Advanced Numerical Simulation for the Safety Demonstration of Nuclear Power Plants

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1. Introduction

Existing commercial nuclear power plants (NPPs) have obtained excellent and outstanding performance records over the past decade. Nevertheless, even though the high safety level already achieved could be maintained without investing new exhaustive research efforts, anticipation of further tighter requirements for even higher standard levels should be made, which implies preparedness for new research. Accordingly, in the near and intermediate future, research will conceivably focus on new emerging trends as a result of further desire to reduce the current uncertainties for better economics and improved safety of the current reactors and requirements of the new reactor designs.

As it has been usual in the past, the research will continue serving the short-term needs of the end-users (regulatory bodies, utilities and vendors) which mainly focus on both emerging and pending issues, but it will also contribute to addressing the long-term safety needs or the questions arising from the changes in plant designs and operating modes, and to preparing the emergence of new concepts. The sensibility of the stakeholders for a continuous enhancement of safety, mainly when dealing with the advanced and innovative concepts, will entail the development of reactor concepts able to intrinsically prevent severe accidents from occurring, and, should that not be possible, reduce either their probability or the level of expected consequences on the environment and the populations. That should be done in first priority by design, and not necessarily by improvements or the addition of safety systems.

Such anticipatory research will involve new generation simulation tools and innovative experimental programs, to be carried out both in the research facilities currently in operation throughout the world and in new dedicated mock-ups supported by suitable laboratory infrastructures. Enhanced or complementary data banks to be generated and further investigations on human and organizational factors will be the primary research activities, from which the end users will definitely profit.

In addition, significant efforts should be devoted to get the maximum benefit from the computation tools already available and start preparing their improvements as well by taking advantage from the development and availability of new computation techniques, such as advanced numerical simulation.

Their applicability should be extended to all types of current and future water cooled reactors and validated under the conditions of new designs. Such an "extrapolation" of the already gathered knowledge in the field of Light Water Reactors (LWRs) would maximize benefit from the work already done and could save some major efforts in the future.

2. Numerical simulation in the current nuclear safety context

In a context of a worldwide renaissance of nuclear energy, the most important pending milestones for the Generation II reactors are the periodic safety review (every ten years in France), which include safety reassessments, as well as the demand for long-term operation of the plants - far beyond their original design lifetime -. Additionally, the safety assessment for Generation III and III+ reactors under construction must be carried out and the safety demonstration for future highly innovative Generation IV (GEN IV) reactors accurately prepared.

On the other hand, over the past decade, considerable progress has been made in the domain of numerical simulation in many fields of endeavor.

In this challenging context, the following two main questions are raised:

- Could the safety demonstration of current and future power plants benefit from the progress currently made in numerical simulation?
- Does the safety demonstration of GEN IV concepts require a breakthrough in terms of numerical simulation?

This chapter is intended to address both questions and provide with preliminary elements of answer. In its first part, through some selected examples, it illustrates the development perspectives for the computation tools that are currently adopted in the safety demonstration of nuclear power plants, and wonders about the future contribution to these tools of the progress made in advanced numerical simulation. In its second part, for a selected sample of GEN IV concepts, it investigates the directions the modeling efforts (including advanced simulation ones) could and/or should be orientated towards.

At least two ways for progress (which are not mutually exclusive) are identified in the development of computation tools already adopted or to be adopted for current reactor concept design and safety studies:

- The first one relies on a progressive sophistication of the physical models, the codes adopted for Loss Of Coolant Accidents (LOCA) transient studies providing a wide field of application.
- The second one holds on advanced detailed modeling. It includes:
  - The investigation of phenomena at a physical scale significantly smaller than for the current generation of safety codes. It may contribute, through the so-called multi-scale approaches, to improving the macroscopic models (as it is presently the case for the fuel), and/or, whenever possible, to replacing them. A pertinent example in the field of severe accidents is the current use of Computational Fluid Dynamics (CFD) codes to investigate the risk of hydrogen explosion in the containment.
  - The coupling of different physical fields. Pertinent examples can be found in the domain of reactivity accidents, including dilution accidents: for these transients, such as un-borated water injection at shutdown, more accurate methodologies are now under development, they allow coupling different fields contributing to the power excursion (neutronics, fuel thermal-mechanical and thermal-hydraulics).

As far as the GEN IV concepts are concerned, today in France only 3 out of the 6 concepts proposed by the GEN IV International Forum (GIF) are currently considered:

- The Sodium Fast Reactor (SFR) that benefits from significant industrial and operating experience in several countries, including France;
- The Gas Fast Reactor (GFR) that possesses a very high potential in terms of uranium sparing, incineration, transmutation and heat production;
- The High or Very High Temperature Reactor (HTR/VHTR) that is the most likely concept to be inherently safe and multi-use and benefits from a first industrial experience in several countries.

Each of these concepts, according to its physical features and operating mode, engenders specific needs in terms of development and assessment of computation tools. Nevertheless, several major trends can be mentioned as relevant to the safety demonstration and widely independent from the design. At the present and first stage of IRSN's investigation, 5 main issues have been pointed out: the consistence and robustness of neutronics design, the demonstration of the actual capacity to passively and safely evacuate the residual power, the fuel integrity, the quantification of activated fission products that might be released to the environment in case of accidental situations, the inquiry upon the significant reduction of a likelihood of severe core damage, particularly the prevention of the "design basis" conditions from degenerating into severe accidents.

All of them could benefit from the current progress in advanced simulation. The chapter accurately investigates the potential contribution of progress in numerical simulation, and more specifically the advanced one, to the above-mentioned safety issues.

3. Current practice of advanced numerical simulation in nuclear safety

Before addressing the numerical simulation for the safety demonstration of GEN IV concepts, it is worthwhile presenting a quick overview of the present status concerning the use of advanced numerical simulation techniques in current nuclear safety analysis. This status has already been discussed and elaborated in specific seminars and workshops, e.g. the meeting organized by OECD and IAEA (OECD IAEA, 2002) for CFD, as well as in a previous IRSN's paper (Livolant, et al. 2003).

In the following, some LWRs safety related topics are addressed such as: Primary circuit thermal-hydraulics and LOCA, Fuel behavior in Design Basis Accident (DBA), Coupled phenomena in DBA, Severe accidents (SA), and Use of CFD codes in other accidents.

