Corium-sodium interaction the development of the SCONE software

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CORIUM-SODIUM INTERACTION: THE DEVELOPMENT OF THE SCONE SOFTWARE

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ABSTRACT

In the frame of the safety studies for the ASTRID reactor, CEA has started the development of the SCONE software. SCONE aims at being a mechanistic code dedicated to the simulation of the molten corium-sodium interaction that could occur in a sodium-cooled reactor. In particular, SCONE must allow studying the configuration of an interaction occurring in the lower plenum of ASTRID in case of massive relocation of corium discharged from the core by dedicated transfer tubes.
In this paper, after a recall of the interaction phenomenology, the physics to represent it with SCONE is described as well as the available modeling approaches. The main gaps in knowledge have been identified and are explained along with the foreseen experimental programs aiming at filling these gaps. The numerical aspects of the SCONE development are also discussed before concluding by giving the status of the SCONE software.

KEYWORDS
SFR - Severe accidents - Corium-sodium interaction - SCONE software

1. INTRODUCTION

The ASTRID reactor (Advanced Sodium Technological Reactor for Industrial Demonstration) is a technological demonstrator, currently designed by CEA and its partners, with very high levels of requirements, especially when it comes to safety. In the frame of the conception of ASTRID, the possible occurrence of a severe accident leading to fuel melting has to be considered. The melting of the fuel assemblies generates a mixture called corium composed, for fast neutron reactors, of molten materials (UO_2-PuO_2 and steel) carrying residual power.

In order to decrease the core reactivity in case of material melt-down, it is foreseen to include, within the ASTRID core, transfer tubes (TTs) dedicated to corium relocation into the lower plenum. The resulting Fuel-Coolant Interaction (FCI) between large masses of corium at ~3000°C and a large volume of sub-cooled sodium (T~400°C) present in the reactor lower plenum would cause the intense fragmentation of corium and the rapid vaporization of sodium. Depending on the physical conditions of both corium and sodium, this sudden vapor production could lead to the formation of a pressure wave able to threaten the reactor structures. The explosive nature of the vapor generation has then to be studied as well as the relocation of the corium particles generated by the interaction to ensure post-accident debris bed cooling and avoid the risk of a return to criticality.

In the past, melt-sodium experiments have been calculated with the SIMMER code ([1] and [2]) which is part of the ASTRID calculation chain for the reactor core degradation calculation in case of a severe

accident [3]. Globally, these FCI calculations reproduce the experimental data but the SIMMER modeling of the FCI remains simplified (see in particular the discussion of the SIMMER FCI models in [2]).

So, in the aim of precisely assess Corium-Sodium Interaction (CSI) and of being as predictive as possible in terms of energy release and features of the generated debris, CEA has started the development of the SCONE software (**S**oftware for **CO**rium-**N**a interaction **E**valuation), a dedicated tool for detailed analysis of the physics of the interaction. With SCONE, we intend to represent the main phenomena occurring during a CSI as accurately as possible, relying on past experiments or devoted future experiments to develop and validate the necessary models.

In the next sections of this paper, after recalling the phenomenology of corium-sodium interaction, we describe the physics of CSI that will have to be simulated and we present the first modeling choices for SCONE.

2. PHENOMENOLOGY AND SOFTWARE REQUIREMENTS

2.1. General phenomenology - Needs for a mechanistic code

During a CSI, the hot dense liquid (corium) transfers its internal energy to the cold, more volatile, liquid (sodium) in a very short timescale. This fast heat transfer is governed by the intense fragmentation of the hot liquid and the resulting drastic increase of the exchange surface area between the two liquids. The temperature and the pressure within the coolant increases along with its compressibility, the vapor production becomes more intense, generating a pressure wave that expands against the inertial constraints of the surroundings and the mixture itself. In other words, during a CSI, the internal energy of the hot liquid is partially transformed into mechanical energy that can threaten the reactor structures [1, 5].

When the corium and the sodium are brought into contact, the corium is firstly coarsely fragmented and a film boiling regime establishes around the fragments. Unlike with water, it is quite difficult with sodium to reach and maintain a stable vapor film configuration, especially when the sodium is far from saturation conditions but such a configuration can be encountered when the sodium is heated up. Then, even if the presence of the vapor film strongly reduces the heat exchanges between the corium fragments and the liquid sodium, the unstable nature of the sodium vapor film rapidly leads to contacts between corium and sodium which enhance the exchanged fluxes and play a major role in vapor production. The total collapse of the vapor film causes the corium to fragment again and the explosive step of the interaction to start [6]. The explosion itself can then be described two main phases.

The first phase corresponds to the pressure rise in the so-called interaction zone (IZ). After the total collapse of the vapor film, the corium finely breaks-up, the exchange surface area between corium and sodium increases again and the vapor production is suddenly intensified. With sodium, the vapor film destabilization and collapse is spontaneous, due to the thermal behavior of both corium and sodium. The temperature and the pressure increase within the system causes the two-phase coolant and the corium to be put into sufficient relative motion which causes corium hydrodynamic fragmentation to occur. The whole fragmentation process leads to the formation of "vapor bubble" and an associated pressure wave that can propagate through the multiphase medium and reach the solid surrounding structures. During that first phase, the local thermodynamic conditions of the materials are major parameters while the surrounding system is of secondary importance.

