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Overview of key thermal–hydraulic phenomena in severe accident unfolding: Current knowledge and further needs

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A B S T R A C T

Severe Accidents (SA) developments are closely and deeply linked with thermal-hydraulics, that is, fluid flow combined with heat and mass transfer. The present paper synthesizes this relation during an accident unfolding and provides an overview of the remaining gaps associated to thermal-hydraulics that need to be addressed to reduce the uncertainties associated to SA and to optimize their management. Some of those thermal–hydraulic phenomena are common to other areas, but most of them are genuine to the SA domain. In addition to thermal–hydraulic phenomena affecting SA development, there are others major SA consequences, like fission product transport and eventual release to the environment, that are heavily affected by thermal–hydraulic boundary conditions and need to be investigated under the anticipated accident conditions. There is a consensus that any investigation to be launched in the coming years should have a direct impact on either reducing the uncertainties associated to their modelling or on optimizing their management, or on both; such consensus was soundly built in the EC EURSAFE project and has been renewed under the frame of the SARNET projects and the SNETP/NUGENIA/TA2 activities.

1. Introduction

Severe Accidents (SA) are the most complex, extreme, and unlikely accident scenarios that might occur in a Nuclear Power Plant (NPP). However, no matter how unlikely they are, the accidents that already occurred in commercial NPPs (TMI-2 (USNRC, 2016), Chernobyl-4 (USNRC, 1987) and Fukushima Daiichi (Units 1 through 3) (TEPCO, 2012)), highlight that "improbable" does not mean "impossible" and, given their potential consequences, their investigation is necessary to prevent and/or mitigate them. The four main distinctive features of a SA, considered within the scope of the present paper, are:

- *Multidisciplinary nature*. SA involve energy generation, heat and mass transfer, fluid flow, solid material mechanical behaviour, aerosol and vapour/gas generation and transport and chemical reactions (including combustion). The present paper is focused on identifying the key thermal–hydraulic (TH) phenomena that still require further research.
- *Strong interaction of different phenomena*. Phenomena of a specific nature may have a key influence on others of a different nature. This means that thermal–hydraulic phenomena might be intrinsically important and/or might pose a crucial initial and/or boundary condition for a non-thermal–hydraulic phenomenon that becomes crucial on the accident unfolding.
- *Time length*. These events may last days or even weeks. Along this time span, the variability of boundary conditions is considerable, so that well-known phenomena under certain circumstances might require further investigation when conditions change significantly.
- *Uncertainty associated to human actions*. Given the high complexity of a SA, implementation of any recommended Accident Management (AM) action introduces additional uncertainty (i.e., right timing and way to implement it, local and global effects on the accident scenario), so that it is anticipated that AM actions might result in highlighting thermal–hydraulic phenomena not investigated so far or, at least, not under the anticipated prevailing conditions.

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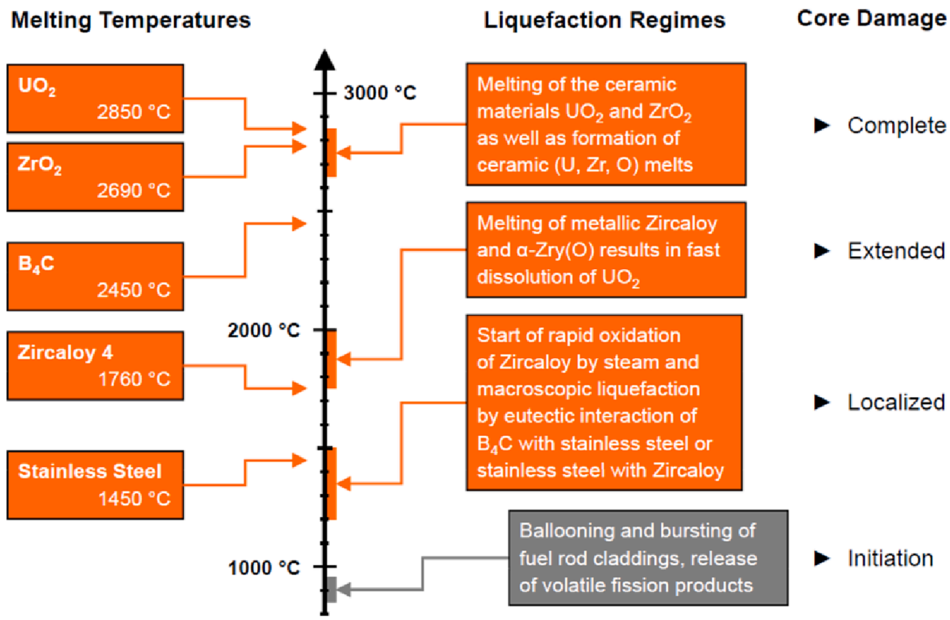

Fig. 1. Thermal diagram of key processes in core degradation (BWR).

The final goal of any item of necessary research identified in the present paper would be to enhance SA predictability; in other words, to reduce uncertainties in the current system codes employed to model SAs and in any method/approach used to assess AM measures. This implicitly requires a proper scaling of data used for model development and code validation.

2. Overview of severe accident unfolding

A SA in water cooled reactors results from a thermal imbalance between the power being generated and the cooling capability to remove it for a time span long enough to cause significant nuclear fuel degradation. Coolant leaking and/or water phase change deteriorate the core cooling, which at this point relies heavily on natural circulation, and make fuel temperature increase and reach around 1200 °C. At this temperature, a strong exothermic metal-steam oxidation leads to a further thermal escalation and hydrogen (H_2) production as well as loss of the clad mechanical properties:

$$Zr + 2\cdot H_2O_{vap} \rightarrow ZrO_2 + 2\cdot H_2 \quad \Delta h \approx 6\cdot 10^6 J/kg_{Zr}$$

Depending on reactor design and accident sequence, the amount of H_2 generated in-vessel could range from tens to hundreds of kilograms and even exceed 1000 kg (OECD/NEA, 2001). During this early phase of the sequence, (liquid) water and steam flows through the reactor core are affected by local ruptures and clad ballooning of the nuclear fuel.