3.1 Primary circuit thermal-hydraulics and Loss Of Coolant Accidents (LOCA)

A key safety problem in LWRs is guaranteeing the coolability of the fuel in any normal operation, incidental and accidental condition, including the worst case of a pipe rupture. The development of codes able to treat the problem with some realism started in the early 70s. At that time, the main challenge was calculating the behavior of a steam-water flow in a hot pressurized circuit, with a breach into the containment building.

Today, various code systems are internationally available. Their physical models are based on experimentally-supported reasonable assumptions on the steam and water flows as well as their mutual interactions. The circuits are represented assembling together 1D pipe elements, 0D volumes, and, whenever possible, 3D components. In the past, intensive experimental programs to validate these codes have been carried out either on the system loops or on components mock-ups. As a consequence, a sufficient and convenient

confidence level exists in their results, at least when they are used within their validation domain and by skilled users.

The calculation results significantly improve the safety analysis and the probabilistic risk analysis. The existing codes are able to offer a satisfactory answer for the reactors in operation and even for the next generation of evolutionary water reactors (GEN-III). The lasting requirements for improvement mainly concern their robustness, reliability and user friendliness.

However, the confidence in the results of these codes widely relies on their experimental validation. Extrapolation to situations out of the validation domain may provide doubtful and sometimes even erroneous results. So, for both design and safety reasons, in presence of significant design and operation changes, it would be worth improving the existing modeling. An international consensus exists on the interest to keep maintaining an R&D activity aimed at achieving that objective.

In the medium term (5 to 10 years), the two-fluid models are expected to improve with extension to fields like droplets, and incorporation of transport equations for the interfacial area, and the 3D modeling should be extended as far as possible. This strategy is likely to sustain a process of progressive improvement, without any significant breakthrough.

Meanwhile, the increasing computer efficiency should allow using refined meshing and capturing smaller scale phenomena, provided that convenient models are made available. In this regard, it is worth recalling that the study of non-azimuthal cold shocks on reactor vessel of the first generation French Pressurized Water Reactors (PWR) (900 MWe) has been performed by the French Utility (EDF - *Electricité de France*) with CFD codes. Nevertheless, conventional system and component codes are likely to remain the basic tools for long, while benefiting from the development of the more refined approaches derived from CFD codes and Direct Numerical Simulation (DNS).

CFD codes will allow zooming on specific zones of a circuit or may be used as a powerful investigation tool to derive new closure relationships for more macroscopic approaches, thereby reducing the need for expensive experimental programs. Coupling between CFD and system codes may also be an efficient way to improve the description of small-scale phenomena while maintaining computer costs and time consumption at reasonably low levels.

Once the underway developments are available, the DNS codes will be adopted to search for a better understanding of small scale physical processes and derive new and more accurate models for averaged approaches.

In conclusion, the strategy for preparing the next generation of thermal-hydraulic tools consists in improving the capabilities of system and component codes by developing new models while extending CFD codes capabilities to all flow regimes and improving DNS techniques. Nevertheless, the concern for the uncertainties in CFD simulations is still to be addressed.

3.2 Fuel behavior in DBA

A major safety concern in LWRs is the possible failure of core fuel rods during transients, such as a LOCA or a RIA (Reactivity Initiated Accident, which can be initiated for example by an uncontrolled control rod withdrawal). Such failures can modify the core geometry and reduce its coolability; they can also engender the ejection of fuel fragments (and consequently radioactivity) in the reactor primary circuit. During the 60s and in the early

70s, several experimental programs were carried out, which provided information about fuel rods behavior. The results were used to develop and assess RIA and LOCA fuel codes.

At that time, the fuel was pure UOX (Uranium Oxide) and the burn-up was limited to 40GWd/kg; data for low burn-up had been included in data bases for code assessment, and it was believed that some extrapolation in burn-up was acceptable. By the mid-1980s, however, significant changes in the pellet microstructure and clad mechanical properties were observed in experiments carried out with fuel at higher burn-up and MOX (Mixed Oxide, i.e. containing both Uranium Oxide and Plutonium Oxide).

Those observations provided evidence that the fuel thermal-mechanical behavior is strongly dependent on the fuel type (UOX, MOX, etc.) and the cladding material, and that extrapolation was not always appropriate. Thus, a large number of experimental and analytical programs were initiated to check the fuel behavior and model the effects of the higher burn-up of fuel elements proposed by fuel designers, mainly under RIA and LOCA conditions.

Fuel codes for RIA analysis include models, correlations, and properties for cladding plastic stress-strain behavior at high temperatures, effects of annealing, behavior of oxides and hydrides during temperature ramps, phase changes, and large cladding deformations such as ballooning. The mechanical description of cladding should preferentially be 2-dimensional, but models of lower dimension are used as well; moreover, it generally includes a failure model. These codes also include fuel pellets thermal-mechanical models that may interact with fission gas models.

The mechanical models of pellets are generally mono-dimensional. Special care is to be paid to the modeling of the so-called pellet RIM-zone (i.e. the very external boundary of it where most of nuclear interactions currently occur) and the MOX due to its heterogeneous nature (the MOX grains – of quite large size - are dispersed in a UOX very thin matrix).

Fuel codes for LOCA analysis usually adopt built-in heat transfer correlations (cladding to coolant), a constant or dynamic gap conductance model, and average values for thermal conductivity and heat capacity. As regards clad thermal-mechanical aspects, these codes typically describe ballooning and include burst and oxidation models. Although simpler in the practice, the LOCA fuel models take into account high burn-up effects and thermal-mechanical characteristics of different types of fuel elements. New specific developments are underway to treat fuel relocation, an important phenomenon recently highlighted in the framework of the OECD-Halden program (OECD/NEA, 2003).