The second phase of the explosion corresponds to the expansion of the "vapor bubble" generated during the first phase. Here, the heat transfer from the IZ to the surroundings takes over from the heat transfer between the corium and the coolant. It is during this second phase that most of the mechanical work is done on the surroundings. This phase is system-dependent which means that the work done is system-

dependent and that the use of yield to extrapolate from experimental results to other situations (reactor for example) is to be avoided. These two phases of the explosion are represented in Figure 1:

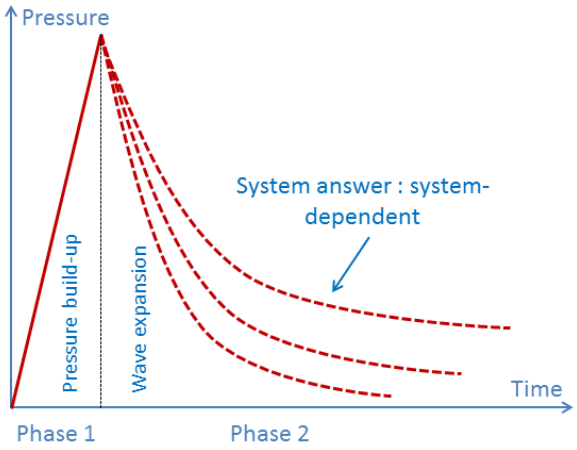

Figure 1: The two phases of the explosion

To summarize:

When corium and sodium are brought into contact, the corium is heavily fragmented and the sodium is suddenly vaporized. The increase of the vapor fraction (also called void fraction) within the system causes opposite behaviors of the pressure. Indeed, when the void fraction increases:

- the coolant compressibility increases, which leads to the increase of the relative velocity between the liquid and the vapor phase enhancing the corium fragmentation and the pressure build-up ;
- the volume of liquid coolant that can interact decreases, the thermal transfers between corium and liquid sodium decrease as well as the pressure.

We are then in front of tight couplings between thermal and hydrodynamic phenomena; a transient multi-phase, multi-component, multi-dimensional software is necessary to calculate the interactions between the different time and space scales involved in the interaction. This led CEA to start the development of the SCONE software.

2.2. Configurations to study

SCONE will be used to pre-calculate/analyze small-scale CSI experiments and perform full-scale reactor simulations. The first configuration that SCONE will have to assess is the arrival of large masses of molten corium into the lower head of the ASTRID reactor via the transfer tubes and the encounter between this hot liquid material (T~3000°C) and the liquid sodium at ~400°C. The discussion in the present paper mainly supposes this configuration, but the software development remains general so that other configurations could be studied.

One of the main features of CSI is that corium cannot penetrate in a well-shaped jet into subcooled sodium. Past experiments have shown that, in subcooled conditions and for this contact configuration (molten UO_2 flowing into sodium) a stepwise penetration is observed with fuel fragmentation and dispersion. In this case, a succession of mild pressure events (multiple small explosions) is usually observed (see [8], [9] and [10] for experimental evidences). Yet, these experiments have also demonstrated that a coherent mass of molten UO_2 could flow through sodium at temperature close to saturation ([11] and [12]). Indeed, when sodium reaches these levels of temperature, a change in the phenomena was exhibited as explained in [6]: smaller pressure rise time and larger mechanical energy release were observed. The overall phenomenon then appeared to be more akin to FCI with water. This behavior is observed when the initial sodium temperature is close to saturation or when sodium

approaches saturation condition after extended or repeated contacts with UO_2 [6]. Concerning fragmentation, generally speaking, the past experimental programs have shown that, whatever the sodium temperature and the pressure level reached, heavy fragmentation of corium was observed and very fine particles (Mean Sauter Diameter ~150 μm) were collected.

Important: If, from a hydraulic point of view, water and sodium can be comparable, from a thermal point of view their behavior is different. As a liquid metal, sodium has a very low Prandtl number which plays a major role in the structure of the thermal boundary layers which are significantly larger. It is then fundamental to establish transfer laws taking into account the appropriate physics in order to correctly predict the vapor production and the pressure levels reached during the interaction.

2.3. Software requirements

With the SCONE software, the future users will have to be able to:

- locate, at each instant of the calculation, the corium within the studied system and know its features: dispersed or continuous form, temperature, composition, velocity and physical properties;
- have access to the vapor production at each instant of the calculation;
- follow the pressure and the temperature evolution within the calculation domain.

To simulate CSI, the main phenomena to calculate are: the fragmentation of a coherent mass of corium (primary fragmentation) and the fragmentation of liquid corium particles (secondary fragmentation) as well as their solidification, the sodium boiling for different regimes and the associated heat transfers between the different constituents of the system, the heat flux partition between vaporization and liquid sodium heating, the expansion of the pressure wave resulting from CSI. Due to the multiple interactions that can occur successively, it is not possible to separate coarse initial mixing, fine fragmentation and propagation wave phenomena: a unique code dealing with compressible phases must be used, with the ability to manage nearly incompressible flows. The model must follow both separated flows (the coherent corium mass) and dispersed flows (corium particle populations, two-phase sodium).

As we have just seen, the different materials present in the domain are under various phases, either due to their physical state liquid/gaseous/solid or their physical form dispersed/continuous. It can then be convenient to be able to describe a phase (for instance the corium dispersed phase) by a more precise representation if needed to account for some specificities of the flow (for instance its polydispersity). Moreover all constitutive laws are not frozen (or even established) yet and the modeling could evolve with future experimental knowledge and theoretical developments. Therefore the software must be versatile enough to deal with any number of phases, each with its proper set of balance equations, and to easily implement evolutions of the models.
The numerical engine must be tolerant of these evolutions in the sense that adding a physical model must not imply a major change for the numerical scheme, whose first quality must be robustness. The software will have to be efficient, from a precision to calculation cost ratio point of view, and allow sensitivity calculations within reasonable time frames. For that aim, capability to run tests on parallel computers is required.

3. PHYSICS TO REPRESENT AND FIRST MODELING CHOICES FOR SCONE

3.1. General modeling and representation of phases

As summarized in the previous paragraph, the physics to represent consists in compressible multiphase flows for liquid sodium, sodium vapor, continuous corium and dispersed corium (particles). For each of these four phases, the balance equations are written in their average time-dependent form for mass,

momentum and energy [13]. Every phase has a representation on a unique common fixed domain on which the equations are written in Eulerian description.

