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**Approaches and Tools for
Severe Accident Analysis
for Nuclear Power Plants**



IAEA

International Atomic Energy Agency

APPROACHES AND TOOLS FOR
SEVERE ACCIDENT ANALYSIS
FOR NUCLEAR POWER PLANTS

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SEVERE ACCIDENT ANALYSIS
FOR NUCLEAR POWER PLANTS

INTERNATIONAL ATOMIC ENERGY AGENCY
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FOREWORD

Severe accidents at nuclear power plants involve very complex physical phenomena that take place sequentially during various stages of accident progression. Computer codes are essential tools for understanding how the reactor and its containment might respond under severe accident conditions. The codes are used as a tool to support engineering judgement, based on which specific measures to mitigate the effects of severe accidents are designed. They are also used to determine accident management strategies and for probabilistic safety assessment. It is very important to use these sophisticated tools in accordance with certain rules derived from knowledge accumulated worldwide.

Severe accidents are addressed in the IAEA Safety Standards Series: in the Safety Requirements for Safety of Nuclear Power Plants (Safety Standards Series Nos NS-R-1 and NS-R-2) and the Safety Guide on Safety Assessment and Verification for Nuclear Power Plants (Safety Standards Series No. NS-G-1.2). These recommend that severe accident sequences be identified, using a combination of engineering judgement and probabilistic methods, to determine those sequences for which reasonably practicable preventive or mitigatory measures should be evaluated and potentially implemented.

The IAEA Safety Report on Accident Analysis for Nuclear Power Plants (Safety Reports Series No. 23) provides practical guidance for performing accident analysis based on present good practices worldwide. All the steps required to perform such an analysis are covered in the report, for example, the selection of initiating events, acceptance criteria, computer codes and modelling assumptions, preparation of input data and presentation of calculation results. It covers both design basis accidents and beyond design basis accidents, including severe accidents, however, only basic guidance is provided for severe accident analysis. Therefore, a specific publication on accident analysis for severe accidents is needed and is provided through this publication.

The objective of this publication is to provide a set of suggestions, using current good practices worldwide, on how to perform deterministic analyses of severe accidents using the available computer codes.

This publication provides a description of factors important to severe accident analysis, an overview of severe accident phenomena and the current status in their modelling, categorization of available computer codes, and differences in approach for various applications of severe accident analysis. The report covers both the in-vessel and ex-vessel phases of severe accidents, and is consistent with the IAEA Safety Report on Accident Analysis for Nuclear

Power Plants. It can be considered a complementary report specifically devoted to the analysis of severe accidents.

Although the publication does not explicitly differentiate between various reactor types, it has been written essentially on the basis of the available knowledge and databases developed for light water reactors. Its application is, therefore, oriented mainly towards pressurized water reactors and boiling water reactors and, to a more limited extent, Russian WWER type reactors and pressurized heavy water reactors.

The IAEA officer responsible for this publication was S. Lee of the Division of Nuclear Installation Safety.

EDITORIAL NOTE

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1. INTRODUCTION

1.1. BACKGROUND

The continued development of economic and environmentally friendly nuclear power plants (NPPs) can play a fundamental role in the improvement of living standards worldwide. As the life of existing NPPs is extended and new plants are designed and built, public perceptions of the safety of these plants will continue to have an important impact on the future of these plants. In many cases, one of the most critical factors in public perception is the potential for the occurrence of severe accidents. As a result of more than two decades of research in the field of severe accidents in NPPs, it has become increasingly clear how the consequences of such accidents can be reduced or even eliminated through the use of improved training, through the development of more realistic accident management strategies and, ultimately, through the development of more advanced reactor designs.

Severe accidents involve very complex physicochemical and radiological phenomena that take place during various stages of the accident. These phenomena and the associated severe accident phases are typically divided into two groups:

- (1) In-vessel phase, covering core heat-up, fuel degradation and material relocation expected to occur inside the reactor pressure vessel up to the failure of the reactor pressure vessel, and subsequent release of molten corium into the containment building.
- (2) Ex-vessel phase, covering thermal and chemical interaction between core debris and containment structures, and containment behaviour (including transport of radioactive substances).

Severe accidents, and specifically their analysis, are addressed in a number of IAEA publications [1–9].

The IAEA Safety Requirement on the design safety of NPPs [1] establishes the following requirements on severe accidents and accident management in the design of nuclear power plants:

“Certain very low probability plant states that are beyond design basis accident conditions and which may arise owing to multiple failures of safety systems leading to significant core degradation may jeopardize the integrity of many or all of the barriers to the release of radioactive materials. These event sequences are called severe accidents. Consideration shall be given to

these severe accident sequences, using a combination of engineering judgement and probabilistic methods, to determine those sequences for which reasonably practicable preventive or mitigative measures can be identified. Acceptable measures need not involve the application of conservative engineering practices used in setting and evaluating design basis accidents, but rather should be based upon realistic or best estimate assumptions, methods and analytical criteria. On the basis of operational experience, relevant safety analysis and results from safety research, design activities for addressing severe accidents shall take into account the following:

