARFITEC, June 2018.

[2] Ségolène JAMET, « *Étude d'un nouveau modèle de transitoire d'interface appliqué à l'interaction corium-béton* », lieu LPSC-Grenoble, funding EDF, April 2017 to Septembre 2018.

[3] Manuele AUFIERO, « *Simulation physique des réacteurs, projet Molten Salt Fast Reactor* », March 2014 to April 2015.

3.5- Publications in Multiphysics since 2015

Publications related to the multiphysics activities are reported in this section.

(i) Journal publications

[J1] F. Acosta, P. Rubiolo, V. Blanc, T. Cadiou, "Application and Benchmarking of a Novel Coupled Methodology for Simulating the Thermomechanical Evolution of Sodium-cooled Fast Reactors Fuel Subassemblies", Nuclear Engineering and Design, Vol. 374 (2021).

[J2] M. Tiberga, R. Gonzalez Gonzaga de Oliveira, E. Cervi, J. A. Blanco, S. Lorenzi, M. Aufiero, D. Lathouwers, P. Rubiolo, "Results from a multi-physics numerical benchmark for codes dedicated to molten salt fast reactors", Annals of Nuclear Energy, Vol. 142, (2020) pp. 1-19.

[J3] J. Giraud J., V. Ghetta V., P. Rubiolo, M. Tano Retamales, "*Development of a Cold Plug Valve with Fluoride Salt*", EPJ Nuclear Sciences & Technologies, Vol. 5 (2019) pp. 1-12.

[J4] F. Acosta, T. Cadiou, V. Blanc, P.R. Rubiolo, "*On the thermal-hydraulics/thermomechanics coupling for the modeling of the behavior of Sodium-cooled Fast Reactors fuel subassemblies under irradiation*", Nuclear Engineering and Design, Vol. 348 (2019) pp. 90-106.

[J5] K. Laureau, D. Heuer, E. Merle-Lucotte, P.R. Rubiolo, M. Allibert, M. Aufiero, "*Transient coupled calculations of the Molten Salt Fast Reactor using the Transient Fission Matrix approach*", Nuclear Engineering and Design Vol. 316 (2017) pp. 112–124.

[J6] M. Tano-Retamales, P.R. Rubiolo, O. Doche, « *Progress in modeling solidification in molten salt coolants* », International Journal of Modelling and Simulation in Materials Science and Engineering, Vol. 5, Issue 7 (2017).

[J7] C. Fiorina, N. Kerkar, K. Mikityuk, P.R. Rubiolo, A. Pautz, « *Development and verification of the neutron diffusion solver for the GeN-Foam multi-physics platform* », Annals of Nuclear Energy, Vol. 96 (2016) pp. 212-222.

[J8] A. Laureau, M. Aufiero, P.R. Rubiolo, E. Merle-Lucotte, D. Heuer, "*Transient Fission Matrix: Kinetic calculation and kinetic parameters βeff and Λeff calculation*", Annals of Nuclear Energy, Vol. 85 (2015) pp. 1035–1044.

[J9] M. Aufiero, A. Bidaud, M. Hursin, J. Leppänen, G. Palmiotti, S. Pelloni, P.R. Rubiolo, "*A collision history-based approach to sensitivity/perturbation calculations in the continuous energy Monte Carlo code SERPENT*", Annals of Nuclear Energy, Vol. 85 (2015) pp. 245-258.

(ii) International conferences

[C1] F. Quinteros, P. Rubiolo, V. Ghetta, J. Giraud, N. Capellan, "*Design Studies of a Molten Salt Reactor for Space Nuclear Electric Propulsion*", *International Conference on Physics of Reactors 2022 (Physor 2022), Pittsburgh, USA, May 2022*.

[C2] P. Rubiolo, M. Tano, J. Blanco, V. Ghetta, J. Giraud, V. Richard, F. Quinteros, "*A Numerical Tool for Space Nuclear Reactor Design based on Molten Salt Reactors (MSRs)*", *Transactions of the American Nuclear Society*, Vol. 122, N°1, pp. 679-681, ANS Virtual Annual Meeting, June, 2020.

[C3] P. Rubiolo, J. Giraud, V. Ghetta, M. Tano, J. Blanco, F. Kovacevich, "*Design of a Flat Channel Experiment to Study Molten Salt Thermal Radiation Heat Transfer*", *Transactions of the American Nuclear Society*, Vol. 122, N°1, pp. 909-912, ANS Virtual Annual Meeting, June, 2020.