For the corium particles, in order to account for a complex distribution of particles, an Eulerian multiple size method (such as the MUSIG method [14]) is envisaged to follow the particles in terms of size, velocity and physical state. In this case, as many balance equations sets will be used as groups of particles. With this representation, an accurate description of particle fragmentation or solidification will be facilitated. Anyway this corresponds to an internal representation of the dispersed phase: a Lagrangian (particulate) description could be used that still will need to communicate to other Eulerian phases through some representation on the Eulerian mesh. By separating, at the computing software level, these two representations (internal, proper to the phase, and external to communicate with other phases on the common mesh), it will be possible to change the internal representation if the Lagrangian appears to be notably advantageous. But, for now, this approach would require to develop specific modules in the software, adding difficulties for efficient parallelization; it has then been decided, for the moment, to promote the implementation of the Eulerian description.

As for the continuous corium phase, tracking the sharp interface with the surrounding multiphase flow is necessary to well capture the flow and the deformation of the coherent mass of corium. Therefore a technique must be implemented to follow the interface with a limited numerical diffusion. Driven by the desire to ensure mass conservation, an Eulerian representation will also be used for the continuous corium phase associated with a technique for tracking the sharp interface.

At every position and time, pressure equilibrium is assumed so that only one pressure field is used for all the phases. However, mechanical equilibrium is not instantaneous in general as velocity fields differ for the different phases. So each phase has its own velocity field and friction terms define the momentum exchanges. Also, non-thermal equilibrium is considered between the phases and the pressure build-up is controlled by the heat exchanges between these phases. Coupling between phases thus consists in sharing the same pressure field in the same control volume (sum of the volume fractions equals to one), together with exchange terms in the balance equations which are described in the following sections: mass exchanges (corium fragmentation/coalescence and sodium vaporization/condensation), momentum exchanges (friction) and energy exchanges (heat due to phase-change, friction work, conduction/convection and radiation). Solving the non-linear system composed by all these elements gives the state of the different phases as well as their volume fractions.

3.2. Fragmentation of a coherent mass of corium

Subcooled sodium

The first contacts between hot liquid fuel and subcooled sodium are still very difficult to model due to the lack of observations and knowledge of the phenomena involved. Dedicated experiments are needed to fully understand this first contact and are under design. In the meantime, we have chosen to progress on this point by developing a numerical (CFD) approach in order to assess the dynamics of fragmentation and identify the major fragmentation mechanisms. The work planned consists in following the corium-sodium interface at a microscopic scale and use a multi-scale method to treat the primary and secondary fragmentation of corium. This model will have to be validated against separate effect tests.

Hot sodium

To treat the cases of coherent molten corium masses entering sodium close to saturation, the CFD work previously mentioned will help us clarifying the phenomena involved. However, since corium interactions with hot sodium exhibit behaviors similar to corium-water interactions, it is foreseen to adapt the model developed by Namiech [16] for corium-water interactions to CSI. Namiech establishes his base flow for the vapor film around the corium jet with a careful estimation of the steam velocity profile within the

film. This base flow calculation relies on the boundary layer theory. A stability analysis of the film is then performed at the corium interface to estimate the jet breakup length and the generated particle diameter. Considering the low Prandtl number of the liquid metals, the boundary layer calculation will have to be reviewed as well as some assumptions used by Namiech but his overall methodology could be used for molten corium jet propagation into hot sodium.

Experimental database:
To validate the models for coherent mass fragmentation, the experimental database is very limited. For oxide corium, the only experimental program is the FARO-TERMOS one [10]. However, in the FARO-TERMOS experiments, the corium was falling through a 20 cm gas slab before impacting the sodium surface. In addition to entraining non-condensable gases, the stepwise UO_2 penetration into sodium led to limiting the melt mass actually in interaction with sodium. This configuration does not correspond to the ASTRID ones where corium is directly injected into the sodium bulk, below the free surface. As for metal (steel) jet fragmentation, no data could be found in literature. Then, to develop pertinent fragmentation modeling and validate it against relevant data, one of the goals of the PLINIUS2 platform is to develop a database by carrying out well instrumented (with an X-Ray imaging system in particular) experiments for the interaction between prototypical oxide or metal, and sodium [15].

3.3 Corium particle fragmentation

As stated by Corradini [5], particle fragmentation models are generally classified depending on the source of the driving force for fragmentation or the contact mode between the hot corium and the liquid coolant. Following this classification we consider the fragmentation mechanisms due to pure hydrodynamics or due to thermal effects even if we are fully aware that these effects are strongly coupled as shown in [17]. A complete review of these models can be found in [5] and [18]. Some elements of model selection for SCONE are given hereunder.

Hydrodynamic effects
This fragmentation process occurs when a population of droplets is suddenly impacted by an external flow with a velocity greater than its own velocity. A droplet then undergoes an acceleration that induces surface forces that may overcome the cohesive forces of its surface tension. This causes droplet deformation and breakup. To evaluate the possibility for a droplet to fragment under hydrodynamic forces, the Weber number is usually evaluated. It is given by the ratio between the inertial forces and the surface tension:

$$We = \frac{\rho_C D_d \left\| \vec{V}_d - \vec{V}_C \right\|^2}{\sigma_d}$$

where $\vec{V}$ is the velocity (m/s), D is the diameter (m), ρ is the mass density (kg/m^3) and σ is the surface tension (N/m). Subscripts: *d* represents the droplet and *c* the coolant.