- (1) Important event sequences that may lead to severe accidents shall be identified using a combination of probabilistic methods, deterministic methods and sound engineering judgement.
- (2) These event sequences shall then be reviewed against a set of criteria aimed at determining which severe accidents shall be addressed in the design.
- (3) Potential design or procedural changes that could either reduce the likelihood of these selected events, or mitigate their consequences should these selected events occur, shall be evaluated and shall be implemented if reasonably practicable.
- (4) Consideration shall be given to the plant's full design capabilities, including the possible use of some systems (i.e. safety and non-safety systems) beyond their originally intended function and anticipated operating conditions, and the use of additional temporary systems to return the plant to a controlled state and to mitigate the consequences of a severe accident, provided that it can be shown that the systems are able to function in the environmental conditions to be expected.
- (5) For multi-unit plants, consideration shall be given to the use of available means or support from other units, provided that the safe operation of the other units is not compromised.
- (6) Accident management procedures shall be established, taking into account representative and dominant severe accident scenarios (Ref. [1], para. 5.31).

The IAEA Safety Requirements for Safety of Nuclear Power Plants: Operation [2] establish the following requirements on severe accidents and accident management in the operation of NPPs:

“Plant staff shall receive instructions in the management of accidents beyond the design basis. The training of operating personnel shall ensure

their familiarity with the symptoms of accidents beyond the design basis and with the procedures for accident management” (Ref. [2], para. 3.12).

“Emergency operating procedures or guidance for managing severe accidents (beyond the design basis) shall be developed” (Ref. [2], para. 5.12).

Severe accident research began in the 1970s with early fuel rod melting experiments, resulting in the development of an extensive experimental database, a firm understanding of important severe accident phenomena and the development of mature severe accident codes. The results of such research programmes have been summarized in a variety of publications, including a series of state of the art reports [10–17] issued within the framework of the programmes of the Nuclear Energy Agency of the Organisation for Economic Co-operation and Development (OECD/NEA). Other suggested references for relevant European Union programmes are included in Refs [18–27], but were not exhaustively reviewed for the purposes of this report. Ongoing research is currently addressing the remaining few technical issues, such as fission product release and transport, the behaviour of core melt in the lower plenum of the reactor pressure vessel, the reflooding of damaged cores, debris coolability, and the mitigation of core melt and hydrogen distribution in the containment.

Among the IAEA publications, the Safety Report on Accident Analysis for Nuclear Power Plants [6], in particular, provides practical guidance for performing accident analysis based on present good practices worldwide. All the steps required to perform such an analysis are covered in the report, for example, the selection of initiating events, acceptance criteria, computer codes and modelling assumptions, preparation of input data and presentation of calculation results. Specific suggestions applicable for individual reactor types, such as pressurized water reactors (PWRs), pressurized heavy water reactors (PHWRs), the Russian RBMK type reactors, boiling water reactors (BWRs) and the Russian WWER type reactors, are given in several appendices to the main report. The report covers both design basis accidents and beyond design basis accidents, including severe accidents, however, only basic guidance is provided for severe accident analysis. Therefore, a specific publication on accident analysis for severe accidents was needed, and is provided through the present report.

1.2. OBJECTIVES AND SCOPE OF THE REPORT

The main objective of this publication is to provide a set of suggestions, based on current good practices worldwide, on how to perform a deterministic analysis of severe accidents using the computer codes available. Since detailed assumptions and requirements associated with severe accident analysis may be driven by: (a) each country's own regulatory requirements; (b) the plant designs to be considered; and (c) the computer codes that are available for use, it was considered inappropriate to provide guidance that was too specific. Rather, it was decided to strike an appropriate balance between general suggestions that could be followed without regard to the specific details of each country, and specific suggestions that would be helpful but might be applicable to specific designs or specific types of computer codes. A more general framework for these suggestions is also provided, including a description of factors important to the analysis, an overview of severe accident phenomena and the status in their modelling, categorization of available computer codes, and differences in approach for various applications of analysis. The publication covers both the in-vessel and ex-vessel phases of severe accidents. This report is consistent with the Safety Report on Accident Analysis for Nuclear Power Plants [6] and can be considered a complementary report specifically devoted to the analysis of severe accidents.

Although the publication does not explicitly distinguish one reactor type from another, it has been written essentially on the basis of available knowledge and databases developed for light water reactors (LWRs). Therefore, its application is oriented mostly towards PWRs and BWRs and, to a more limited extent, WWERs, since WWERs are expected to exhibit a response similar to that of LWRs, once core uncovering has started. However, it can also be used as preliminary guidance for other types of reactors (PHWRs, RBMKs), the most important potential differences in severe accident behaviour of other reactor types being briefly discussed in this report. In the future, additional reports may be issued to provide more specific guidance for the other reactor types.

The publication is intended primarily for code users or reviewers involved in the analysis of severe accidents for NPPs. It is applicable mainly to countries with a developing nuclear energy sector. In the preparation of this publication, it was assumed that its users will have some knowledge of severe accident phenomena and also of the use of computer codes for accident analysis, although such users may not have been actively involved in severe accident research or analysis activities. Although the publication is intended as a stand-alone report, it is suggested that the user read the previous general report on accident analysis [6].