At higher fuel temperatures (1700 °C), but still far from the melting temperatures of the individual materials in the reactor core, the formation of eutectics leads to their partial liquefaction and to an uncontrolled downward motion of the molten materials. Around 2200 °C the molten cladding is even capable of dissolving the nuclear fuel pellets and the core geometry may be locally or grossly lost. Solid fragments and molten materials may lead to in-core blockages, which deeply affect the cooling flow patterns. Local or large molten pools, a complex material mixture called *corium*, may be formed and, if so, heat transfer in the core region becomes drastically distorted (compared with the initial configuration). A fraction of the molten corium may proceed downwards, finally slumping into the Reactor Pressure Vessel (RPV) lower head. Fig. 1 illustrates a schematic correspondence between the key temperature and the key core degradation process for a BWR design (Sornette et al., 2019).

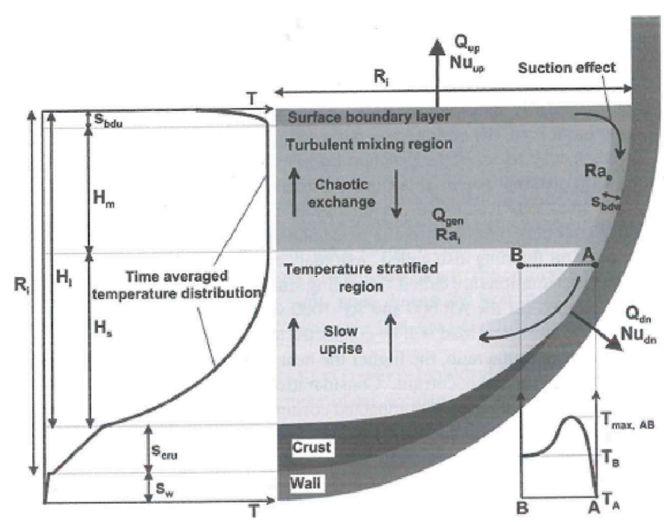

Fig. 2. Natural convection flow in a homogeneous corium pool (Sehgal, 2012).

In-vessel relocation of molten materials and corium throughout the core is highly uncertain (Pellegrini et al., 2020). This might have a strong effect on the TH phenomena occurring in the core degradation phase of a SA and on related processes, like H_2 generation.

The presence of remaining water inside the RPV lower plenum is a key factor for the accident unfolding. If water is available, the Fuel Coolant Interaction (FCI) process may lead to the fragmentation of the molten corium and a possible Steam Explosion (SE), with formation of high pressure vapour peaks (either spikes or explosions) having as a consequence the mechanical loading on the RPV (OECD Research Programme on Fuel-Coolant Interaction and Resolution, 2006). Otherwise, the molten materials directly attack the RPV structures. Natural convection induced by temperature gradients inside the corium pool governs the heat and mass transfer phenomena in the lower head (Fig. 2, an example of possible in-vessel configuration).

The slumping of molten materials and debris into the lower plenum of the RPV as well as the internal mass motion and the complex heat transfer patterns give rise to thermal and mechanical loading on the RPV surfaces. In case that the RPV eventually fails, a fraction of the corium

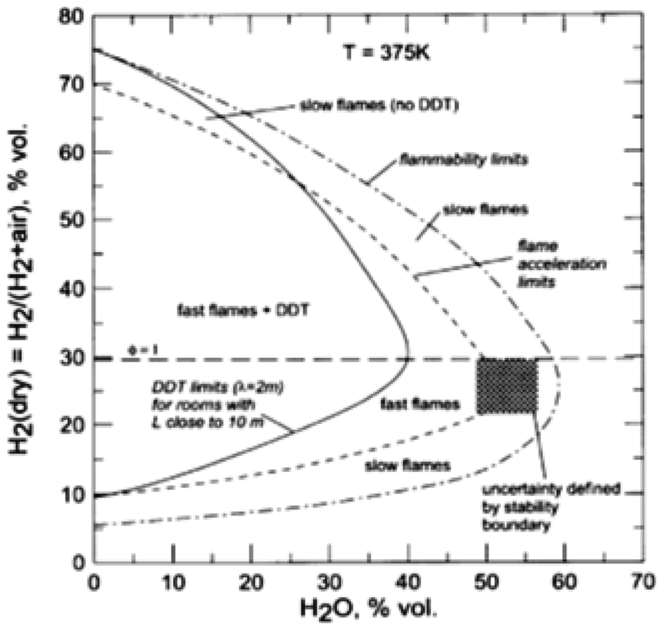

Fig. 3. Limits and combustion regimes for H_2-air–steam mixtures at 375 K and 1.01 bar.

previously relocated in the lower head would be transferred towards the reactor cavity, this being the onset of what is called "ex-vessel phase" of the SA.

In the ex-vessel phase, the containment integrity might be challenged by a number of TH phenomena: Steam Explosions/spikes, corium spreading, containment basemat ablation due to thermal attack of the concrete by corium melts (Molten Core Concrete Interaction, MCCI), over-pressurization resulting from the steam/gas production by the MCCI (H_2O, CO_2, H_2 and CO due to concrete ablation and melt/gases reactions), and fast deflagration and/or detonation of combustible gases (H_2 and CO). MCCI is a good representation of the strong coupling of TH and other phenomena: concrete ablation; immiscible liquids (metallic and oxides) thermal-hydraulics and heat transfer of the corium pool agitated by gas bubbles; physico-chemistry of the multi-component corium melt with a continuously-changing composition due to the admixture of molten concrete, and wide solidification ranges (of the order of 1000 °C); oxidation of metals, and partial or total solidification of the melt at the interface between corium and concrete (Cranga et al., 2014).