Among others, Pilch and Erdman [19] have studied the fragmentation of a liquid droplet in a gas or liquid flow at high flow velocity and mass density lower than the droplet. Carrying flow and droplets being at the same temperature, only hydrodynamics effects are investigated by the authors. They proposed a classification of the breakup processes with respect to the Weber number and their work is widely used in the frame of the vapor explosion modeling. However, in [20] the authors propose a more detailed map of the hydrodynamic fragmentation regimes by considering both the Weber and the Ohnesorge numbers. This classification may guide us sorting out more precisely the fragmentation mechanisms especially for the expected high Weber numbers.
To calculate the hydrodynamic fragmentation of the droplets in SCONE, we intend to base our modeling on these two approaches ([19] and [20]).

Thermal effects

Thermal stress: for oxide fuels, the analysis of the debris issuing from past experiments (mainly in subcooled sodium) has exhibited a majority of particles with a fractured shape and a small proportion of round-shaped debris ([9] or [21] for example). From these observations, it is usually concluded that two fragmentation mechanisms co-exist: the fractured shape suggests solid state fragmentation due to stress while cooling, whereas the round shape debris probably come from liquid state fragmentation (hydrodynamics). However, as pointed out in [21], the thermal stress breakup is a delayed process taking place as a second step and may not contribute directly to the pressure build-up. A thorough analysis will also have to consider that, for the UO_2/Na couple at the temperatures of interest for CSI, the solidification kinetics is faster than the heat transfer kinetics. This point is discussed in [22] where the authors indicate that a UO_2 fragmentation model has to take into account superficial, even partial, solidification.

Different approaches are proposed in literature: Cronenberg and Chawla [23] base their model on the calculation of a thermal stress at the particle surface; Haraldsson [24] develops a linear stability analysis at the interface of the two liquids and considers the appearance of a fine crust; Berthoud and Newman [25] consider that the fragmentation is related to the development of a solid crust that fissures to the fragile/ductile transition to form fragments that break off; in a similar way, Corradini and Todreas [26] propose a model based on a thermal stress analysis and a brittle fracture mechanics approach to determine the minimum UO_2 particle size due to thermal stress.

These models give us hints for SCONE. They will have to be studied as well as their level of validation. The future PLINIUS2 analytical experiments will help selecting a modeling approach and extend the validation database.

Fragmentation and boiling regimes: either for a coherent mass or for particles, the corium fragmentation is also related to boiling regimes. Some experiments have shown that a violent transition boiling regime was initiated at contact between corium and subcooled sodium. It is described as a cyclic process of vapor bubble growth/collapse on the hot body surface. Such a phenomenon is presented as the most probable mechanism inducing fragmentation for subcooled sodium [21]. In other documents, the high pressure pulses recorded during experiments are explained by the occurrence of a vapor film boiling regime and the destabilization of the film [27]. Whatever the boiling regime, the fragmentation would be caused by the direct contacts between the two liquids and the impact of liquid sodium micro-jets onto the liquid fuel surface.

From these observations, two classes of micro-jet models were developed in the literature. For some authors [28], the coolant micro-jets penetrate underneath the fuel surface, are trapped, and vaporize causing the fuel to break up. Others [29] consider it difficult for a light fluid such as the coolant to penetrate into a much more dense fluid (the fuel). Moreover, in [29] the authors explains that it would be necessary for the micro-jets to have a kinetic energy large enough to overcome the surface tension effects during deformation and get through the fuel surface. In the theory they propose, based on the so-called splash theory [30], they describe: the development of Rayleigh-Taylor instabilities at the vapor/liquid interface and the formation of coolant micro-jets impacting the corium surface, the melt surface pressurization due to the nucleation of coolant bubbles, the deformation and the resulting fragmentation of the melt.

Just like for the fragmentation model for a coherent corium mass, this last approach should be considered for the fragmentation of corium droplets in SCONE but will have to be adapted to sodium properties and thermal behavior.

Experimental database:

For droplet fragmentation in a sodium pool, even if literature proposes models relying on some experimental observations, uncertainties remain concerning the relative significance of the different mechanisms with respect to the sodium temperature. A precise data bank needs to be built for model development and validation. Future droplet experiments in the PLINIUS2 platform (where an X-Ray

imaging system is foreseen) will help understanding the phenomena, identifying the leading effects and specifying the modeling to be implemented in SCONE.

3.4 Exchange laws

During a CSI, alongside with the coherent mass of corium, the IZ is composed of three phases: the corium particles, the liquid sodium and the sodium vapor. Non-thermal equilibrium is considered between the phases and the pressure build-up is controlled by the heat exchanges between these phases. From a modeling point of view, the exchanging phases have to be identified so that momentum and energy transfer laws can be written as the product of a transfer coefficient, an exchange surface area and a driving difference. In particular, the surface exchange area strongly depends on the local topology of the flow. In order to specify the appropriate closure laws, two main flow configurations are usually considered depending on the vapor volume fraction (void fraction) within the domain (see Figure 2):

- bubbly flow: the carrier continuous phase is liquid sodium, sodium vapor is the discrete phase in the form of films around the corium particles and bubbles carried by the liquid,
- droplet flow: the carrier continuous phase is vapor, dispersed liquid sodium droplets represent the discrete phase along with the corium particles.

This flow map is established according to only one criterion, the void fraction within the calculated area. The bounding values between the different regimes come from earlier studies for channel water flows, $\alpha_B = 0.3$ and $\alpha_D = 0.7$ are usually used in corium water interaction calculation codes [31].
The transition regime between these two types of flow is considered to be a mix of both, so that contributions of the closures from both flows are taken into account, without looking at the precise topology in such zones. Even if this flow map is generally used in FCI codes, uncertainties remain, especially on the transition bounds (α_B and α_D) and on the representation of the transition zone, as discussed in [31]. For SCONE, the interpolation procedure used to smooth the transition will be a logarithmic average, which is more appropriate than an arithmetic one in case of exchange terms varying by several orders of magnitude [32].