1.3. STRUCTURE OF THE REPORT

Following the introduction, the report is divided into seven main sections. Sections 2 and 3 provide an explanation of phenomena important to the analysis of the in-vessel and ex-vessel phases of severe accidents, respectively. Sections 4 and 5 describe the present status in modelling of individual phenomena for the in-vessel and ex-vessel phases, respectively. An overview of presently available computer codes with their basic characteristics, categorization, capabilities and limitations is provided in Section 6. Issues related to the verification and validation of computer codes, to user qualification and user effects on accident analysis, as well as to uncertainties in the analysis of severe accidents, are also discussed in this section. Section 7 summarizes approaches for various applications of severe accident analysis and codes, and gives advice on the selection of computer codes and acceptance criteria for these applications. Specific suggestions on how to perform the analysis of severe accident scenarios are included in Section 8. Basic steps in developing input data and performing calculations, the validation of input models, essential design characteristics influencing the results of analyses, main requirements for best estimate analysis, consideration of uncertainties and the presentation of results are addressed. Section 9 contains a summary of the approaches and tools for severe accident analysis and related conclusions. Appendix I provides specific guidance on developing containment noding schemes. Appendices II and III present examples of specific severe accident analyses to demonstrate the steps and techniques discussed in the report. A discussion of frequently used computer codes and the status of their validation is provided in Annex I, and Annex II describes an approach to combining lumped parameter and computational fluid dynamics (CFD) models for hydrogen combustion analysis.

2. IMPORTANT IN-VESSEL PHENOMENA

As a result of the research started after the accident at Unit 2, Three Mile Island (TMI-2), there has been a significant increase in the ability to understand and model severe accident phenomena and to apply the resultant severe accident codes to the analysis of plant behaviour during severe accidents [13, 14]. Important trends have been identified through a wide range of experiments, the examination of the TMI-2 core and vessel, as well as the analysis of representative reactor designs. In this section, the in-vessel phase of severe

accident phenomena, as well as other factors that should be considered in the analysis of severe accidents, are discussed. For a more detailed description of these severe accident trends and phenomena, there are more comprehensive reviews contained in Refs [10–17].

2.1. THERMOHYDRAULICS

The ability to accurately predict the overall thermohydraulic response of the plant during a severe accident is one of the most significant contributors to a successful analysis. However, since the thermohydraulic response of the plant is also very sensitive to: (a) the plant design; (b) the response of the plant systems and components to the initiating events; and (c) other external events such as operator actions, it is impossible in this report to define general trends for the thermohydraulic response of all plant types and conditions. Nevertheless, once a specific reactor design and accident conditions are known, it should be possible to accurately predict the thermohydraulic response using currently available severe accident codes and models.

There is a wide range of phenomena that can have an impact on the thermohydraulic response of the plant. One of the most dominant factors for the management of severe accidents is the effect of the core and vessel reflood, which is considered one of the remaining few outstanding technical issues in severe accident analysis. Some of the important trends associated with this process are discussed in Section 2 on reflooding.

2.1.1. Natural circulation of steam and non-condensable gases

For typical PWR designs, there are three general modes of natural circulation that may have an impact on the response of the plant during a severe accident: in-vessel natural circulation, circulation within the hot leg and associated piping, and circulation through the primary loops.

For in-vessel natural circulation, experiments and detailed code calculations have shown that the natural circulation flow patterns are typically formed in the vessel as a direct result of the variation in temperature within the core and vessel. These flow patterns can be initially influenced by the ballooning and rupture of the fuel rod cladding, the formation of blockages formed over a long time period, and other damage inside the core. The primary impact of in-vessel natural circulation is to delay the overall heating of the core, due to the more effective heat removal from the hotter core regions to the colder core structures. As a result, radial temperature gradients in the core are reduced and the resultant heating pattern becomes much more uniform. Once the peak core

temperature approaches 1500 K, the effect of natural circulation is somewhat reduced due to the accelerating oxidation process of the hotter core region that is driven by the strong positive influence of temperature on the reaction rates.

The circulation within the hot leg and associated piping can also have a significant impact on the subsequent response of the plant. This is particularly important if the heating of the piping results in a mechanical failure. Prototypic experiments and detailed code calculations have shown that counter-current natural circulation can be significant in the hot leg. In hot leg counter-current flow, the hotter vapour flows along the upper surface of the piping up through a portion of the steam generator tubes and then returns to the vessel along the lower surface of the piping. If hot leg counter-current natural circulation does occur, the impact on the response of the plant, particularly for high pressure transients, can be dramatic because the circulation can result in the heating and failure of the hot leg, associated piping, or steam generator tubes. In US PWR designs, an analysis performed by SCDAP/RELAP5 [28–30] showed that the surge lines were typically the first components to fail during high pressure sequences such as station blackout, resulting in the early depressurization of the reactor coolant system. In turn, the depressurization of the reactor coolant system reduced the likelihood of vessel failure. Although steam generator tube failure was typically precluded by the earlier failure of the surge line or hot leg piping in the calculations for the PWRs, the potential for steam generator tube heating and failure may exist for other reactor designs.