It is worth noting that some of the phenomena mentioned above, like the behaviour of molten pools or MCCI, involve complex and aggressive corium fluids at very high temperature (1220 °C < T < 2400 °C) other than water in which complex heat transfer and fluid motion mechanisms take place.

Depending on in-vessel or ex-vessel accident scenario and the associated boundary conditions, fission product of different chemical and physical nature are formed and transported into the containment. In addition to chemical interactions or reactions with containment surfaces, Reactor Coolant System (RCS) and containment thermal-hydraulics plays a major role in defining the types and amounts of radioactive material which could be released to the environment (Source term) in case of containment failure or controlled opening, like venting with or without mitigation filters. The TH conditions which will have major influence on source term (ST) include flow characteristics (e.g., gas composition and concentration of gas constituents, flow velocity) and thermal parameters like gas, surfaces and sump/water pool temperatures. For the reduction of the ST related uncertainties, a correct description of underlying thermal hydraulic phenomena is there necessary, as the fission product distribution inside the containment system will be influenced directly due to heat transfer (gas–gas or gas-wall) or due to mass transfers (e.g. bulk- or wall condensation).

The main issue of the presence of hydrogen (H_2) and carbon monoxide (CO) in the containment atmosphere is the possibility of formation of flammable mixtures in regions of the building where oxygen is present at the onset of the accident (i.e., inside non-inert containments) or might reach in the course of the accident (even in inert-designed containments or compartments). Fig. 3 illustrates the H_2 flammability limits and combustion regimes (OECD/NEA Report, 2000) for hydrogen-steam-air mixtures. After a flammable mixture ignition, initially laminar deflagrations (with a flame velocity of about few m/s) may accelerate and develop into a fast deflagration (first laminar with a flame velocity of a few m/s, then turbulent with much faster flame) or even into a detonation (with a flame velocity over 1000 m/s) due to hydrodynamic instabilities and turbulence (this transition is known as Deflagration-to-Detonation Transition, DDT). Even though the containment structures should withstand a pressure spike caused by a combustible gas deflagration (the most likely form of combustion, since triggering directly a stable detonation would require an energy supply –MIE, Minimum Ignition Energy – at least 108 times higher), such an event would still significantly disrupt accident management, as it could affect the safety component systems functionality needed for SA management. In all these possible events, the relevance of the gas mixture composition turns combustible gas (H_2 and CO) transport and distribution (uniform or not) into a key feature of the accident progression.

During the core degradation phase, most volatile fission product vapours and aerosols are released together with structural and control rod materials. Additionally, a secondary fission product source could enter into the containment atmosphere from the molten materials transferred to the containment basemat once RPV fails and MCCI starts. In both cases, their release kinetics, amount and speciation and, particularly, their transport through the RCS to the containment (and eventually to the environment) are strongly affected by a number of factors (i.e., volatility, pathway, engineering safeguards, etc.), among which TH boundary conditions stand out. Just to give a few examples: in the RCS, the steam production during the core reflooding may lead to flows (i.e., mostly turbulent) that remobilize the materials previously deposited on the systems surfaces; in the containment, the steam condensation is responsible for removing a significant fraction of fission products, either airborne or pre-deposited on containment surfaces, to the containment sump or to elevated water pools, not just by processes like diffusiophoresis but also by the adsorption/desorption of iodine on/from containment painted surfaces, and indirectly for enhancing the dominant aerosol removal mechanism (sedimentation) by making aerosol particles in the gas phase grow and be subject to gravity. In the specific case of iodine in containment, mass transfer of iodine to the gas phase from ponds or surfaces is heavily impacted by TH boundary conditions, like flow regimes. This strong influence of TH on fission product behaviour and then on the ST is even enhanced when engineering safety systems come into operation, like containment spray systems or in-containment suppression pools.

There are some specific examples where the close bond between TH and ST is remarkably illustrated. In accidents like the Fukushima one, the fission products trapping was found mostly governed by the steam condensation and by the inertial particle impaction under a jet injection regime, both of them occurring at the inlet of the suppression pool (Herranz et al., 2020); likewise, in case of a boiling pool (highly expected during the late phase of a SA), a late FPs release may happen. Moreover, the highly turbulent flow and the elevated temperatures associated with a combustion process may play a significant role due to the remobilization of pre-deposited aerosols on containment surfaces and/or the thermal decomposition of the metal iodide aerosols.

Along SA unfolding, some actions (Accident Management, AM) are foreseen to be undertaken by NPP operators aimed at preventing a significant core damage, terminate the core degradation once initiated, maintain the containment integrity, minimize the external releases, and achieve a long-term stable state. Some of them involve a water injection at different time and locations (i.e., in-reactor, in-containment, in-cavity, etc.) and may give rise to THc phenomena affecting the subsequent accident progression, like severely damaged core reflooding that may produce large amounts of steam and H_2 or in-cavity steam explosions. Others, like the containment venting, might indirectly cause TH phenomena, like pool boiling and/or turbulent flows along the system. All those TH phenomena resulting from AMs might play a key role in the accident progression.

3. Thermal-hydraulic research needs

The most recent update of the Severe Accident Research Priority (SARP) ranking conducted under the frame of NUGENIA/TA2 (Manara et al., 2019), includes TH phenomena and other non-thermal–hydraulic phenomena that are strongly conditioned by thermal-hydraulics. It is worth emphasizing that the main aim of further research is either reducing the uncertainties in current analytical tools or enhancing the AM capability. This section synthesizes the remaining investigation needs on thermal–hydraulic aspects of a SA.