DRACCAR is currently developed at IRSN for the simulation of the thermal-mechanical behavior of a rod bundle under LOCA conditions, with a 3D multi-rod description (Figure 1). The objectives are to simulate mechanical and thermal interactions between rods, to evaluate the blockage ratio, as well as the structure embrittlement and the coolability of the fuel assembly. The reflooding phase of a fuel rod assembly during a LOCA transient can be calculated when DRACCAR is coupled with a suitable thermal-hydraulics code. The models are applicable to any kind of fuel (UO_2, MOX …), cladding (Zircaloy 4, Zirlo, M5 …), core loading and management (burn-up …) and types of water-cooled reactor (PWR, Boiling Water Reactor or BWR, …). It is also applicable to fuel handling or spent fuel pool draining accidents. A version for GEN IV SFR is planned. The flexibility of the DRACCAR code allows to model from one single rod to a fuel assembly. Each structure is in mechanical and thermal interaction with others, including contacts between fuel rods and eventually with guide tubes. Each rod has a 3D description and is coupled with a sub-channel thermal-hydraulics. The code uses 3D non structured meshing to describe the fuel assembly.
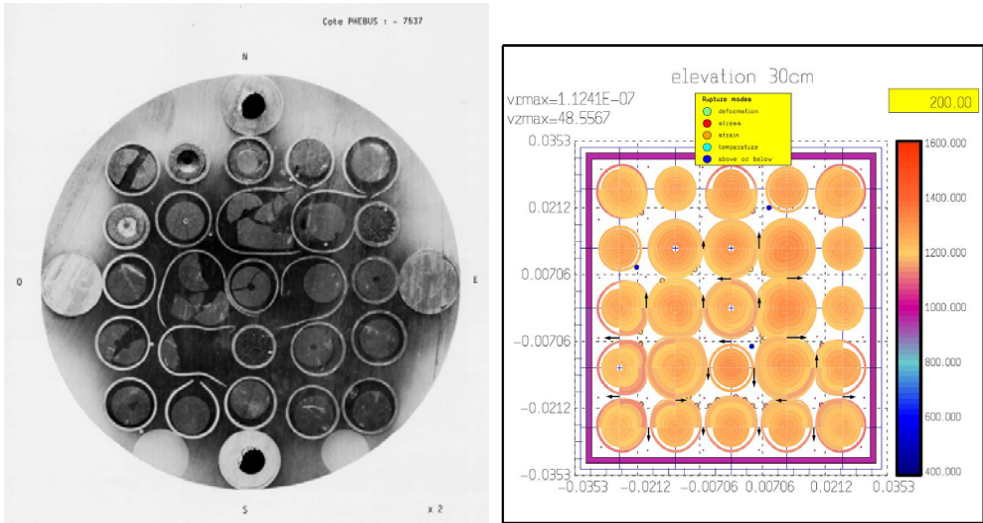
Fig. 1. Bundle deformation obtained during Phebus LOCA tests (run 215), 5 x 5 rod bundle; experimental results and DRACCAR simulation

Even if a limited number of model improvements are still judged necessary in the fuel codes, it is widely agreed that these developments could be achieved without any major breakthrough; however, it is to be mentioned that in order to improve the physical basis of models and consequently to give some confidence in extrapolations (beyond the domain covered by experimental results) the fuel models are more and more often backed up by the above-mentioned multi-scale approach.
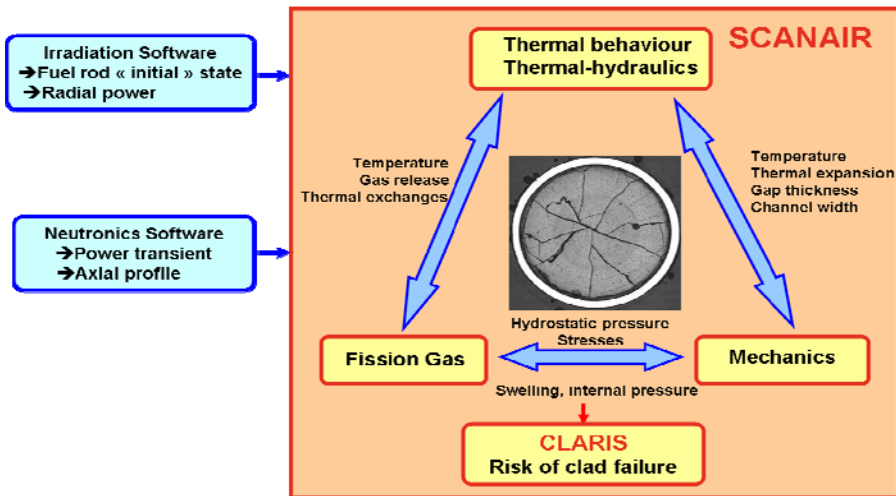

Fig. 2. The SCANAIR computation principle

A typical application of such an approach can be found in the work carried out at IRSN to improve the modeling of the Zircaloy clad behavior. This entails modeling cladding behavior on a micro-scale that represents the structures composing the cladding. In this case, the characteristic size is set by the thickness of the zirconium hydride disks (form in which the hydrogen diffused in the cladding precipitates). As the structure is subdivided into elementary units, behavior laws have to be established for each one of them. Homogenization methods were used to determine the current volume behavior of the material.

These improvements were undertaken to develop an anisotropic elastoplastic behavior model for hydride Zircaloy that may be used at macro-scale in current RIA fuel codes such as SCANAIR developed by IRSN in the framework of a collaboration with EDF, and globally assessed on CABRI REP-Na (Papin et al., 2007) and NSRR (Suzuki et al., 2006) in-pile or integral experiments.

SCANAIR is a thermo-mechanical code simulating a fuel rod surrounded by coolant that undergoes an RIA (Figure 2). The SCANAIR code couples three modules: the first one calculates fission gas migration and release into the rod gap, the second one deals with mechanics (it calculates the stresses and strains in the fuel and in the cladding) and the third one evaluates the fuel, cladding and coolant temperatures.