Natural circulation through the primary loops may also have some impact on the subsequent response of the plant, but the importance of this process is limited by two factors. Firstly, in PWR designs, the impact of natural circulation in the primary loop may be overshadowed by the influence of hot leg natural circulation. Secondly, it is necessary for the primary loop seals placed in the cold leg sides to clear of water before the flow of hot steam and gases can circulate through the loops. Under conditions allowing natural circulation to occur, the heating of the piping and steam generator tubes may be a key factor in the failure of these structures. If these structures fail, the subsequent response of the plant could be significantly changed, particularly for high pressure severe accident sequences.

Under severe accident conditions, the study of natural circulation associated with non-US PWR designs has been much more limited. Although detailed code calculations could be performed, the lack of relevant experimental data on the conditions of interest for severe accident analysis may limit the general acceptance of such calculations, particularly when the impact could be so significant.

2.1.2. Reflooding of hot, damaged cores

The reflooding of high temperature (above 1500 K) but relatively intact fuel rods may result in sharp increases in the temperatures of the fuel rods and surrounding core regions, as well as in hydrogen production, fission product release and melting. (This sounds counter-intuitive, but the increases in temperature are caused by the oxidation of the regions of the core that have not yet been quenched but are exposed to large quantities of hot steam produced by the quenching process.) Although this is still an area of active research, a wide range of reflooding experimental data as well as data from TMI-2 have demonstrated these characteristic trends. The data have shown that this behaviour occurs as a direct consequence of the accelerated oxidation of the zircaloy structures due to the cracking of protective oxide films and the oxidation of freshly exposed zircaloy layers and any molten zircaloy that may be present in the coolant channels. In addition, more limited experiments that have included B_4C control rods or blades have shown similar increases due to rapid oxidation. As a result, local hydrogen production rates may increase by an order of magnitude relative to the rates produced during the initial heating and melting of the core. In turn, the local heat generation rates in the core also increase by an order of magnitude, completely overshadowing the local decay heat contributions by factors of 10 to 20. The heat generation due to zircaloy oxidation during typical heating and melting conditions can exceed the decay heat generation by more than a factor of two at temperatures near the melting point of zircaloy.

The rapid heating and cooling, and the associated high hydrogen production rates, can also affect other processes in the reactor system. Fission product release rates can increase rapidly due to the release of fission products on the grain boundaries during quench, and the pressure in the system can also be increased because of the additional steam and hydrogen produced during quenching. For example, the rapid increase in fission product release was observed in the only two experiments where irradiated fuel rods were quenched under severe accident conditions, SFD-ST and OECD LOFT-FP-2. These two experiments used trace irradiated fuel. The rapid increase in pressure was observed in TMI-2 under similar conditions when one of the reactor pumps was turned on briefly after initial core melting had started.

The prior temperature history of the core, as well as the core design, can have a significant impact on the quantitative nature of the process although qualitatively the results will be the same. Transients leading to the heavy oxidation of the core prior to reflood will reduce the consequence of oxidation during reflood since there will be less zircaloy to oxidize during reflood. The presence of B_4C structures, as noted above, or zircaloy fuel assembly shrouds in

certain BWR and WWER designs will have the opposite consequence because of the additional oxidation potential of these structures (e.g. the heat generation rate due to the oxidation is greater than that of zircaloy oxidation).

After large blockages of molten fuel have been formed, the consequence of core reflooding is not well known from a quantitative point of view. However, the TMI-2 accident analysis and other supporting calculations have shown that, after peak core temperatures exceed 2800 K and large melts of UO_2 and ZrO_2 have been formed, reflooding the core is not effective in arresting sustained core heating and growth of molten pools. This is mainly due to the reduced heat transfer area and the low thermal conductivity of the ceramic crust surrounding the melt. In the case of the TMI-2 accident, the molten pool situated in the upper core region continued to grow, and ultimately a portion of the melt was relocated into the reactor lower plenum, even after the core had been totally covered with water. In addition, the existing mechanical analysis of the molten pool crust has shown that the stability of the crust depends on its configuration and thickness, and variations in system pressure. While the thickness of crust is determined from the local heat transfer from the crust surface to the surrounding water, the other two parameters are dependent on the prior temperature history of the core and external thermohydraulic boundary conditions [28].

The reflooding of regions of the core with temperatures above the melting point of the zircaloy cladding but below the melting point of the fuel is expected to show trends somewhat in between the previous two extremes. At the higher end of the temperature range, at temperatures between 2200 and 2800 K, intact fuel columns may collapse due to the thermal shock associated with quenching, but will not produce any significant quantities of hydrogen since much of the remaining zircaloy may be either completely oxidized or melted and relocated in the lower temperature regions of the core. The collapse of the fuel may result in an increased release of the fission products trapped inside the fuel rods. Additional hydrogen may be produced in the lower temperature core regions where molten zircaloy may have refrozen or accumulated in the form of metallic layers, but this hydrogen production rate will be limited by the reduced surface area of zircaloy.

The consequence of reflooding of the lower plenum region and structures is not well known and, as discussed in a later section, is an active area of current research. Examination of the TMI-2 lower head and similar experiments using stimulant materials have shown the potential for enhanced cooling of the debris and vessel structures due to the combination of the formation of gaps between the debris and the vessel structures, and the cracking of the debris itself.