3.1. In-vessel

During the in-vessel phase of the accident, phenomena initiated by core reflooding and RPV wall mechanical behaviour stand out. As for reflooding, aside the conceptual benefit of cooling through water injection, the potential steaming and subsequent additional cladding oxidation might lead to further heating and H_2 generation. In addition, if the core is reflooded at later accident stages, the cooling capability of corium pools and debris by water injection is not known and may be even questioned. In particular, the still existing lack of knowledge on the morphology of core debris as core degradation progresses represents the dominant source of uncertainty when considering the quenching of the debris during reflooding. In order to reduce such uncertainties, several research activities have been performing since years on this subject (Bürger et al., 2010; Karbojian et al., 2009; Modak, 2022) as well as dedicated analyses are going on at the Fukushima site (Mizokami, 2022). It is therefore necessary to consolidate the dedicated physical models embedded in the integral codes in order to properly predict core heat evacuation and hydrogen production in realistic corium and debris configurations.

Enhancing the capability to reduce the in-vessel consequences of a SA is the main driver of the current worldwide investigations on Accident Tolerant Fuels (ATFs) (NEA, 2018; IAEA, 2020). Activities related to design, development, and testing of innovative fuels, claddings, and absorber material are currently going on in the framework of OECD/NEA (OECD/NEA, QUENCH-ATF Project) and IAEA (IAEA CRP 2236) projects. The main goal of the research investigations on such innovative cladding materials is the reduction of the clad-steam oxidation reaction, in order to limit the amount of hydrogen produced in the vessel during the accident as well as to delay the failure of the first safety barrier.

Having this in mind, single tests and bundle experiments have performed and are planned in the near future to investigate the behaviour of different innovative materials, i.e. FeCrAl(Y), SiC. In this framework, the QUENCH-19 experiment has been conducted in 2018 at the QUENCH facility at the Karlsruhe Institute of Technology (Stuckert and Grosse, 2019; Kim et al., 2021). In the experiment, the analysis of the effect of water reflooding in a pre-heated PWR-like rod bundle composed of 24 heated rods simulators with FeCrAl(Y) cladding and 8 corner rods made of FeCrAl (Kantal APM) has been investigated. The results of the QUENCH-19 test have been compared with the outcomes of the QUENCH-15 test where a similar transient has been analysed for the same rod bundle where ZIRLO™ claddings have been employed (Stuckert and Grosse, 2019; Kim et al., 2021). The analysis reveals that the employment of FeCrAl(Y) claddings leads to a reduction of about 80% of the total amount of hydrogen produced during the test as well as no thermal excursion observation. In particular, the FeCrAl(Y) material in such experimental conditions show a lower initial oxidation rate before the clad melting, despite a potential for significant oxidation after the melting. As above mentioned, single test tests are going on for, i.e. SiC, (Steinbrueck et al., 2021), and related integral experiments are planned in the framework of OECD/NEA QUENCH-ATF project.

At the same time, activities are already going on to better understand how ATFs may affect the SA progression and the ST. Having this in mind, a Phenomena Identification Ranking Table (PIRT) has been developed by USNRC (United States Nuclear Regulatory Research, 2021a,b) to address the significant phenomenological issues under SA conditions for various ATF designs, also including the impact of high burnup/enrichment fuels. The understanding of the behaviour of such innovative components and their effects on the in-vessel thermal-hydraulics is therefore worth to be investigated also in view of the envisaged employment of such materials in innovative concepts, i.e. Small Modular Reactors (SMRs). It poses new challenges for the development of the corresponding physical models in the integral codes, which are mainly based on the employment of Zr-clads. Having this in mind, code development and validation activities are planned in the above mentioned projects. As an example, the analyses of the performance the SA codes ASTEC (Chatelard et al., 2014), MELCOR, and AC2/ATHLET-CD when employing FeCrAl clad material are currently going on (Hollands et al., 2022).

The potential loss of integrity of the RPV is a cliff-edge process in the accident unfolding. The current information of the Fukushima events, based on local inspections, show that the accident progressions in units 1, 2, and 3 are different from each other depending on the different availability of systems and operator actions. More details can be found in (Mizokami, 2022; OECD/NEA, 2021; OECD/NEA, 2017). In addition, it is worth noting significant differences in aspects such as the breaching or failure of the RPV, the material relocation in the pedestal floor, and the position of the RPV breach itself. These insights are quite unique and have triggered research aiming at developing and improving the degree of confidence of Severe Accident Management (SAM) strategies. In particular, the In-Vessel Melt Retention (IVMR) strategy, which aims at stabilizing and isolating molten materials and fission products inside the RPV to minimize the radiological consequences by flooding the reactor pit (cavity), has been and it is being paid substantial attention (Fichot et al., 2018; IVMR Project).

The IVMR Project meant to provide a step forward on both the knowledge of the phenomena occurring as well as the level of predictive abilities of the integral codes, particularly ASTEC (Chatelard et al., 2014). A new methodology has been proposed based on the use of mechanistic codes and the residual thickness of the vessel as safety criterion. Furthermore, a PIRT table has been assessed in the project for a better understanding the complex phenomena governing the IVMR mitigation strategy. Such work is the basis of a current going on IAEA CRP on IVMR (IAEA CRP 2283; Carenini et al., 2022). However, the predictability of possible inversions of the corium layers (stratification) is still an open issue. In addition, still rather large uncertainties exist on some key phenomena, i.e., molten pool formation, heat transfer correlations in the upper metal layer, metal/oxide crusts chemical interactions. Finally, additional efforts should be performed in improving the predictability of the RPV failure, in particular for RPV lower heads embedding a high number of penetrations.