The use of multi-scale approaches should increase the confidence in the extrapolations from experimental conditions to reactor ones. It should also contribute to optimizing the definition of the experimental programs and decreasing their global cost; nevertheless, the necessity of code assessment against so-called "integral" experiments (i.e. experiments involving all the major phenomena that could occur in reactor conditions) will remain to verify the consistency of the different models (in particular models that have been independently derived by multi-scale approaches) and check that there is no important omission.
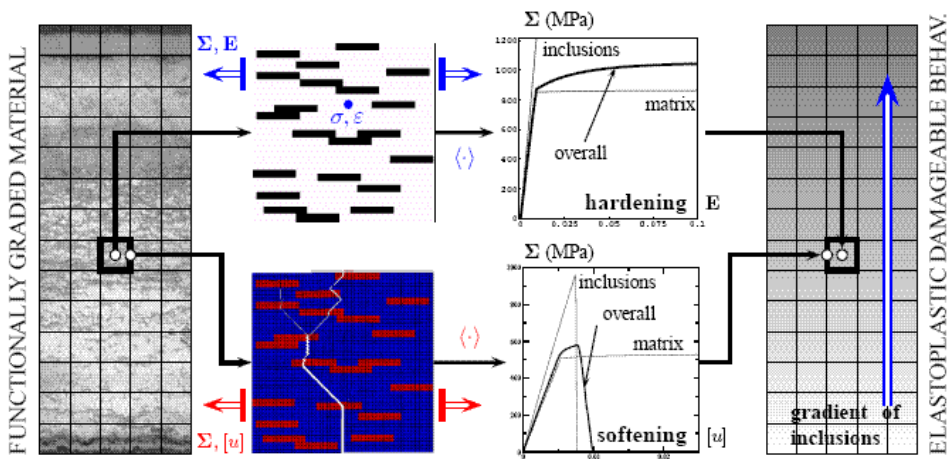

Fig. 3. Principle of the multiscale cohesive-volumetric approach for the study of the overall elastoplastic and damageable behavior of a functionally graded material

In the recent years, a new approach has been developed to predict the ductile fracture of heterogeneous materials during transient loadings. This approach is based on the so-called cohesive volumetric finite element (CVFE) method in the periodic homogenization framework (Perales et al., 2008). The coupling of this numerical approach to some analytical homogenization models allows predicting the behavior of heterogeneous materials from elasticity to ductile damage up to failure.

The framework of this coupling has been applied to a material from the nuclear industry: the highly irradiated Zircaloy cladding. This application illustrates a coupled approach where the overall hardening behavior of a composite material (as elastoplasticity) is incorporated into the bulk behavior and the overall softening behavior (as damage and fracture) is incorporated into some cohesive zone models.

The highly irradiated Zircaloy cladding is a functionally graded material composed of a metal matrix and aligned brittle hydride inclusions (Figure 3). The overall elastoplastic and damageable behavior of this material is obtained using the CVFE method where both the mean volumetric and cohesive properties arise from homogenization techniques at the micro-scale. The volumetric hardening behavior is obtained adopting a homogenization model based on a variational approach, and the cohesive softening behavior comes from a periodic CVFE modeling (Perales et al., 2006).

3.3 Coupled phenomena in DBA

Compliance with safety criteria in DBA and, more generally, in any operation, incidental and accidental circumstance of the reactor life requires the development of neutronics, fuel thermal-mechanical and thermal-hydraulics models. In principle, these three fields should be accounted for simultaneously because:

- The neutron cross-sections depend on the fuel temperature and the moderator density;
- The fuel temperature depends on the fuel element geometry, the neutronics power and the thermal exchange with the moderator fluid;
- The thermal-hydraulics depends on the fuel element geometry, the "source term" corresponding to the power released by convection and by γ radiation.

Up to now, due to the heaviness and complexity of computations, the methods adopted in the safety analysis have assumed these three fields as more or less decoupled. The major disadvantage of this assumption is the impossibility to accurately compute the pin-wise power distribution of the core. Thus, power peaking factors are adopted for design and safety analysis. Whereas they are evaluated in steady-state conditions, they are used for transient studies adding some corrections to ensure conservatism.

Incorporating full three-dimensional (3D) models of the core in the system transient codes enables the interactions between the core behavior and the plant dynamics to be accounted for in a more consistent way. Recent progress in computer technology has been achieved in the development of coupled thermal-hydraulics, fuel thermo-mechanical behavior, neutron kinetics and system codes.

Developments of several multi-physics code systems are currently underway, among which the NURESIM platform being developed in the frame of the 6th Framework R&D program of the European Commission and the HEMERA (Highly Evolutionary Methods for Extensive Reactor Analyses) coupled chain, developed jointly by IRSN and CEA (Figure 4). The HEMERA chain (Bruna et al., 2007) features are intended to allow performing more accurate calculations for the safety assessment of the thermal nuclear reactors in operation, in association with uncertainty and sensitivity studies and penalization techniques.

The HEMERA computation chain is a fully coupled 3D code system developed jointly by IRSN and CEA. It comprises the CRONOS neutronics code, the FLICA thermal-hydraulics code and the CATHARE system code. The ISAS supervisor manages the coupling. The nuclear data (neutron cross-sections) are provided to HEMERA by the APOLLO-2 code. HEMERA allows performing coupled (neutronics/thermal-hydraulics) calculations.
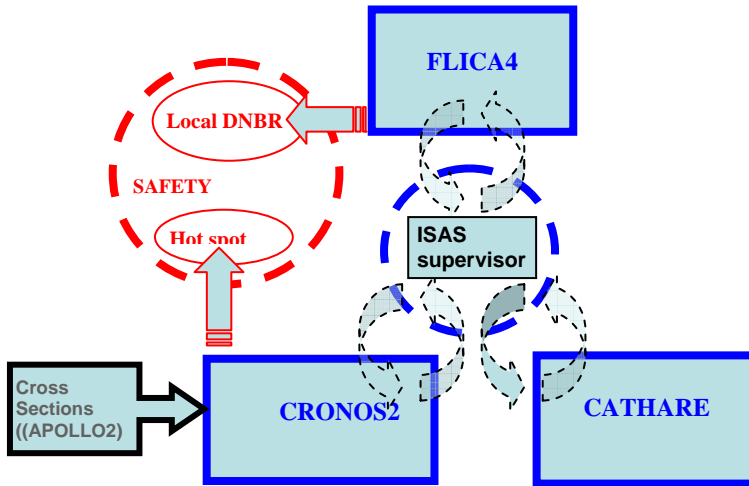

Fig. 4. The HEMERA computation chain

Accident analyses should demonstrate compliance with safety criteria. As far as the simulation of transients is concerned, the traditional French approach compels adopting the most penalizing initiators, so that neutronics, thermal and thermal-hydraulics calculations have to be either externally or internally coupled. HEMERA provides this coupling internally through the multi-level and multi-dimensional models which have been implemented to account for neutronics, core thermal-hydraulics, fuel thermal analysis and system thermal-hydraulics phenomena with best estimate and/or conservative assumptions (Clergeau et al. 2010).