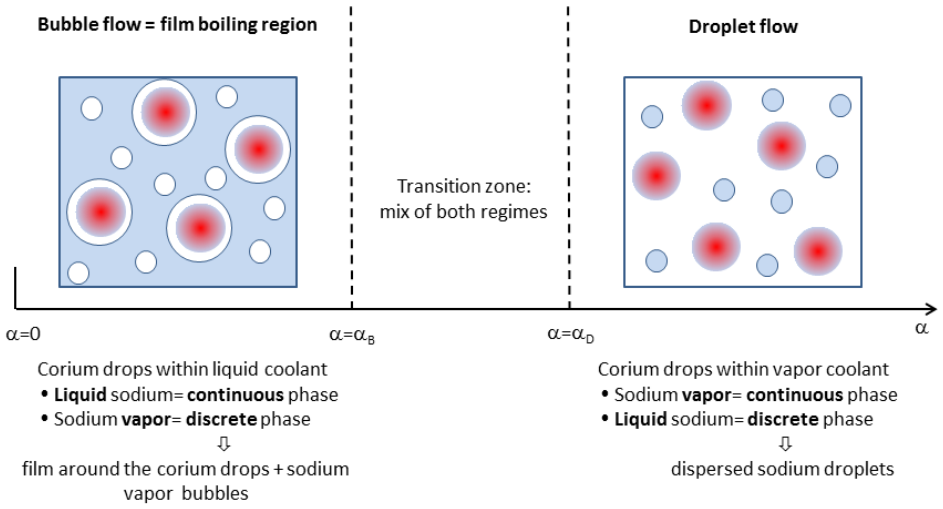

Figure 2: Three-phase flow pattern map

Heat exchanges

When liquid sodium is the continuous phase ($\alpha < \alpha_B$), the corium droplets are isolated from liquid sodium by a vapor film that, as discussed before, is rather unstable. Some sodium bubbles escaping from the films also exist in this configuration. The heat transfer in film boiling is then the major heat transfer

mode existing. It includes a forced convection film boiling contribution and a radiation contribution. Heat from the corium droplet is directly transferred to the vapor/liquid interface to produce vapor. The sodium vapor is considered transparent whereas the liquid sodium is supposed opaque [33].
A model has been developed at CEA for stable sodium film boiling around a hot sphere [7]. The model was partially validated against the Farahat experiment [34] where a hot Tantalum sphere was immersed into a sodium pool. This was the only sodium film boiling experiment available. In [7], the rigorous re-analysis of the Farahat results highlighted the existence of a stable film boiling regime and an unstable one during which contacts between the liquid sodium and the hot sphere enhance the heat exchanges. Following that work, it is planned to perform the analytical stability analysis of the base flow established in [7] in order to understand the conditions of appearance of the unstable film boiling regime (more likely to occur especially in subcooled sodium) which leads, if the contacts become "too" numerous and/or "too" long, to fine fuel fragmentation and violent vapor production. In the meantime, a new experimental program is under study, based on a setup similar to Farahat's one, with extended experimental parameters (forced convection, smaller sphere diameters, pressure effects, and wider range of sodium and sphere temperatures) and improved measurement methods in order to provide more precise data. The objective of this new program is to fill the gaps in the understanding of the stable and unstable sodium film boiling regimes (sodium boiling curve) in terms of physical conditions of appearance, impact on the exchanged heat fluxes and transition toward the explosive phase.
The aim of these analytical and experimental developments is to establish, for SCONE, reliable sodium film boiling correlations (which do not exist in literature) so that the vapor production, pressure build-up and peaks could be correctly estimated.

Heat exchanges due to mass transfer by vaporization/condensation at the interface between the sodium bubbles and the liquid sodium will also be treated by writing energy balances at the interface and using literature correlations.

When sodium vapor is the continuous phase ($\alpha > \alpha_D$), in droplet flow configuration, convective heat transfer between corium particles and vapor has to be taken into account and will be calculated according to classical correlations from literature [35]. The radiative heat transfer from corium particles to liquid sodium droplets will have to be considered and will be included in the energy balance at the vapor/liquid interface.

Momentum exchanges

The driving difference taking part in the interfacial drag coefficients is the velocity difference between the exchanging phases. In our three-phase system, we will establish momentum exchanges between the different phases using here again the flow pattern map (Figure 2) to identify the exchanging phases. The formulation of the drag coefficients is performed in two steps: the drag coefficient has to be precisely written for one single particle (droplet (corium or sodium) and sodium vapor bubble) then the collective effects have to be taken into account, that is, the interactions between the particles [36]. The Ishii and Zuber formulation will be used [38], more specifically the extension to our three-phase systems as proposed in [39].

Mass exchanges

The mass exchange terms will come from vaporization and condensation processes as well as fragmentation and coalescence.
For the sodium, which can be considered similar to water on a hydraulic point of view, fragmentation and coalescence models can be found in literature [40]. As for the mass transfers by vaporization and condensation, they will be estimated by writing energy balances at the liquid/vapor interfaces.
For the corium, the mass exchange source terms will be due to the fragmentation and coalescence of the molten corium which was discussed earlier for corium coherent masses and particles.

3.5 Structure response

In the SCONE software, the structures surrounding the IZ will be represented mainly for the geometry (bounding of the domain) and the thermal aspects: sodium vapor re-condensation will be considered as well as the structure heat-up. This aspect cannot be neglected since, as shown in the CORECT II program a large amount of energy can be transferred to the structures leading to their melting [6].
The detailed mechanical response of the structures needs to take into account their deformation which is not planned for SCONE. A coupling of SCONE with a dedicated software such as EUROPLEXUS [41] is foreseen in order to evaluate the impact of the impulsion generated by the pressure wave onto the structures.