3.2. Ex-vessel

The severe accidents of Chernobyl and Fukushima confirmed that ex-vessel configurations have to be take into account in SAM regarding different phenomena involving thermal–hydraulic such as corium spreading or corium concrete interaction. After the RPV failure, there are two ex-vessel configurations possible: dry cavity and wet cavity. Both of them pose challenges requiring further research (Bechta et al., 2019).

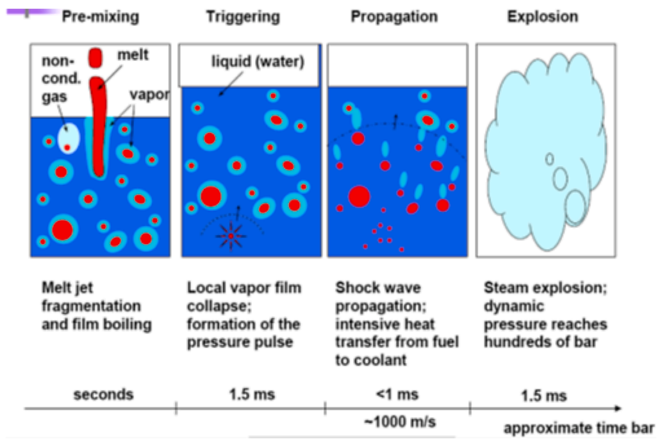

Fig. 4. The four phases of Fuel Coolant Interaction (FCI).

In absence of water, in addition to the effect of specific compositions of the material (i.e., oxide-metal or pure oxidic phase), there are still some phenomena not well known, like melt ejections from MCCI, short-term top flooding, cooling (including the use of core catchers). The thermal-hydraulics of the corium pool and the different pool configuration (for example immiscible oxide and metallic phases, stratification or emulsion – i.e., metallic droplets in a corium oxidic melts) will play an important role on the ability of cooling pool and stopping the progression of the concrete ablation. Another still open issue concerns the coupling between corium thermal-hydraulics and nature of the concrete: isotropic (lime-siliceous) or anisotropic (basaltic, siliceous) ablation has been observed without any clear understanding (Journeau and Piluso, 2020). One explanation could be the concrete degradation process in advance of the ablation/dissolution of the concrete by the corium (Mastori et al., 2019).

In the long-run MCCI, improved knowledge is essential to assess mitigation measures dedicated to arrest the concrete erosion while limiting containment over-pressurization. Experimental data are still needed, particularly for the behaviour of oxide-metallic immiscible phases during a fast reflooding. These topics are being addressed in the OECD/ROSAU program (Licht et al., 2022), which specifically focuses on underwater cooling and melt spreading and in the MIT3bars project (Journeau et al., 2022) which focuses on corium (oxide and metallic melts) underwater cooling. The upper cooling and water ingression process efficiency will be able to be qualified in these experiments for configurations representative of reactor case.

In presence of water, as a result of either cavity design or AM actions (cavity flooding), two phenomena draw research attention: Fuel-Coolant Interaction, ex-vessel Steam Explosions included; and, corium spreading under water.

Ex-vessel steam explosion and its mechanical short-term consequences on the containment building are still an open issue (Piluso, 2017). In particular, in case that the "focusing effect" (i.e., the high local thermal loading of RPV lower head side walls due to preferred thermal conduction through the metallic layer overlying the oxidic pool underneath) ends up with the RPV failure, a metallic melt (Fe-U-Zr) will be formed and interact with water. This kind of interaction is not known in terms of fragmentation, hydrogen produced and energy release. Especially, it will be necessary to better know the dynamic fragmentation mechanism (3 phases) to more accurately calculate energy exchanges in this configuration (Fig. 4). Separate effect tests such as steam oxidation on corium melt are on-going studies (Thilliez et al., 2022) and integral tests varying composition, including iron, non-volatile radio-nuclide such as barium, are on-going R&D activities (Meignen et al., 2022). Furthermore, thermophysical properties -density, surface tension, and viscosity - are playing a key-role in the fragmentation process. The COPS (COrium Properties for reactor Simulation and uncertainties) (Piluso, 2022) proposal is currently under construction at OECD/NEA to produce reliable data and modelling of these properties. Several sensitive analyses studies (BSAF, 2015, BSAF, 2021; Journeau et al., 2016) have been devoted to identify the main sources of uncertainties in SA code calculation and nuclear safety assessment. Among the identified sources, uncertainties on corium thermophysical properties have been assessed as being one important source of uncertainty on simulation, as it has been shown in the OECD/NEA TCOFF-1 project (TCOFF-1, 2021).

The Fuel Coolant Interaction (FCI)/Steam Explosion (SE), so-called ICE program (Piluso et al., 2015), addresses various gaps, identified after the OECD SERENA-2 and EC SARNET-2 network programs, in both understanding and modelling of the phenomena: the melt fragmentation during premixing; detailed process of pressurization during the explosion; melt properties and impact on solidification; extent and impact of oxidation. The research issues were addressed thanks in particular to combined Direct Numerical Simulation (DNS), analytical experiments, and experiments. A series of FCI/SE tests with prototypic corium have been performed (Kudinov et al., 2017) in the improved PLINIUS KROTOS installation, simulating different reactor case configurations. Some thermophysical and thermodynamic properties have been measured in the ATTHILA facility and VITI facility. Separate effect tests on oxidation have been performed in the VITOX facility, allowing the establishment of new oxidation laws. New insights on the process of fragmentation and a clarification of the secondary process of fragmentation, applicable for both premixing and explosion stages have been reached. A revised modelling of oxidation, including variation of the melt thermodynamic properties, has been achieved. As for the issue of the steam explosion load build up, the work was based on separate DNS simulations related to the boiling and fragmentation processes. This work is being pursued by investigating with details the heat transfer during the fragmentation process, still without boiling.