[C4] C. Fiorina, P. Shriwise, A. Dufresne, J. Ragusa, K. Ivanov, T. Valentine, B. Lindley, S. Kelm, E. Shwageraus, S. Monti, C. Batra, A. Pautz, S. Lorenzi, P. Rubiolo, I. Clifford, "*An Initiative for the Development and Application of Open-source Multi-physics Simulation in Support of R&D and E&T in Nuclear Science and Technology*", International Conference on Physics of Reactors 2020: Transition to a Scalable Nuclear Future (Physor 2020), Cambridge, United Kingdom, March 2020.

[C5] J.A. Blanco, P. Rubiolo, E. Dumonteil, "*Neutronic modeling strategies for a liquid fuel transient calculation*", International Conference on Physics of Reactors 2020: Transition to a Scalable Nuclear Future (Physor 2020), Cambridge, United Kingdom, March 2020.

[C6] J.A. Blanco, P.R. Rubiolo, E. Dumonteil, "*Multiphysics Coupling Analysis for Spent Fuel Pool Loss of Coolant Accident*", ICNC 2019 - 11th International conference on Nuclear Criticality Safety, Paris (France), September 2019.

[C7] M. Tano, P.R. Rubiolo, J. Ragusa, "*Direct Numerical Simulations of Turbulence in Molten Salt Coolants*", ANS Topical Meeting on Mathematics and Computations (MC 2019), Portland (USA), August 2019.

[C8] F. Acosta, V. Blanc, P. Rubiolo, T. Cadiou, "*Simulating the Thermomechanical Evolution of SFR Fuel Bundles with a Coupled Approach*", 25th Conference on Structural Mechanics in Reactor Technology (SMIRT25), Charlotte (USA), August 2019.

[C9] M. Tano, P.R. Rubiolo, J. Ragusa, "*Non-linear Eddy Viscosity Models for the Turbulent Phenomena in Molten Salt Reactors*", ANS Topical Meeting on Mathematics and Computations (MC 2019), Portland (USA), August 2019.

[C10] M. Tano, P.R. Rubiolo, J. Ragusa, "*Accuracy Analysis of Near Wall Thermal-Hydraulics Modeling of Molten Salt Reactors*", 18th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-18), Portland (USA), August 2019.

[C11] M. Tano, P.R. Rubiolo, J. Ragusa, "*Progress in Thermal-hydraulics Modeling of the Molten Salt Fast Reactor*", 18th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-18), Portland (USA), August 2019.

[C12] P.R. Rubiolo, M. Tano Retamales, V. Ghetta, N. Capellan, J. Giraud, J. Blanco, S. David « Molten Salt Reactors for Nuclear Electric Propulsion », Nuclear and Emerging Technologies for Space, American Nuclear Society Topical Meeting, Richland, WA, February 2019.

[C13] J.A. Blanco, P.R. Rubiolo, E. Dumonteil, "Quasi-static methods performance comparison for neutronics transient calculations", *Transactions of the American Nuclear Society*, Vol. 119, pp. 1145-1145, Orlando (Etats Unis), Novembre, 2018.

[C14] P.R. Rubiolo, M. Tano-Retamales, J. Giraud, V. Ghetta, J. Blanco, "Numerical and Experimental Thermal Hydraulics Studies of High Temperature Molten Salts for Generation IV Nuclear reactors", *Proceedings of the GIF Symposium*, Paris (France), Octobre 2018.

[C15] J. Giraud, V. Ghetta, P.R. Rubiolo, M. Tano-Retamales, "Development and Test of a Cold Plug Valve with Fluoride Salt", *12th International Topical Meeting on Reactor Thermal-Hydraulics, Operation, and Safety (NUTHOS-12)*, Qingdao City, Shandong Province, China, Octobre 2018.

[C16] S. Jamet, J.M. Seiler, P.R. Rubiolo, B. Tourniaire, "Progress in the Modeling of Molten Corium Concrete Interaction", *12th International Topical Meeting on Reactor Thermal-Hydraulics, Operation, and Safety (NUTHOS-12)*, Qingdao City, Shandong Province, China, Octobre 2018.

[C17] F. Acosta, T. Cadiou, V. Blanc, P.R. Rubiolo, "Evaluation of thermal-hydraulics/thermomechanics coupling strategies for the modeling of the behavior of Sodium-cooled Fast Reactors fuel assemblies under irradiation", *12th International Topical Meeting on Reactor Thermal-Hydraulics, Operation, and Safety (NUTHOS-12)*, Qingdao City, Shandong Province, China, Octobre 2018.