2.2. OXIDATION OF CORE MATERIALS

The oxidation of core materials is important in view of the severe accident progression due to the production of hydrogen, the generation of heat that may exceed the decay heat at high temperatures, and the transition of the metallic materials (e.g. Zr) into ceramic materials (e.g. ZrO_2). Of them, the oxidation of zircaloy by steam is considered as the most important contributor to the behaviour of the core, although the oxidation of other materials, particularly B_4C , can be important in some cases. It should be noted that other Zr alloys behave differently from zircaloy. When the oxidation kinetics of different alloys is considered, thus, the quantitative trends may be somewhat altered.

2.2.1. Zircaloy oxidation in steam

During a severe accident, the oxidation of the zircaloy structures in the core has a significant consequence on the overall behaviour of the LWR core. Although the specific consequence depends to some degree on the type of transient being analysed, the exponential increase of the zircaloy oxidation in fuel rod temperatures exceeding 1500 K is a characteristic feature of representative severe accident experiments and plant simulations. In addition, the sharp increase in fuel temperatures is a direct result of the positive feedback between temperature and the oxidation of zircaloy in the presence of steam. In the LOFT-FP-2 experiment, the rate of core heat-up (less than 1 K/s) driven by decay heat was rapidly increased by an order of magnitude, due to additional heat released by zircaloy oxidation. As a result, temperatures of the fuel rods and intact core structures increase rapidly to above the melting point of zircaloy. Once the peak temperatures of the core exceed the melting point of zircaloy, the subsequent thermal response of the core, particularly peak or average core temperature, is strongly dependent on the sustained oxidation of the zircaloy. Since the total heat generated by the zircaloy oxidation process is enough to drive the peak core temperature above 3000 K or the melting point of the fuel rod, the total amount of oxidation energy added to the core is limited by the maximum rate of zircaloy oxidation.

On the other hand, the oxidation rate of zircaloy is governed by the availability of steam in the core and the diffusion of oxygen into the zircaloy. In general, the diffusion coefficient for zircaloy is characterized by an exponential function of temperature. For typical transient sequences, the diffusion of oxygen into the zircaloy tends to limit the oxidation process at lower temperatures. Once the peak temperature exceeds 1500 K, however, the positive feedback between core temperature and oxidation rate results in little

constraint on the heat-up and oxidation rate. More specifically, the rate of oxidation decreases as the oxide thickness grows (the rate is inversely proportional to the oxide film thickness). However, the increase of the diffusion rate with temperature completely overwhelms the consequence of the protective film, at least until the zircaloy is completely oxidized. As the core temperature becomes higher, the availability of steam and the diffusion of steam to the surface of the zircaloy limit the oxidation rate. In that case, the in-vessel thermohydraulic conditions become more important than temperature dependence of the oxidation process. In particular, the increase of hydrogen concentration in the upper core region and the decrease of steam generation rate due to the decreased water level become more effective in limiting the maximum oxidation rates, especially in the upper core region.

The total amount of oxidation at a given location is limited by the amount of zircaloy present at that location and two additional factors. Firstly, the oxidation of the zircaloy is limited by the melting and relocation of the zircaloy cladding, especially for transient sequences characterized by relatively rapid initial heating rates. For heating rates above 0.3–0.5 K/s, the buildup of a protective oxide layer on the outer surface of the zircaloy cladding is limited, allowing the hot zircaloy to melt and relocate to the lower core region just after the melting temperature of zircaloy is exceeded. In this case, the oxidation process is terminated at the original location of the zircaloy because the zircaloy has been completely removed. Although the relocating zircaloy can continue to oxidize, in addition, the enhanced cooling as the melt moves towards cooler regions of the core tends to rapidly cool the material, in turn terminating the oxidation process as the material moves lower in the core. The second limiting factor is considered for slower heating rates, typically lower than 0.3–0.5 K/s. At lower temperatures, the formation of a protective oxide film prevents the relocation of the molten zircaloy and, as a result, the zircaloy is completely oxidized in place. For intermediate initial heating rates, a combination of relocating zircaloy and complete consumption of the zircaloy tends to control the oxidation process.

The total amount of hydrogen released to the reactor coolant system and containment building is also related to the total oxidation of the zircaloy. Although the oxidation of the core structures can contribute to the total amount of hydrogen generated in the vessel, the early melting of the structures tends to limit their contribution. The oxidation of the fuel can also contribute to the total hydrogen, but is limited by the exposure to steam and the rate of oxidation of UO_2 .

The temperature response of the core can also be directly related to the oxidation process. Although the maximum core temperature is ultimately limited by the melting of the fuel, the peak core temperature is limited by the

peak oxidation rate. At rapid heating rates, the peak core temperature occurring during rapid oxidation will approach the melting point of zircaloy. At slow heating rates, the peak core temperature will be limited by the melting point of the oxidized cladding material. This effect is more noticeable in bundle heating and melting experiments: The experiments are normally terminated just after rapid oxidation and melting occurs, and the peak core temperature measured in the experiments is directly related to the peak oxidation rate.