Another ex-vessel configuration can lead to a steam explosion: this is the so-called "stratified steam explosion" observed several time at KTH with simulant materials (Kudinov et al., 2017). Several experiments, carried out in Pouring and Under-water Liquid Melt Spreading (PULiMS) facility (78 kg of simulant materials), have resulted in spontaneous explosions with relatively high conversion ratios (order of one percent). There are today same hypothesis to explain this specific behaviour, but there are no clear understanding.

In the long-run MCCI, deep knowledge is essential to implement proper measures to arrest the concrete erosion and to limit the containment over-pressurization. Experimental data are still needed, particularly for the behaviour of oxide-metallic immiscible phases during a fast reflooding. These topics are being addressed in the foreseen OECD/ROSAU program, which specifically focuses on underwater cooling and melt spreading.

In any of these configurations, corium melt properties play a key-role. Properties such as surface tension or viscosity for various corium composition and temperatures should be determined along with the corium solidification temperature, which depends on its composition and cooling conditions. The lack of knowledge in this field is one important source of uncertainties on SA code assessment. An experimental program on corium thermophysical properties needs to be developed in the next years to solve this important SA issue.

Other generic topics involving thermalhaydraulics concern the lack of knowledge for FP release and transport during all the ex-vessel phenomena and the corium mid and long term behaviour under leaching conditions as it is the case for Fukushima Daiichi.

3.3. Containment

The accumulation of H_2 and CO in the containment may lead to combustion, with different regimes already described in section 2. Both gas transport in the containment atmosphere, which may lead to the formation of flammable mixtures, as well as combustion are thermal–hydraulic phenomena with some aspects that still need to be investigated further. As combustion cannot be stopped after starting, investigations should be primarily directed towards preventing it to occur in the first place. However, different modes of combustion can have markedly different consequences. Specifically, detonation could cause pressure spikes exceeding the containment design pressure by far. Therefore, investigations directed towards preventing combustion modes with the severest consequences are also necessary. As an example, by a thorough understanding of the flame acceleration process, the conditions leading to potential endangerment of the integrity of the containment structure or safety systems components might be prevented. To this end, experimental investigations are being carried out in facilities with a geometric shape that mimics that of some parts of the containment (AMHYCO Project, Proposal number: 945057, European Commission, September 2021). In addition, the results of these studies contribute to the improvement of SAMG by updating flammability limits and flame acceleration criteria for both in-vessel and ex-vessel representative conditions.

The process of flammable gas distribution in the containment results from gas flow, possibly induced by a break flow from the RCS, but later sustained by heat and mass transfer, as well as (possibly) interaction with mitigation systems. The relevant gas flow phenomena are: convective flows (plumes or jets) released from the RCS; density-driven buoyant flows; interactions with mitigation systems: Passive Autocatalytic Recombiners (PARs), sprays and fan coolers; Stefan flow induced by steam condensation on structures; diffusion. Among heat transfer phenomena, both forced and natural convection play a role along the entire accident unfolding. Thus, the relationships between cause and effect in the formation of zones with high local flammable gas concentration are much too complex for predictions based on physical intuition and engineering judgment. One way to predict the evolution of the containment atmosphere structure is to solve the basic equations of fluid mechanics on the local instantaneous scale, that is, to perform so-called numerical simulations. These have been used to simulate various experiments, performed in relatively large vessels (Containment Code Validation Matrix, 2014). Although discrepancies are still present, the general agreement between experimental and theoretical results is, from the point of view of nuclear safety and predicting the course of a severe accident, satisfactory (NEA, 2007). As to simulations of (expected) processes in actual containments, these should in principle be feasible using the same approach but with much more powerful computers. However, as actual containments are a few orders of magnitudes larger than experimental vessels in which local measurements were performed so that experimental results are suitable for validation of models on the local instantaneous scale (few tens of thousands of m^3 compared to at most 200 m^3), such a possibility is at present hypothetical. For the time being, the most adequate approach seems to be so-called sub-grid modelling, that is, the solving of basic equations of fluid mechanics using relatively coarse numerical grids, with the influence of processes taking place on the sub-grid scale taken into account in source/sink terms, included in the solved equations.

Another way to predict the formation of flammable zones could be the scaling-up of experimental results, obtained in experimental vessels, to actual containments. Namely, at present, the results are supposed to be scaled-up (at least, in principle) by first validating theoretical models on experiments and then applying these models to actual containments. The much larger volumes should not be an issue, as relevant physical phenomena are local. However, the open question is whether experimental results could be scaled-up "directly", without using theoretical simulations as intermediary. Even though this issue was addressed within the ERCOSAM project (Paladino et al., 2016), a consistent universal methodology to scale-up experimental measurements to actual containments has not been proposed yet; by such a development, the existing large experimental database of hydrogen distribution (that is, helium distribution, as it is used in experiments instead of hydrogen for safety reasons) could be fully exploited and, as a consequence, the predictability of the severe accident development in the containment improved.

The performance of PARs (that might have a determining influence in the prevention of flammable zones) has been thoroughly characterized through performed experiments. In such experiments, scaled-down PARs were placed in a containment experimental facility with hydrogen present in the atmosphere, and the ensuing decrease of hydrogen concentration due to recombination was observed (Gupta et al., 2021). Although the volume of such experimental vessels is much smaller than the volume of actual containments, the local phenomena (that is, in the vicinity of the PAR) can be considered to take place also in the vicinity of the PAR in an actual containment. Nevertheless, further research of PAR performance under combined challenging conditions (i.e., lean O_2 mixtures, high pressure, temperature and humidity, and presence of both CO and H_2) is still necessary.