3.4 Severe accidents

Historically, for a long time the LOCA has been considered as the maximum credible accident in LWRs. Accordingly, their main safety design features have been defined to prevent it or, at least, to limit its consequences, through keeping the core geometry coolable as long as possible, and strictly limiting the fission products release to the environment.

However, since the 70s, and mainly as a consequence of the TMI2 accident, it was internationally agreed that it is necessary to account for accidental situations in which the core cooling cannot be guaranteed.

Should it be the case, the loss of core coolability engenders a chained sequence of physical phenomena which can end up in core meltdown and the dispersion of contaminants into the environment and the ground. A typical sequence can be as follows: the fuel cladding is oxidized by the steam, which generates hydrogen in the containment; the cladding loses its integrity, and a large part of the fission products is released into the vessel and, through the

circuit and the breach, reaches the containment; the cladding and the fuel lose their geometrical integrity, disaggregate and fall down to a colder region of the core, so that molten "corium" (mixture of core molten materials) is contained inside a solidified crucible; the crucible breaks and the corium falls down into the vessel bottom; if no extra cooling is available after a time, the vessel bottom breaks and the corium falls down and spreads over the basemat of the containment; depending on the chemical, geometrical and thermal conditions, the corium can be either confined and cooled down in the containment, or erodes the basemat and flows down to the ground; the hydrogen in the containment could generate severe damage if its concentration is such that it can cause either detonation or fast deflagration (suitable devices which ignite it as soon as it expands can be added to prevent and mitigate such events); eventually, in case of loss of integrity of the containment, the fission products may be released to the environment, the rate of released radioactivity depending on all the physical-chemical processes that may affect the fission products in the reactor circuits and containment.

All the phenomena involved in a severe accident scenario being very complex and quite coupled, a great difficulty for modeling arises from the lack of precise knowledge of the laws governing them, notably the dynamics of the great number of physical-chemical reactions.

Suitable integral codes have been developed in recent years to perform realistic studies on the accidental scenarios, also - at least partially - accounting for their probabilistic aspects. A typical example of such move is the ASTEC code (Van Dorsselaere et al., March 2009), jointly developed by IRSN and GRS (Gesellschaft für Anlagen- und Reaktorsicherheit mbH), and assessed by 30 organizations in the framework of the SARNET Network of Excellence dedicated to Severe Accidents (Micaelli et al., 2005) and backed by the European Commission in the 6th and 7th Framework Programs. The code is now considered as the European reference for severe accident analysis.

Such integral codes describe all the physical phenomena governing the reactor behavior, in space and time, from the core melting up to the possible release of contaminants to the environment, as well as the behavior of all safety systems and of the operators' procedures (see the scheme of ASTEC code in Figure 5). They must be (relatively) fast running to enable sufficient number of simulations of different scenarios to be performed, accompanied by studies on the uncertainties and on potential cliff-effects. In most codes, the structure is modular enough in order to make easier the validation process, for instance applying only a limited set of modules on experiments devoted to a few physical phenomena (see Fig. 5 for the modular structure of the ASTEC code). As the integral code approaches emphasize the overall plant response, interactions and feedback between separate phenomena occurring at the same time play an important role: e.g. fluid flows, heat transfers, phase changes (melting, freezing, vaporization) and chemical reactions. Another important feature of such codes is that they gather very diverse scientific domains like thermal-hydraulics, chemistry, mechanics of solid structures, neutronics, etc.

Each phenomenon is represented through simplified models, often empirically adjusted on experiments. These codes are globally assessed on integral tests such as those carried out within the PHEBUS FP programs (Clément et al., 2003). Some specific parts of the accident are addressed via the so-called mechanistic codes, which model the local equations more precisely, with a much refined geometrical description. Such codes calculate the behavior of both the core during the degradation process and the corium molten pool in the bottom of

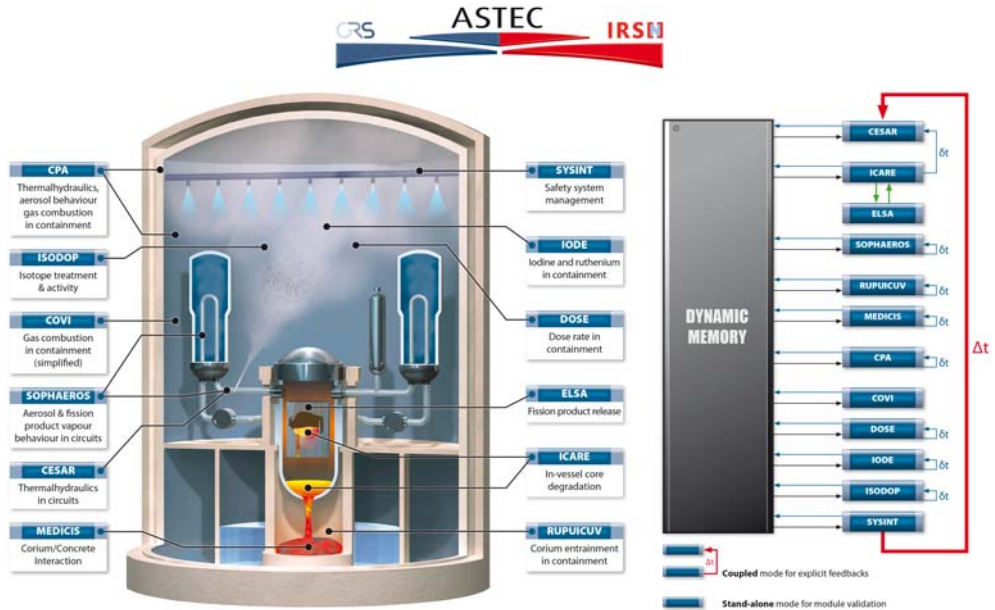the vessel and in the cavity, as well as the steam and hydrogen distribution in the reactor containment.