2.2.2. Oxidation of B₄C in steam

As discussed in the previous section on core reflood, a limited number of reflooding experiments with fuel rod bundles and B₄C control blades have shown that the oxidation of B₄C may be an important contributor to the production of hydrogen and other combustible gases during reflood. In addition, the methane generated by the oxidation of B₄C may react with the iodine released from the fuel to form organic iodines and thus influence the source term considerably. However, it should be noted that the amount of B₄C is relatively small compared to the amount of zircaloy in typical NPPs, so that the consequences of B₄C will be less important. Although the oxidation of B₄C during the normal heating and melting of the core could also be theoretically important because of the reaction of B₄C with steam, experiments without reflooding have not clearly shown any significant difference in the hydrogen production in assemblies with and without B₄C.

2.3. LOSS OF CORE GEOMETRY

Loss of the original core geometry can occur gradually over a period of minutes to hours, covering a range of temperatures from 1000 to 3000 K. The specific timing and temperatures are very strongly dependent on types of core materials, the initial uncover and heating rates of the core, system pressure, and overall thermohydraulic response of the plant, so the ranges quoted apply strictly to western LWR designs with UO₂ zircaloy fuel rods, and Ag-In-Cd or B₄C control rods or blades. Other reactor designs may respond differently as a consequence of different melting temperatures or the formation of lower melting point alloys. Since the core geometry is changed primarily with the local core temperature, many of these changes can occur simultaneously in different regions of the core. However, typical transient sequences involve a general increase in the maximum and average core temperatures with time; the geometrical changes, such as ballooning and rupture of the fuel rods that are expected at lower temperatures, also occur at the early phase of the transient

sequence. The most notable exception would be the geometrical change associated with the core reflooding and the possible fragmentation of heavily oxidized materials. This kind of geometrical change can occur at any time once the core structures have absorbed a sufficient amount of oxygen to become brittle.

2.3.1. Ballooning and rupture of the cladding

For low pressure accident sequences, the zircaloy cladding starts to balloon and rupture once the core temperature reaches 1000–1200 K. In that case, the timing and temperature of ballooning and rupture depend on the internal pressure of the fuel rods (including any fission gases that may be released into the gap), and the mechanical characteristics of the cladding material. For high pressure accident sequences, the failure of zircaloy cladding may be delayed until the core temperature reaches above 1500 K, due to the collapse of cladding onto the fuel rather than ballooning. Even though the cladding does not fail mechanically in that case, chemical interactions between the zircaloy cladding and other core materials cause local failures of the cladding due to the formation of low melting temperature alloys.

At this stage of core damage, the most significant consequences of ballooning cladding and rupture are the release of fission products, the exposure of the inner surface of the cladding to steam, and changes in the melting and relocation of fuel rod materials later in the transient. Ballooning and rupture may also alter subsequent flow patterns in the core, particularly when the deformation is extensive.

2.3.2. Liquefaction and relocation of control and structural materials

For typical LWR designs and at temperatures between 1500 and 1700 K, chemical interactions between Fe–Zr, B₄C–Fe, Ag–Zr, and others, can result in the early liquefaction and relocation of grid spacers, control structures, and portions of the zircaloy cladding material in direct contact with the other materials. For rapid transient sequences where the chemical interactions are enhanced, the failure can occur at temperatures near 1500 K. For slower transients, the failure will be delayed until temperatures near 1700 K are reached. In the latter case, the formation of protective oxides on the zircaloy tends to restrict the strength of chemical interactions.

At this stage of core damage, the most significant consequence of the material interactions is that the control materials can become segregated from the fuel, increasing the potential for recriticality at the instant of core reflooding. The secondary consequence is the loss of Inconel or stainless steel

spacer grids which in turn alters the subsequent formation of local blockages and flow patterns in the core.

2.3.3. Liquefaction and relocation of zircaloy cladding

At temperatures above 2000 K, the zircaloy cladding can melt and, in some cases, drain into the lower core regions or reactor lower plenum. Since the relocation of the molten zircaloy cladding may be delayed or prevented by the formation of protective oxides on the outer surface of the cladding, the drainage of molten zircaloy depends to a large extent on the early temperature history. For fast transients with heating rates in excess of 0.3–0.5 K/s, or transients with low core water level, the zircaloy cladding will melt and drain into the lower core regions. The melting point of zircaloy typically ranges between 2000 and 2200 K, depending on the alloy and oxidation content of the material. For much slower transients (typically with heat-up rates below 0.3–0.5 K/s), the relocation of molten zircaloy is inhibited by the formation of a protective oxide on the outer surface of the cladding. The formation of a protective oxide film can be also enhanced, and the relocation of molten zircaloy is inhibited by transients characterized by multiple events of core heating and cooling with peak temperatures remaining below 2000 K. Examples might include the cycling of relief valves or periodic accumulator injection.

The most significant consequence of the drainage of molten zircaloy is a reduction in the hydrogen production and heat generation due to the oxidation of the zircaloy. Although the draining zircaloy can continue to oxidize as it moves lower in the core, the rate of oxidation is typically reduced for two reasons. Firstly, since the oxidation rate is strongly dependent on temperature, the movement of the zircaloy into the lower cooler regions of the core causes a reduction in the oxidation rates. Secondly, once the molten zircaloy freezes, the subsequent oxidation is further reduced because the blockages of metallic zircaloy have greatly reduced surface areas exposed to the steam. A secondary consequence of this change is the possibility of enhanced fission product release that can occur due to the dissolution of the fuel by the molten zircaloy.