Even though theoretical models, embedded in SA computer codes, are able to reproduce major footprints of combustion processes (such as pressure and temperature increase), they still seem unable to properly determine the flame propagation regimes, which indicates that flame propagation mechanisms are still uncertain (both in the sense of aleatoric and epistemic uncertainty) under anticipated SA conditions. In particular, attention should be paid to scenarios in which turbulence generated by the flame-obstacles interaction is sufficiently high (in the sense of turbulent kinetic energy) to trigger Deflagration-to- Detonation Transition (including scenarios not yet considered, such as use of containment venting systems and combustion in locations beyond the primary containment). More specifically, additional investigations should address: a priori discrimination of gas mixtures prone to flame acceleration through more accurate experimental determination of critical conditions (i.e., mixture expansion ratio, detonation cell size, laminar burning velocity and flame thickness, and turbulent flame velocity); extension of flame acceleration criteria to stratified conditions (in $H_2/O_2/N_2/CO/CO_2/H_2O$ mixtures); flame interactions with sprays or structures; determination of flammability domains and required ignition energy at specific ex-vessel conditions (in contrast to generic conditions) for $H_2/O_2/N_2/CO/CO_2/H_2O$ mixtures.

3.4. Source term

During the past 10 years, several projects involving ST related issues have been conducted in the framework of OECD/NEA joint nuclear safety projects (i.e., BIP, STEM, THAI, BSAF), CSNI/WGAMA activities (e.g., FCVS status report) and EC projects (e.g., PASSAM, FASTNET, SARNET) (NEA, 2020, 2014; Van Dorsselaere et al., 2017). Experiments conducted as part of these projects revealed the importance of considering thermal–hydraulic conditions on distribution and release behaviour of fission products. As an example under RCS conditions, atmosphere composition showed an important effect on the release of iodine from the FP deposits on surfaces. Increasing concentration of oxygen seemed to enhance the formation of gaseous iodine, on the other hand, reducing conditions favour release of HI (NEA, 2020). Thermal-hydraulic conditions also present important mechanisms for fission product remobilization inside containment, i.e. highly transient flow and high temperature. Recently performed experiments in OECD/NEA THAI-3 project (Gupta et al., 2021) revealed that, in parallel to the resuspension of aerosol particles due to high transient flows, CsI aerosols can be thermally decomposed at high temperatures occurring during hydrogen deflagrations.

Pool scrubbing include coupled interactions among bubble hydrodynamics, aerosols and gaseous radionuclides retention mechanisms under a broad range of TH conditions as per accident scenarios. As per current status of knowledge gathered through, e.g., Fukushima accident analysis (Pellegrini et al., 2020), there remains several accident specific conditions requiring further research both on experimental and analytical aspects (Herranz, 2023), e.g. pool scrubbing under high-velocity flow regime, impact of impurities-additives in water pools. An inadequate modelling of pool scrubbing phenomena can limit reliable assessment of AM measures. As an example, safety analyses codes show large deviations in calculating high decontamination factors like relevant for wet-FCVS, regardless of experimental conditions. The uncertainties associated with the pool scrubbing phenomena (Herranz et al., 2020) and related boundary conditions are therefore important to be further evaluated and reduced not only to support validation and further improvement of pool scrubbing modelling towards reactor application but also to facilitate performance behaviour of installed safety and accident mitigation systems, e.g. PARs, Spray, Venting. International activities are currently underway for systematic integration of experimental and modelling research activities related to pool scrubbing, e.g. SNETP-NUGENIA IPRESCA project (Gupta et al., 2023). In addition to the operating fleet of reactors, advanced reactor designs, e.g. SMRs, are being developed by using multiple layers of (passive) mitigation systems to allow enhanced safety. In some of the SMR designs with containment vessel submerged in a water pool, pool scrubbing will be of high safety relevance as fission product scrubbing potential of water pools provide additional defence-in-depth to further reduce the potential for external releases.

Even though some important insights have been gained, the experiments conducted have only partly covered relevant boundary conditions and the database should be extended to the entire range of anticipated SA conditions. This is sometimes hard to achieve given the extreme conditions that prevail in case of SA, as high velocity flows, high temperatures, high radiation fields, etc. There are two scenarios on which investigation should be focused on the coming years and thermal-hydraulics is deeply involved: late remobilization of fission products and particle/vapour-gas–liquid interaction in pools. At least, a part of the answers to the remaining questions will be given by the ongoing OECD/NEA projects (i.e., ESTER and THEMIS (Gupta et al., 2021)) and, at the same time, new SA analysis methodologies are being explored in projects like EC-MUSA (Herranz et al., 2021), from which how much thermal–hydraulic uncertainties affect ST is a potential outcome. The recently funded projects in the framework of EC Horizon like ASSAS, SASPAM-SA, and SEAKNOT also aim to provide necessary input on the emerging ST issues relevant for management and mitigation of SAs in both operating fleet as well as advanced reactor designs.

3.5. Accident management

SA investigations have been lately focused on AM and a variety of SAM techniques have been developed worldwide (IAEA, 2009). However, some mitigation techniques (as the reactor cavity flooding or the containment spray activation during the long term phase of a SA scenario) still have uncertainties; their potential success depends on the proper moment to initiate the different AM actions and some of them even can have negative effects if not implemented properly (i.e., steam explosions or de-inertization of the containment atmosphere, respectively for the previous examples). Therefore, a substantial and detailed knowledge of the SA phenomenology, particularly those closely related to thermal hydraulics, should be gathered to support the right implementation of SAM Guidelines (SAMGs). After the Fukushima accident in 2011, the related investigation has been oriented particularly on the prolonged absence of the DC/AC electric power and of the ultimate heat sink for the decay heat removal, on the effect of an injection of untreated water for RCS and containment, and on the long term cooling and thermal hydraulics of spent fuel pools (SFP). The emphasis on the absence of electric power has strengthened the concept of passive systems to cope with SAs; however, the reliability of these systems should still be thoroughly tested and validated models should be implemented in the current SA analysis codes to soundly assess their actual effect on postulated accident scenarios.