Fig. 5. The ASTEC integral code for simulation of severe accidents

The majority of these codes is still making strong approximations on the geometry of the core and its evolution during the degradation process, and remains very sensitive to the physical-chemical uncertainties, due to the large number of components in interaction and the very high temperature. Such insufficient mastering of the uncertainties, which is at least partially due to the poor knowledge of the behavior and properties of the materials, does not encourage going through further development of very detailed models considering that the outcome of the development efforts should show up quite low.

Nevertheless, selected efforts could be devoted to improving the computation features of the transient parts where the geometry-related effects are widely dominant on the physical uncertainties. In such situations, CFD codes can give interesting results, and in fact they are becoming more and more widely used in problems like the hydrogen repartition and combustion in the containment (TONUS code jointly developed by CEA and IRSN (Bielert et al., 2001)) or the corium pool behavior in the vessel bottom, or the corium spreading and solidification process out of the vessel (CROCO code developed by IRSN (Gastaldo et al., 2006)).

The multi-scale approach has tentatively been adopted at IRSN to investigate the physical phenomena in the regions where the solid particles form a porous bed of debris (Fichot et al., 2006) and where the molten materials build up and accumulate, forming a molten pool (Roux et al. 2006). The progression and growth of the molten pool is a major threat for the vessel wall and, therefore, an important source of concern for the safety experts. One of the most efficient ways to stop its growth is to re-flood it with water but this process involves complex steam and water flows through the porous debris bed. It also forms a solidification

front at the edges of the molten pool where coupled heat transfer and material transport engender major modeling difficulties which challenge the validity of simple models.

The details of the processes (steam and water flow in porous debris and solidification of molten mixtures) should be studied numerically at a small scale; models suitable for implementation in industrial codes could then be derived thanks to a volume averaging method (Fichot et al., 2006; Roux et al., 2006). As previously mentioned in section 3.2, such an approach does not exempt from validating the codes against experiments that involve simultaneously all the phenomena contributing to the process to be modeled. For this reason, in the framework of SARNET, IRSN and partner organizations are building an experimental program that addresses the issue of debris bed quenching by water injection (Van Dorsselaere et al., October 2006).

3.5 Use of CFD codes for other accident studies

Some transients, even if not explicitly included in the set of severe accident initiators, may have important safety consequences and must therefore be studied very carefully. That is the case for the reactivity swing resulting from the injection of clear water into a core at shutdown for reloading. The core is under-critical in these conditions, due to the huge soluble boron poisoning of the water. The injection of clear water generates a RIA–type transient and the core can go back critical quite quickly (and, maybe, even prompt-critical, depending on the clear-water injection amount and location). Immediately, the power of the core begins to increase and it still does until the Doppler feedback is able to shut the reactor down. Then, the cooling-down can start a reactivity-driven oscillation.

Past studies showed that such situations, due to operation and maintenance errors, may be quite likely and significantly contribute to the risk space. Operating procedures were modified to reduce the probability of such events, and probabilistic safety analyses were performed to evaluate their consequences. Nevertheless, they remain a major safety issue and have to be conveniently addressed through computation.

A typical event of this kind is as follows: one of the loops of the reactor provides pure water and the other loops provide water with normal boron concentration level. The main modeling problem is to evaluate the map of boron concentration at the core entry, accounting for the fact that the flow entering into the vessel is highly turbulent, and there are many obstacles opposing the flow, such as tubes and plates in the vessel bottom. A neutron dynamics code can then calculate the core power distribution and evolution with time. Calculations of that kind are already performed with CFD computer codes. To gain full confidence and access to fully realistic results, they need improvements in turbulence models and geometrical modeling, which implies the use of high computing power.

Other studies of operational transient adopt CFD techniques to complement the usual tools and obtain a more precise description of local and complex phenomena such as the flow stratification in pipes and tees, the cold plumes touching hot walls, the impinging jets with temperature differences and the pressurized thermal shocks.

4. Advanced numerical simulation and safety demonstration of GEN IV concepts

Specific needs in terms of development and assessment of advanced computation tools could show up for each GEN IV design, depending on its physical features and operating mode. Nevertheless, several trends can be pointed out as relevant to the safety

demonstration and widely independent from the design. They would claim a major effort of computer code development and assessment, which should impulse new experimental programs.

As mentioned above, particular care is paid in this paper to three out of the six GEN IV concepts:

- The SFR that can benefit from a significant experience in France, Great-Britain, Japan, Russia (and some other countries of the former USSR) and the USA,
- The GFR that presents a very high potential in terms of uranium sparing, incineration, transmutation and heat production; however, even if the concept principles are not new in Europe or in the USA, no GFR has ever been built in the world,
- The HTR/VHTR that can benefit from a first experience in Germany, Great-Britain, China, Japan and the USA.

At the present stage of the investigation of the 3 above-mentioned concepts, five main issues have been retained by IRSN as major ones:

- The consistence and robustness of neutronics design of such systems, the behavior of which is quite different from current PWRs and conventional experimental facilities, due to an increased coupling among neutron and temperature fields, the new design of the core, with heterogeneities, an advanced fuel technology, and a very different operation mode;
- The demonstration of the actual capacity of such systems to passively and safely evacuate the residual power, in any circumstance;
- The features of reactor fuel, with specific emphasis on its transient behavior, mainly as regards either the TRISO particle for HTRs/VHTRs or the advanced carbide and nitrite fuels for fast neutron reactors;
- The features of the source term produced by the migration of activated fission products inside the reactors and likely to be released to the environment in case of accidental situations;
- The inquiry upon either the significant reduction or the risk of a generalized and severe damage of the core, which founds the whole safety approach for these plants.

All these issues are widely addressed in the SRA (Strategic Research Agenda) of the European SNETP Sustainable Nuclear Energy Technology Platform (Bruna et al., 2009) and in several connected presentations and articles, such as (Bruna, 2008). They will not be investigated here. In the following, only the computation-related aspect will be discussed, mainly in the perspective of the improvements expected from either an extended use or the adoption of the CFD methodologies.

All these fields claim for a new effort in R&D. In order to achieve an optimum management of the resources, a priority scale is to be established in agreement with the technological choices and the objective dictated by each country's policies. In the following, we shortly assess each of them before focusing on specific needs for the safety demonstration of the systems which are most likely to be constructed in a relatively near future. It is remembered, for completeness sake, that numerical simulation for the development of specific non destructive examination methods is not addressed in this chapter.