[C18] M. Aufiero, P.R. Rubiolo, "Testing and verification of multiphysics tools for fast-spectrum MSRs: the CNRS benchmark", *International Seminar on Nuclear Reactor Core Thermal Hydraulics Analysis (IS-ReCTHA 2018)*, Lecco, August 29-31, 2018.

[C19] H. Geiser, J.L. Vacher, P.R. Rubiolo, « Sensitivity Analysis Applied to LOCA Integral Effects Tests for the Justification of the BEPU Approach », Proceedings of the *2018 ANS International Conference on Best-Estimate Plus Uncertainties Methods (BEPU-2018)*, Lucca (Italie), Mai 2018.

[C20] M. Tano-Retamales, P.R. Rubiolo, O. Doche, « Multiphysics study of the draining transients in the Molten Salt Fast Reactor », *2018 International Congress on Advances in Nuclear Power Plants* (ICAPP 18), pp.215-225, Charlotte (Etats Unis), Avril 2018.

[C21] M. Tano-Retamales, P.R. Rubiolo, J. Giraud, V. Ghetta, « On the use of inverse problem methods in nuclear reactors design applications », *2018 International Congress on Advances in Nuclear Power Plants* (ICAPP 18), pp.701-711, Charlotte (Etats Unis), Avril 2018.

[C22] P.R. Rubiolo, M. Tano-Retamales, J. Giraud, V. Ghetta, J. Blanco, O. Doche, N. Capellan, « Design of close and open channel experiments to study molten salt flows », *2018 International Congress on Advances in Nuclear Power Plants* (ICAPP 18), Charlotte (USA), Avril 2018.

[C23] M. Aufiero, P.R. Rubiolo, M. Fratoni, « Monte Carlo/CFD coupling for accurate modeling of the delayed neutron precursors and compressibility effects in molten salt reactors », *Transactions of the American Nuclear Society*, Vol. 119, pp. 1183-1186, San Francisco (Etats Unis), June 2017.

[C24] H. Geiser, J.-L. Vacher, P.R. Rubiolo, "The use of Integral Effects Tests for the justification of new evaluation models based on the BEPU approach", *Proceedings of 17th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH17)*, Xi'an (China), September 2017.

[C25] P.R. Rubiolo, M. Tano Retamales, V. Ghetta and J. Giraud, "High temperature thermal hydraulics modeling of a molten salt: application to a molten salt fast reactor (MSFR)", *ESAIM: Proceedings and surveys*, Vol. 58, pp. 98-117 (2017).

[C26] M. Tano-Retamales, P.R. Rubiolo, O. Doche, « Development of solidification models for molten salts coolants », *Proceedings 8th International Conference on Multiscale Materials Modeling*, Vol. 1, pp. 815-826, Dijon (France), October 2016.

[C27] M. Tano-Retamales, P.R. Rubiolo, O. Doche, « Development of Data-Driven Turbulence Models in OpenFOAM - Application to liquid fuel nuclear reactors », *Proceedings 11th OpenFOAM worksho*p, pp. 106-118, Guimaraes (Portugal), November 2016.

[C28] P.R. Rubiolo, M. Tano, J. Giraud, V. Ghetta, « Overview of the Salt at WAll Thermal ExcHanges (SWATH) Experiment », *Transactions of the American Nuclear Society*, Vol. 115 pp. 1705-1708, Las Vegas (USA), November 2016.

[C29] A. Laureau, M. Aufiero, P.R. Rubiolo, E. Merle-Lucotte, D. Heuer, "Coupled Neutronics and Thermal Hydraulics Transient Calculations Based on a Fission Matrix Approach: Application to the Molten Salt Fast Reactor", *Joint International Conference on Mathematics and Computation (M&C), Supercomputing in Nuclear Applications (SNA) and the Monte Carlo (MC) Method*, Nashville (USA), Avril 2015.

[C30] M. Aufiero, C. Fiorina, A. Laureau, P.R. Rubiolo, V. Valtavirta, "Serpent-OpenFOAM coupling in transient mode: simulation of a Godiva prompt critical burst", *Joint International Conference on Mathematics and Computation (M&C), Supercomputing in Nuclear Applications (SNA) and the Monte Carlo (MC) Method*, Nashville (USA), Avril 2015.