4. NUMERICAL ASPECTS

4.1 Software design

To develop the numerical and physical models of SCONE, we chose to rely on a software architecture with a high level of abstraction. Its design is based upon an object-oriented analysis step of the capability requirements for the software. The necessary classes and packages have been created as well as the different links identified during the analysis step. The implementation is carried out in modern C++ language and relies on several design patterns to describe the different class managers useful to work with a generic number of phases, materials, fields, physical laws, and algorithmic models.

In order to reduce the development efforts regarding the numerical aspects of SCONE, it was decided to use an open source environment that could offer the necessary tools for meshing and parallelism management. The selected environment is the DUNE platform [43, 44]. Based on a C++ template programming, the library allows working with an abstract definition of grids, conformal or not, which offers the possibility to change the type of meshes on which the code is built. In this way, it could be convenient to use unstructured meshes if needed for future applications of SCONE, provided that the numerical scheme is adapted to those. Right now the code only supports Cartesian meshes in relation to the chosen numerical scheme, briefly described hereunder.

4.2 Numerical scheme

To limit the development work of a dedicated numerical scheme for the discretization and the solving of the conservation equations, it was decided to use a variant of the ICE scheme [42]: the semi-implicit method described in [36, 37] has been used quite robustly in the specific FCI applications. The discretization is based on a structured, staggered, Cartesian grid where:

- the temperatures, the material properties, the energies and the pressure are stored at the mesh centers;
- the normal velocities are evaluated at the mesh faces.

The ICE family of schemes, with these degrees of freedom, has gained some popularity as they are dedicated to compressible flows, applicable to all Mach regimes, and tend, in the low-Mach limit, to the well-known MAC discretization for incompressible flows.

The conservation equations for mass and energy are discretized using the finite volume method whereas the momentum balance equations are expressed with finite differences. Second order reconstruction of the variables will be used in order to get an accurate enough advection scheme, stability being ensured through upwinding.

As stated before, it will be necessary to follow the sharp interface defining the coherent mass of corium. Rather than developing complex (in the sense of algorithmics, for 3D notably) geometrical tools such as a VOF/PLIC method, it is planned to rely on sharpening or anti-diffusive advection schemes which are now

rid of the numerical artefacts that limited their use in the past (see for instance [45]). The implementation of such techniques is significantly simpler when it comes to 3D and cylindrical geometries.

The time dependencies of the various quantities in the balance equations lead to the following main steps:

- the use of the momentum conservation equations to link the velocities to the pressure gradient;
- the use of the expressions of the velocities into the mass and energy equations and combination of these equations together with equations of state to assembly the system pressure;
- the linearization of the system and its solving at each time step with a Newton-Raphson method (the unknowns of the problem are the system unique pressure field, the phase volume fractions and temperatures, from which the velocities are deduced).

Since SCONE must propagate properly large pressure waves, possibly shock waves, (explosion phenomenon), the scheme must be corrected to be conservative in momentum and total energy at discrete level. This is indeed required to get a convergent, and so a more reliable, scheme in presence of shock discontinuities. Such a correction has been proposed while preserving the previous features of the ICE scheme [39].

5. SUMMARY: WHERE DO WE STAND?

SCONE is a numerical tool under development at CEA, dedicated to the simulation of corium-sodium interaction. It is a mechanistic software that will have to precisely represent the phenomena involved in CSI in the context of the ASTRID sodium-cooled reactor: corium fragmentation (coherent mass and particles), intense heat transfers and vapor production, pressure build-up and wave expansion.

From the computational environment point of view, a flexible object-oriented architecture is in place. The DUNE tool has been encapsulated into the SCONE architecture as a library dedicated to the mesh and parallelism management.

From the numerical point of view, an explicit version of the ICE scheme has been coded to solve the mass, momentum and energy balance equations; it has been corrected for convergence errors while calculating shocks [46]; a shock tube could be simulated (1D, one phase flow) and validated against an analytical solution (Figure 3); the ability to follow the motion of a polydispersed phase (different sizes and velocities) into a continuous phase has been tested (Figure 4).

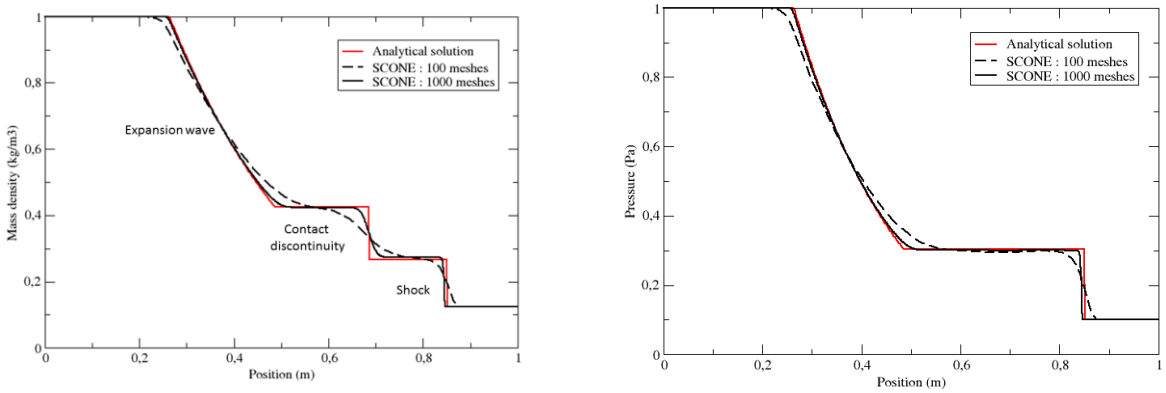

Figure 3: Density and pressure profiles within a shock tube - SCONE calculations and analytical solution (given in [47])