4.1 Reactor physics and core design

GEN IV reactors are very different from each other as regards neutron design, core physics and operating mode. They span a very large spectrum of configurations, including small

and large size cores, fast-neutron and moderated ones, gas, water and liquid metal cooled systems, each one matching more or less completely and comprehensively the general objectives of GEN IV. Sustainability and actinide transmutation are the most affordable goals for systems with fast neutron flux, such as SFRs and GFRs. On the contrary, graphite-moderated gas-cooled thermal-flux reactors, such HTRs and VHTRs, are most likely to be inherently safe and to allow a diversified energy production (electricity, but also industrial steam and hydrogen).

In addition to the overall design, the core size and the operating modes, the fuel, the materials for internals and vessel, the coolant features generate specific problems which must be assessed in computations. Moreover, a strong coupling among neutron and temperature fields can show up in large-size systems. Simulation challenges can be sharpened by the coupling with conventional energy production systems, which can propagate instability and perturbation to the reactors, through the intermediate heat exchanger.

Accordingly, the requirements in terms of simulation for core physics and operation studies would be quite different. A sometimes massive heterogeneity in space and energy and the mutual interactions between the neutron and temperature fields claim for new and enlarged 3D capabilities, and an increased coupling for design and normal operation calculations.

Integrated systems permitting a full description of coupled neutronics, thermal and mechanical transients, such as the SIMMER III/IV code (Tobita et al., 2006), should be very useful for safety studies of strongly coupled, fast-kinetics systems, such as SFR and GFR systems. On the other hand, for HTR and VHTR systems, due to the strong dependence of the core equilibrium on the temperatures, focus should be put on bulk codes enabling a full coupling among the core and the reflector temperature and neutron fields.

Moreover, specific needs exist for SFRs, which mainly concern the risk of a generalized and severe damage of the core, due to either reactivity-driven transients, such as the coolant void (mainly the sodium), or mechanically-initiated transients, such as the blockage of a coolant in a subassembly.

Last but not least, a major safety concern for PBMR (Peddle Bed Modular Reactor) type reactors (particular type of HTR) is the confidence in the evaluation of power peak within an heterogeneous core, where neither the local composition nor the lattice is precisely known during reactor operation, due to the stochastic distribution of the pebbles and the wide burn-up spread among them. Specific developments are needed, which involve a massive use of probabilistic techniques and a careful appreciation of uncertainties. All these items claim for a strong R&D effort devoted both to code development, qualification and validation and to measurement campaigns in ad hoc mock-up experiments.

So as to manage resources as best as possible, a priority scale must be established in agreement with the political and technological choices: emphasis should be put on each item according to its relevance to the safety demonstration of the forerunning concepts likely to be industrialized in a near future.

4.2 Residual power evacuation

For GEN IV concepts as for many other existing ones, the verification of the sufficient cooling of the core in various accidental situations is one of the most important tasks of the safety analysis. Such verification should be supported by the numerical simulation of two processes:

- Fuel cooling by liquid (e.g. sodium) or gas (e.g. helium) natural convection and heat radiation;
- Heat evacuation by water safety circuits.

The difficulty will of course depend on the design (complexity, safety margins, etc.). However, we could reasonably consider that already existing tools like thermal-hydraulics system codes (already developed for light water reactors) and CFD codes for more local evaluation (with radiation models) should be sufficient. Adequate design-oriented experiments will surely have to be performed in order to assess the codes validity for some specificity of the circuits, but this will remain in a strict continuation of current actions aiming at improving capabilities of thermal-hydraulics codes and extending CFD use in reactor safety analysis.

4.3 Fuel integrity

As already mentioned, the integrity of reactor fuel will be an important issue for GEN IV concepts. The challenge will be comparable to that encountered with current generation ones. With a view to enforcing the demonstration of the robustness of the fuel and its resistance to the operation and accidental transients, improvements and adjustments will have to be made in computation tools and devoted experimental programs developed for physical assessment and qualification needs. According to the fuel features and design, it is straightforward that such updating and experiments should be reactor concept-oriented.

The larger effort is foreseeable for HTR/VHTR concepts which, despite their ancient design, have accumulated a quite limited operating experience and, far more, for GFRs, the fuel design of which is new (and is an essential source for performance improvement in terms of both operation and safety, through the achievement of ISO-generation conditions) and does not benefit from any operation feedback.

However, the simulation strategy should be the same as for the current reactor generations: simplified models shall be derived for industrial and well assessed simulation tools and the derivation of these models shall be backed up by a multi-scale approach. It could be recommended to put in place such a strategy as soon as possible in order to more efficiently define the experiments against which the elementary and global assessment of models will be performed.

4.4 Fission products release

All the phenomena involved in the transfer of fission products from the fuel elements to the containment and from the containment to the environment are very complex. As for the current generation of reactors, difficulties come from the great number of involved physical-chemical reactions that make a detailed mechanistic approach almost impossible.

Since the risk of a severe accident and of significant fission products release should be lowered for GEN IV concepts, it does not appear as a necessity to significantly increase the precision we have today when predicting the potential consequences of a severe accident.

Thus, for this topic, it is not judged necessary, from the safety point of view, to have any breakthrough in terms of modeling, apart from the necessity to develop specific models of fission products release for some GEN IV fuels (TRISO for HTRs/VHTRs, carbide for SFRs, specific fuel for GFRs). Simplified models should be sufficient although they will have to be assessed against an appropriate experimental data base including separate effect tests and integral effect tests to make sure that no major important phenomenon has been forgotten.

However, as for the simulation of severe accidents in the current reactor generation, it could be recommended to follow up the current strategy and back up the simplified models by detailed models when it is possible.

4.5 Reduction of the major risk of generalized and severe core damage

As regards the problem of the exclusion of transients likely to result in core melting, it is quite obvious that concepts such as the HTR/VHTR are much more inherently protected against high fuel damaging than others, such as the SFR and the GFR, due to a far slower kinetics, a wider thermal inertia (due to the huge amount of graphite), a capacity to passively evacuate residual heat in almost any circumstance, and a high thermal robustness of the fuel particles.