(ii) European projects deliverables

[D1] V. Ghetta, V, J. Giraud, P.R. Rubiolo, M. Tano-Retamales, « D3.1 MSFR Fuel Salt Conditions During Typical Draining Transients», *Deliverable 3.1 EURATOM H-2020 European SAMOFAR (Grant Agreement number: 661891)*, pp. 1-62 (2017).

[D2] V. Ghetta, V, J. Giraud, P.R. Rubiolo, M. Tano-Retamales, « D3.3 Design and Building of SWATH Experiment (Shut-Down System)», *Deliverable 3.3 EURATOM H-2020 European SAMOFAR (Grant Agreement number: 661891)*, pp. 1-63 (2017).

[D3] V. Ghetta, V, J. Giraud, P.R. Rubiolo, M. Tano-Retamales, « D3.5 Experimental campaign in the SWATH facility and validation of numerical models », *Deliverable 3.5 EURATOM H-2020 European SAMOFAR (Grant Agreement number: 661891)*, pp. 1-62 (2018).

[D4] V. Ghetta, V, J. Giraud, P.R. Rubiolo, M. Tano-Retamales, « D3.7 Recommendations for the MSFR shut down and DHR passive system », *Deliverable 3.7 EURATOM H-2020 European SAMOFAR (Grant Agreement number: 661891)*, pp. 1-29 (2019).

3.6- Funding and manpower (since 2015)

(i) Funding

Up to now, the principal sources of funding of the numerical and experimental multiphysics activities have been by far the H2020 Euratom projects SAMOFAR (2015-2019) and SAMOSAFER (2019-2023). The SAMOFAR project provided the funding for the design and construction of the SWATH facilities (SWATH-W using water and SWATH-S using a FLiNaK molten salt). SAMOFAR also provided funding for the development of the experimental sections that were studied in these two facilities: the Backward Facing Step (BFS), the circular channel section, the cold plug experiment and the solidification experiment. At present, the SAMOSAFER project is providing funding for the operation of SWATH and also for developing three experiments: the Flat Squared Close Channel (FSCC), the Open Channel (OC) and a natural convection experiment.

Funding for the PhD thesis have always been obtained outside from these European projects and include diverses sources such the Grenoble I-MEP2 Doctoral School (2.5 bourses), internal funding from the team budget (1 bourse) and the IN2P3 (0.5 bourse). Three industrial collaborations have also contribute with funding for the graduate students: (i) A collaboration on criticality accidents with the IRSN who funded 50% of the PhD of J. Blanco, (ii) The CIFRE PhD of H. GEISER fully funded by EDF and (iii) The Postdoc of S. JAMET on corium-concrete interaction also fully funded by EDF.

(ii) Manpower

The team involved in the multiphysics numerical and experimental activities at the LPSC is relatively small and composed by the following personnel from the LPSC-Grenoble:

- Nicolas CAPELLAN (Grenoble INP assistant professor)
- Véronique GHETTA (CNRS researcher)
- Julien GIRAUD (CNRS research engineer)
- Pablo RUBIOLO (Grenoble INP professor)

3.7- Perspectives

The current and future efforts will remain focused in the four activities described in section 3.2. For the MSR modeling will be completing the numerical and experimental tasks of the SAMOSAFER project

(2019-2023). In particular, the open channel and the natural convection experiments. Multiphysics activities related to MSRs will continue in the framework of the PIA4 project ISAC (Innovative System for Actinides Conversion, 2022-2026). Partners of this project include the CEA, CNRS, EDF, FRAMATOME and ORANO. Our main task in ISAC will be to develop an experimental and numerical study of the production, transport and separation of fission products in the molten fuel salt of reactor concept studied in this project.

Concerning nuclear space propulsion, our goal is to continue exploring different reactor designs beyond Molten Salt Reactors (MSRs). The objective will be to enhance the current numerical tools to include other possible reactor designs such as Heat Pipe Reactors and eventually perform small-scale thermal experiments at FEST. We will pursue collaborations with international partners such as POLIMI and with national partners such as the CNES, CEA and TECHNICATOME.

On the safety domain, it would be suitable to develop a new collaboration with the IRSN in order to maintain develop effort for the use of the multiphysics tool for criticality accident analyses. Indeed, important improvements are still necessary to be able to cover the different systems that could be study in criticality accidents.

Finally, the prospect of the multiphysics activities related to nuclear targets seems to be more uncertain at this time. They will likely benefit from the other activities developed by the program but their development will ultimately depend on whether the AB-BNCT activity is continued.