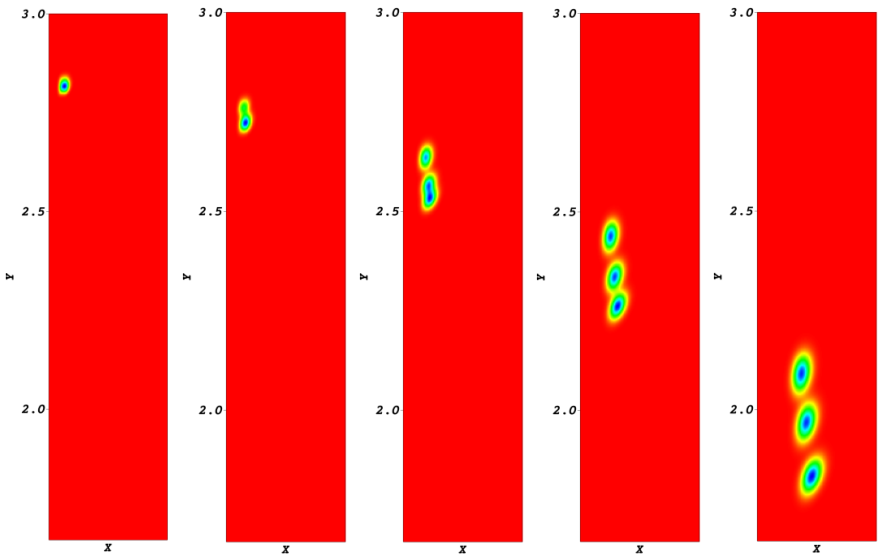

Figure 4: Separation of a polydispersed phase due to different drag coefficents (only the mass balance equation is solved, the velocities are updated according to a simplified evolution equation)

From the physical point of view, the main mechanisms to be represented have been specified and presented in this paper. Work has already been performed on the different modeling approaches proposed in literature or in previous CEA studies. The most appropriate ones will be implemented in SCONE. Some knowledge gaps also have been identified and dedicated, well instrumented, experimental programs are needed at different scales. Analytical experiments are under design and will have to be performed to answer questions regarding:

- sodium film boiling around a hot sphere representing a corium particle: the outcome of such an experiment would allow to fully understand the occurrence and the heat exchanges in "film boiling with contacts" situations as well as the transition to the explosive phase of the CSI.
- UO_2 and steel particle fragmentation in subcooled and hot sodium: the aim is here to investigate the part played by hydrodynamics and thermal effects in the oxide and metal particle fragmentation mechanism.

These detailed programs will help us writing physically grounded models and correlations for SCONE, so we can be confident in the extrapolation to reactor-scale situations.
Then, in order to qualify SCONE in more representative configurations and verify the relevance of the software with all models working together, more global (medium and large scale) tests are foreseen in the PLINIUS2 platform with more important masses involved [15].

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REFERENCES

1. Morita K., Kondo S. Tobita Y., Brear D.J., "SIMMER-III applications to fuel-coolant interactions", Nucl. Engr. Des., **189** (1999)
2. Le Belguet A., Jeanne T., Journeau C., Bataille F., "A new analysis of the large scale fuel-sodium interaction in the FARO-TERMOS experiment with the SIMMER-III code", SFEN Conference, Charlotte (NC), USA (2012)

3. Bertrand F., Marie N., Prulhière G., Lecerf Y., Seiler J.M., "Comparison of the behaviour of two core designs for ASTRID in case of severe accident", *Nucl. Engr. Des*., **297** (2016)
4. Berthoud G., "Vapor explosions", *Annu. Rev. Fluid Mech*., **32** (2000).
5. Corradini M.L., Kim G.J., Oh M.D., "Vapor explosions in light water reactors: a review of theory and modelling", *Progr. Nucl. Energy*, **22**(1) (1988).
6. Berthoud G., Jacobs H., Knowles J.B. "Large scale fuel-sodium interactions: synthesis of European programs", *Fast Reactor Coordinating Committee / Safety Working Group*, WAC(94)-D375 (1994).
7. Le Belguet A., "Etude de l'ébullition en film du sodium autour d'une sphère à haute température, *Thèse de l'Université de Grenoble*, France (2013).
8. Gross S., Vollath D., "Characterization of fragmented fuel from a thermal fuel-sodium interaction", *Nucl. Techn*., **42** (1979).
9. Chu T.Y., Beattie A.G., Drotning W.D, Powers D.A, "Medium scale melt-sodium fragmentation experiments", *International meeting on fast reactor safety technology*, Seattle, USA (1979).
10. Magallon D., Hohmann H., Schins H., "Pouring of 100-kg-scale molten UO_2 into sodium", *Nucl. Techn*., **98** (1992).
11. Magallon D., "An analysis of the melt penetration into sodium in the FARO-TERMOS experiments", *14th meeting of the Liquid Metal Boiling Working Group*, Brasimone, Italy (1991).
12. Chu T.Y., "Fragmentation of molten-core material by sodium", *International topical meeting on LMFBR safety*, Lyon, France, SAND-82-0300C; CONF-820704-10 (1982).
13. Ishii M., Mishima K., "Two-fluid model and hydrodynamic constitutive relations", *Nucl. Engr. Des*., **82** (1984).
14. Krepper E., Lucas D., Franck T. Prasser H-M, Zwart P.J., "The inhomogeneous MUSIG model for the simulation of polydispersed flows", *Nucl. Engr. Des*., **238** (2008).
15. Journeau C., Buffe L., Haquet J.F., Piluso P., Willermoz G., "Needs for large mass prototypic corium experiments: the PLINIUS2 platform", *NURETH-16*, Chicago (2015).
16. Namiech J., Berthoud G., Coutris N., "Fragmentation of a molten corium jet falling into water" *Nucl. Engr. Des*., **229** (2) (2004).
17. De Malmazet E., "Etude de la fragmentationde gouttes chaudes en ebullition en film dans un écoulement d'eau", *Thèse de l'Institut Polytechnique de Grenoble*, France (2009)
18. Cronenberg A.W., Golmes M.A., "A review of fragmentation models relative to molten UO_2 breakup when quenched in sodium coolant", *3rd Specialists' Meeting on Sodium-Fuel Interactions in Fast Reactors*, Tokyo (1976).
19. Pilch M., Erdman C.A., "Use of breakup time date and velocity history data to predict the maximum size of stable fragments for acceleration-induced breakup of a liquid drop", *Int. J. Multiphase Flow*, **13**(6) (1987).
20. Hsiang L.P., Faeth G.M., "Drop deformation and breakup due to shock wave and steady disturbances", *Int. J. Multiphase Flow*, **21**, n°4 (1995)
21. Schins H., Gunnerson F.S., "Boiling and fragmentation behavior during fuel-sodium interactions", *Nucl. Engr. Des*., **91** (1986).
22. Cronenberg A.W., Fauske H.K., "UO_2 solidification phenomena associated with rapid cooling in liquid sodium", *J. Nucl. Mater*., **52** (1974).
23. Cronenberg A.W., Chawla H.K., Fauske H.K., "A thermal stress mechanism for the fragmentation of molten UO_2 upon contact with sodium coolant", *Nucl. Engr. Des*., **30** (1974).
24. Haraldsson H.O., Li H.X., Yang Z.L., Dinh T.N., Sehgal B. R., "Effect of solidification on drop fragmentation in liquid-liquid media", *Heat and Mass Transfer*, **37** (2001).
25. Berthoud G., Newman W.H. "A description of a fuel-coolant thermal interaction model with application in the interpretation of experimental results", *Nucl. Engr, Des*., **8 (**1984).
26. Corradini M., Todreas N.E., "Prediction of minimum UO_2 particle size based on thermal stress initiated fracture model", *Nucl. Engr. Des*., **53** (1979).
27. Schins H. "A critical review of fuel coolant interactions with particular reference to UO_2-Na", *Res Mechanica*, **23** (1988).