However, even if the designers' target is to make a whole core melting or high damaging highly hypothetical, a wise strategy would be, in particular for SFRs and GFRs, to investigate

- the mechanisms that could prevent a core local meltdown from degenerating into a whole core meltdown,
- the consequences of a whole core meltdown on containment integrity (including the release of radioactive elements into the environment).

Codes based on simplified models have been developed and used for the previous generations of reactors (LWRs and SFRs). Appropriate experimental programs have been initiated in the 80s to assess these models. The question of the adequacy of these codes and of their assessment for GEN IV concepts can be considered as an open one. It is likely that codes already developed for previous generations of SFRs will be applicable to GEN IV SFRs, provided some complementary developments and assessment are done (the demonstration on core re-criticality risk was not easy and will not be easier for GEN IV, the demonstration of corium retention, etc.).

The adaptation of LWR codes to HTR/VHTR concepts seems possible although, as the core materials are significantly different, all the elementary models will have to be revised and reassessed against a new and appropriate experimental data base.

Phenomena involved in a severe accident are and will remain very complex due to the tight coupling among several phenomena that intervene as driving ones at different instants of the transients: multiphase flows, heat and mass transfers, thermo-chemistry, mechanic resistance of metallic structures, material melting and freezing, core physics and neutron kinetics, etc.

This complexity makes it nearly impossible to envisage in the coming twenty years any revolution in the numerical simulation of these accidents and the conclusions of section 3.4 for LWRs should be considered valid for GEN IV concept severe accidents: the use of advanced numerical simulation could be introduced by CFD or DNS computation in realistic geometries, for calculation of basic averaged values or limited parts of the accident, in support to "integral" codes based on simplified models such as those adopted for the current generations of severe accident codes.

5. Conclusion

Almost all the codes developed during the last twenty-year period for the analysis of the safety problems of nuclear reactors in operation adopt simplified geometry descriptions and

quite simple physical models, stressing the major physical phenomena in some detail only, and either addressing in a quite approximate way or even neglecting the minor ones, as it is the case for the LWR LOCA codes.

That is undoubtedly a drawback to be overcome from the performance point of view since it implies the adoption of operating and safety margins at any stage of the reactor design and operation. Nevertheless, no major changes are expected in the near future as far as the safety analysis of current reactors is concerned, mainly because the computation systems currently in use benefits from a large validation against a set of diversified and extended experimental results. Moreover, the industrial safety applications need to rely on methods agreed by the safety expert organizations. Quite a long time is therefore generally needed before the advanced methods developed by researchers can be adopted in practice to address actual safety cases.

Advanced simulation is undoubtedly able to provide extended capability to calculate local parameters and, accordingly, it allows deeper insights in many problems, contributes to a better understanding of the physics, and thus leads to more reliable designs, reduced costs and/or more precisely quantified safety margins. For system analysis, advanced simulation has thus a complementary role to play in nuclear safety applications in combination with system codes, particularly in those areas where multi-dimensional aspects are relevant. Moreover, combined applications, supported by proper experiments may guarantee a more precise evaluation of safety margins.

Single-phase CFD applications are already reasonably mature although some models (e.g. turbulence and combustion)   need improvements. Two-phase and multi-phase CFD modeling still require considerable research efforts even though some aspects may be already reasonably well addressed through the advanced models. In addition, a lot of work in terms of experimentation, model development and assessment has still to be done before practical applications in nuclear safety studies can be made. Thus, as far as the current reactor safety analysis is concerned, the adoption of CFD techniques should mostly be limited to achieving a more detailed understanding of the physical phenomena and supporting the methodology currently in use rather than to supporting the development of fully new computation systems.

Multi-scale techniques are more and more used to consolidate the physical bases of simplified models. The use of these techniques allows progressing more rapidly in the understanding of physical processes and contributes to optimizing experimental programs. However, these techniques are applicable for a limited number of phenomena; they provide models that shall be globally assessed against integral experiments.

On the other hand, as for incoming GEN IV concepts, even if it is assumed that the development pace of computing power keeps constant, due to the complexity of the phenomena and the wideness of the investigation fields, a significant breakthrough in the development of computational tools dedicated to the safety demonstration seems quite unlikely in the short term (roughly within 10 to 15 years).

Moreover, the preliminary studies of some of these concepts now underway allow believing that there is no specific need for profound modifications to the current code development and assessment strategies. The key element will remain the adequate validation of the computation chains against appropriate analytical and integral tests, which means *in fine* uncertainty and design margins.

Accordingly, it seems likely that large improvements of computation tools, including an extensive adoption of CFD methodologies, are scheduled for the intermediate future (within the next 25 years).

Nevertheless, it is likely that the use of advanced modeling will be extended and reinforced for GEN IV fields of endeavor, alongside with the expansion of the application for current reactors.

The most challenging issues in the methodology to GEN IV computation should be:

- The extended adoption of CFD techniques for single-phase application, addressing core cooling in particular, with the support of some specific experimentation assessing models and calculation methodologies;
- The development of multi-physics computational tools with a tight coupling among core physics, fuel thermal-hydraulics and thermo-mechanics, as well as systems description;
- The increase in the predictability of fuel codes for fuel integrity issues. To comply with the expected continuous process of fuel improvement, this should be backed by the development of a multi-scale strategy (already initiated for LWR fuel) and supported by a suitable experimental activity as well;
- The achievement, in the severe accident and source term evaluation issues, of a modeling level close to that achieved for LWRs, for which the advanced modeling is only seen as a support for a better understanding of some physical aspects of involved phenomena.

As a general conclusion, in the present state of knowledge, no major breakthroughs seem necessary in terms of modeling for reactors in operation, at least whether if it is postulated that no significant changes are adopted in their design features and operation. Simplified models should still be satisfactory enough, provided that they are validated on appropriate and representative experimental data, including results from both analytical and integral tests.

As far as the future GEN IV concepts are concerned, it must be emphasized that the current wide effort for updating models should provide opportunity for "boosting" advanced numerical simulation that is undoubtedly a source for better understanding of the system physics and consequently improving the concept design and future operation. Nevertheless, the safety analysis being strictly dependent on reactor design, a further investigation on this relevant topic is to be carried out once the main design and operation options for those systems is definitely known.

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