In addition, the remaining open issues related to thermal-hydraulics, as highlighted in previous sections, should be investigated to reduce uncertainties in SA modelling so that the analytical tools can be used to support AM effects on SA progression.

Table 1
Research needs on Thermal-hydraulics from the SA perspective.

SA Process/ Phenomenon	Domain	Motivation	Safety relevance
Core reflooding	In-vessel	Accident management	Arrest of core degradation at early stages of the sequence. Uncertain drawbacks: additional heat-up and H_2 generation
Steam-metal reaction with ATFs	In-vessel	Accident prevention	Reduction of core heat-up and H_2 generation. Uncertain drawbacks: side effects still to be investigated
Corium dynamics in RPV lower plenum	In-vessel	Accident management	In-Vessel melt retention by external cooling. Uncertain drawbacks: RPV thermo-mechanic loading
Focusing effect	In-vessel	Accident management	Determination of maximum heat flux able to be extracted without vessel failure in case of focusing effect configuration (external cooling)
Melt ejections from MCCI (no overlay water)	Ex-vessel	Incomplete understanding	Coolability of molten materials in reactor cavity. Uncertain drawbacks: release of fission products
Short-term corium top flooding	Ex-vessel	Accident management	Arrest of corium fell in the cavity from RPV. Uncertain drawbacks: corium insulation by crust formation and corium cooling Recriticality
Anisotropy /isotropy of MCCI, /concretes,	Ex-vessel	Accident management	Criterion for the minimum concrete thickness to stop the ablation and to avoid containment failure (horizontal wall, vertical ablation)
Fuel coolant interaction/ Steam Explosion	Ex-vessel	Incomplete understanding	Evolution of hot materials releases and their consequences in containment different zones. Uncertain drawbacks: mechanical consequences on

(continued on next page)

Table 1 (*continued*)

SA Process/ Phenomenon	Domain	Motivation	Safety relevance
			equipment and containment building
Corium spreading under water	Ex-vessel	Accident management/ Incomplete understanding	Arrest concrete erosion and limit pressure in containment and fission product releases.
Corium fission products release and leaching	Ex-vessel	Accident management (short-mid-long term)	Assessment of fission products release in the containment (short term)- Radionuclide leaching (mid-long term)
H_2 distribution: scale-up methodology to bring data and models to reactor scale	Containment	Accident management	Prevention of flammable mixtures and efficiency of containment passive cooling systems. Uncertain drawbacks: intrinsic dependence on local conditions
Turbulence-driven DDT	Containment	Accident management	Mechanical threats to equipment and building
Gas flows resulting in late fission products remobilization	Source Term	Accident management	Potential radioactivity release to the external environment through a failed containment at a late stage of an accident.
Multiphase and multi-component interactions and flow regimes in pools	Source Term	Accident management	Retention (short term)/emission (long term) of radioactivity in/from pools.
Reliability of passive systems	Accident Management	Accident management	Multiple, depending on the specific system design.
Thermal-hydraulic uncertainties effect on modeling accident unfolding	Accident Management	Accident management	Awareness of the actual capability of SA simulation (system and CFD codes). Identification of TH uncertainties dominating SA modeling.

Note that any phenomena concerning corium involves an accurate determination of the corium thermos-physical properties.

4. Final remarks

The close and deep link between SA and thermal-hydraulics has been illustrated. Despite the progress made through research in understanding SA unfolding and, consequently, the thermal–hydraulic processes involved, there are still gaps that need to be addressed to reduce the uncertainties associated to SA and to optimize SA management. Most of the TH processes highlighted are intrinsic to the SA unfolding and the physical systems resulting, like corium, debris, combustible gas mixtures and others. It has been also discussed that thermal-hydraulics strongly affects processes that govern the SA consequences and the effectiveness of AM measures, hence, an accurate TH characterization should be pursued. Table 1 synthesizes the insights gained concerning the thermal–hydraulic research to be address from a SA motivation.

In summary, any investigation to be launched in the coming years should have a direct impact on reducing the uncertainties associated to SA modelling and/or on optimizing SA management. In this regard, emphasis is being placed on two aspects: achievement of experimental scenarios as close as possible to anticipated ones, in terms of materials and conditions; and overcoming the limitations set by the experimental scales, either by testing at different scales or by developing and validating suitable scaling methodologies. No less important, as already happened in the area of thermal-hydraulics, the SA modelling should move from single best estimate calculations (as presently done) towards including uncertainties and sensitivity analyses in a systematic way. Application of systematic BEPU (Best Estimate Plus Uncertainties) methodologies, compatible with the intrinsic complexity of severe accidents, might result into key insights into current predictive capability and key areas on which research should focus on. In addition, the technological progress coming in NPPs along with ATFs and SMRs, might bring up further SA thermal–hydraulic issues worth investigating.

CRediT authorship contribution statement

Luis E. Herranz: Conceptualization, Writing – original draft, Writing – review & editing, Supervision. **Ahmed Bentaib:** Writing – original draft, Writing – review & editing, Supervision. **Fabrizio Gabrielli:** Writing – original draft, Writing – review & editing, Supervision. **Sanjeev Gupta:** Writing – original draft, Writing – review & editing, Supervision. **Ivo Kljenak:** Writing – original draft, Writing – review & editing, Supervision. **Sandro Paci:** Writing – original draft, Writing – review & editing, Supervision. **Pascal Piluso:** Writing – original draft, Writing – review & editing, Supervision.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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