28. Kim B., Corradini M.L., "Modeling of small-scale single droplet fuel/coolant interactions", *Nucl. Sci. Engr*., **98** (1988).
29. Leclerc E., Berthoud G., "Modeling of melt droplet fragmentation following vapor film destabilization by a trigger pulse", *Nucl. Techn*., **144** (2003).
30. Ochiai M., Bankoff S.G., "Liquid-liquid contact in vapor explosions" *ANS/ENS Int. Mtg. Fast Reactor Safety*, **4**, pp.1842, Chicago (1976).
31. Meignen R., Magallon D. et al., "Comparative review of FCI Computer Models Used in the OECD-SERENA program", ICAPP-05, Seoul, South Korea, Paper 5087 (2005).
32. Tobita Y. et al, "Interfacial Area Modeling for a Multiphase, Multicomponent Fluid-Dynamics Code," Int. Conf. on Multiphase Flows, Tsubaka, Japan (1991).
33. Vanderhaegen M. Le Belguet A., "A review on sodium boiling phenomena in reactor systems", *Nucl. Sci. Engr*., **176**, pp.115-137 (2014).
34. Farahat M.M.K., "Transient-boiling heat transfer from spheres to sodium", *Ph-D, Argone National Laboratory*, University of Alexandria (1972).
35. Knudsen J.G., Katz D.L., "Fluid dynamics and heat transfer", *Mc Graw-Hill Book Company* (1958).
36. Berthoud G., Valette M. "Development of a multidimensional model for the premixing phase of a fuel-coolant interaction", *Nucl. Engr. Des*., **149** (1994).
37. Valette M., "MC3D V3.2: résolution numérique des équations", CEA internal technical note SMTH/LDTA-2000-015 (2000).
38. Ishii M., Zuber N., "Drag coefficient and relative velocity in bubbly, droplet and particulate flows", *AIChE Journal*, **25** (5) (1979).
39. Berthoud G., Valette M., Meignen R., Picchi S., Description des lois constitutives de la version 3.3 du logiciel de prémélange MC3D, CEA internal technical note SMTH/LDTA/2001-019 (2001).
40. Bohl W.R., Wilhelm D. Parker F.R., Berthier J., Goutagny L., Ninokata H., "AFDM: an Advanced Fluid-Dynamics Model", Laboratory report LA--11692 MS Vol. II (1990).
41. EUROPLEXUS(2012). europlexus.jrc.ec.europa.eu.
42. Harlow F.H., Amsden A.A., "Numerical calculation of almost incompressible flow", *J. Comput. Phys*., **3** (1968).
43. Bastian P., Blatt M., Dedner A., Engwer C., Klöfkorn R., Ohlberger M., Sander O., "A Generic Grid Interface for Parallel and Adaptive Scientific Computing, Part I: Abstract Framework"**.** *Computing,* **82**(2-3) (2008a).
44. Bastian P., Blatt M., Dedner A., Engwer C., Klöfkorn R., Ohlberger M., Sander O., "A Generic Grid Interface for Parallel and Adaptive Scientific Computing. Part II: Implementation and tests in DUNE", *Computing*, **82**(2-3) (2008b).
45. De Vuyst F., Béchereau M., Gasc T., Motte R., Peybernes M., Poncet R., Stable and accurate low-diffusive interface capturing advection schemes, Preprint ArXiv (2016).
46. Fochesato C., Zabiégo M., "Implementation of the ICE scheme in the parallel DUNE framework", *International Conference on Multiphase Flow (ICMF)*, Italy (2016).
47. Sod G.A., "A survey of several finite difference methods for systems of nonlinear hyperbolic conservation laws", *J. Comput. Phys*., **27** (1978).