In addition, the subsequent heat-up of the core can be altered due to the fact that natural circulation flow patterns change as the coolant channels fill up with molten material. These regions of localized flow blockages or restrictions are typically located at the original grid spacer elevations. In the event that the water level is high enough to cool the lower portion of the core, these blockages will typically form just above the level of the water. It was originally thought that the formation of blockages composed of the metallic components of the core, such as zircaloy and structural materials, was a necessary step in the

subsequent formation of blockages of molten fuel and remaining oxidized cladding materials. However, existing experiments indicate that the formation of metallic blockages was not necessary to the formation of regions of frozen or molten pools of fuel or other oxidized materials. Since the fuel and other oxidized materials are ceramics, stable, although perhaps mechanically brittle, crusts can form as a direct result of the convective and radiative heat transfer to the steam or adjacent structures.

2.3.4. Liquefaction and slumping of the fuel

The fourth significant change in core geometry occurs when the temperatures of the fuel or oxidized cladding material reach their melting points. At this point, the fuel and remaining oxidized cladding material start to slump lower in the core. In some cases, if the fuel has a sufficient level of burnup and the pressure is low enough, the fuel can swell, causing additional reductions in the flow area, as initial porosity of the fuel increases. Depending on the location of the slumping material, and the temperature gradients in the core, the ceramic fuel and oxidized cladding material will relocate to cooler regions of the core until it freezes, resulting in the formation of large blockages. These blockages can then trap molten materials formed subsequently higher in the core or upper plenum. Although the specific temperature range depends on the composition of the fuel and oxidized cladding material, the formation of ceramic melts will occur at temperatures below the melting point of the fuel and as low as 2870 K for ceramic (U, Zr, O).

The consequence of the formation of blockages and molten pools of ceramic material can be significant. Because of the size of the blockages, typically extending over a large portion of the core, the flow patterns in the core can be greatly altered. However, the blockages may result in enhanced cooling of other unrestricted core regions, slowing the heat-up of cooler, typically lower powered core regions. Since the molten core pool may be surrounded by the peripheral frozen crust, fission products may be retained inside the fuel even though the fuel rod reaches above its melting point. When the size of the molten pool is relatively large, the resultant molten pool natural circulation can affect the heat transfer rate to the peripheral boundary, including the molten pool crust. The most notable impact of the molten pool natural circulation is that the heat transfer rate to its sides and top may be much greater than to the bottom. Thus, the frozen crust becomes thinner on the sides and top of the molten pool than the bottom, resulting in preferential failure of the corresponding crusts.

2.3.5. Relocation of molten pool materials into the lower plenum

The fifth significant change in the core geometry occurs as the molten pool trapped in the core moves lower in the core or lower plenum. In the case of TMI-2, the melt moved through core bypass into the lower plenum. Although there are limited data for this process under prototypic conditions, the TMI-2 accident progression analysis indicates that the melt relocation is initiated by the penetration of the molten pool to the outer or lower periphery of the core and the failure of the frozen crust enclosing the melt. Prior to a more dramatic relocation to the outside of the core, the molten material can move radially and axially in the core region, but the movement appears to be a sporadic expansion of the frozen crust and molten pool due to the limited core flow areas. Melt relocation can occur even if the core is completely covered with water although the additional cooling may slow or even prevent the further movement of the melt. In the case of TMI-2, the core was reflooded prior to the relocation of a significant amount of the melt into the lower plenum. Although the exact details of the melt relocation in TMI-2 are not known, it was postulated that the melt relocation into the lower plenum was initiated by a variation in the system pressure. This pressure variation resulted in a mechanical failure of the crust, the melting of a hole in the core former walls by the hot melt, and subsequent drainage of the melt through the bypass into the lower plenum. This mechanical failure of the crust and relocation of a portion of the melt was accompanied by the partial collapse of loose debris and fuel rod fragments supported by the upper crust. Although confirmatory data are not available for prototypic core materials and scale, in the case of accidents where the core is not reflooded and the core is uncovered, the molten pool will continue to grow axially and radially until it reaches the boundary of the core. The fraction of the core that is molten at this stage and the ultimate relocation path into the lower plenum will depend on the power distribution in the core, the design of the core and surrounding structures, and the thermo-hydraulic boundary.

Because of the difference in axial peaking factors in the BWR core with a relatively flat flux distribution during some stages of the burnup history, and in the PWR core with a more pronounced cosine shape distribution, it has been postulated that the molten pool is more likely to drain into the lower plenum due to the failure of the lower core plate in the BWR case and through the core bypass region in the PWR case. Drainage of the melt due to core plate failure is also made more likely in BWRs since many severe accident sequences in BWRs also result in the earlier depressurization of the system, resulting in a relatively low water level at the start of initial core heat-up.

The consequence of relocation of the melt into the lower plenum will depend strongly on the amount of water available in the lower plenum. In the unlikely case that the lower plenum is steam filled, the melt can directly contact the lower head structures and may melt through the structures relatively quickly. In the more likely case where water is present in the lower plenum, the heating of the lower head structures will be delayed but the system pressure may increase sharply because of the contact of the melt and the water. Although the likelihood of an energetic melt–water interaction within the vessel is considered to be low, any fragmentation of the melt due to the enhanced heat transfer between the melt and the water can alter the longer term coolability of the debris and vessel wall. The relative timing and nature of the relocation process also has an important effect on the stratification of molten core materials in the lower plenum of the vessel. For example, the early relocation of ceramic material from the upper core portion may result in the formation of multiple layers of ceramic and metallic materials in the lower plenum, whereas late relocation may promote the mixing of core materials in the lower plenum, resulting in a reduction of the number of different material layers.

2.3.6. Fragmentation of embrittled core materials

The sixth major change in core geometry, unlike most of the other changes, results from the addition of water to the core and the fragmentation of embrittled materials. At temperatures below 1500 K, the fragmentation of fuel rod materials has been relatively well characterized due to the research on cladding embrittlement under design basis accident conditions. Experiments have shown that, in this case, the cladding will fail and fuel pellets may fragment. At temperatures above 1500 K, the change in geometry is very much dependent on the geometry at the time of reflood. For regions where either molten metallic or ceramic melts have refrozen, there may be some cracking of the refrozen material but there is little overall change in the geometry of the material. For regions where the fuel rods are relatively intact and peak temperatures remain below the melting point of zircaloy, the fuel and cladding may fragment and partially collapse. For regions where fuel rods are relatively intact but the peak temperatures have exceeded the melting point of the zircaloy cladding, the fuel pellets will remain relatively unchanged even though much of the zircaloy cladding has melted away.

The relative stability of the columns of fuel pellets, once zircaloy melting temperatures have been reached, has been attributed to the interactions between the molten zircaloy and UO_2 , resulting in penetration of molten Zr into cladding cracks and gaps between fuel pellet and cladding. This process

effectively welds the fuel pellets together. Two notable exceptions have been noted. Firstly, if the melting and draining of the molten zircaloy occurs very quickly, the fuel pellets collapse during the addition of water. This has been attributed to the fact that there is insufficient time for the molten zircaloy to penetrate into the pellet interfaces and cracks. Secondly, if the fuel is exposed to steam for an extended period of time, the oxidation of the UO_2 tends to cause the fuel to break apart on grain boundaries on quenching.

The primary consequence of this change in geometry is associated with the break-up of the protective oxide layer on the zircaloy cladding. As discussed in more detail in a previous section on reflooding, this break-up can result in a dramatic increase in the oxidation rate of the zircaloy under some circumstances. The break-up of fuel rods can also result in a dramatic increase in fission product release, as the fuel is exposed to hot steam and the break-up of the fuel at grain boundaries is enhanced. A secondary consequence of the fuel rod break-up is that the resulting rubble debris bed may alter the flow patterns in the core and the heat transfer from the fuel. However, since the flow area within the loose rubble is comparable to that of the original geometry, this impact is relatively small compared to the other factors noted previously.

2.4. HEATING AND FAILURE OF THE LOWER HEAD

Once a portion of the molten core materials or debris has relocated into the lower plenum, the subsequent response will also depend on the water present in the lower plenum, the type of structures present and, in the case where additional water is added to cool the vessel walls or debris, the location and mode of water addition. If additional water is not added, the debris or melt will continue to heat and ultimately the vessel may fail. In the case where the lower plenum is not dry or additional water is added prior to the vessel failure, the situation is less clear. Some research suggests that water added either inside or outside the vessel may be effective in preventing the vessel failure. In the case of water addition to the vessel, some experiments and the evidence from TMI-2 have shown that the water is able to penetrate into the debris cracks and gaps between the debris and vessel wall. As a result, vessel failure was prevented. However, the research is still inconclusive about the general applicability of such a conclusion. Although the consequences of external flooding (or ex-vessel cooling) for vessel failure are even more uncertain, some research has shown that external cooling can prevent vessel failure particularly if the power density in the melt is low. For reactors with high core power density, however, the possibility of vessel failure cannot be ruled out, even in the presence of in-vessel and ex-vessel flooding. Recently, a third alternative has

been proposed for BWR designs where a separate water cooling system is used to cool the control rod drive entering from the vessel lower head. In this proposal, the control rod drive system would be used to inject water through the control rod drives in the bottom of the vessel so the lower plenum debris and vessel wall could be cooled directly, as long as the lower portion of the control drive structures could be protected and plugging of the structures by molten debris could be prevented. Although analytically shown to be a viable approach, prototypic experiments have not yet been performed to confirm these conclusions.

2.5. OTHER FACTORS

As discussed in the latter part of this report, there are many other factors that must be considered when analysing severe accidents. In this section, it is not necessary to explicitly discuss the relative importance of each of those factors needed for a better understanding of severe accident phenomena, except for three additional factors. Of them, the most important is the potential impact of alternative core and vessel designs since many of the studies performed to date have focused on the behaviour of fuel assemblies and materials typical of western BWRs and PWRs. Although the quantitative nature of the phenomenological trends described in the preceding sections may vary for other core and vessel designs, these trends also offer valuable insights into the expected performance of these other designs as well. Two additional factors are: (1) the potential impact of recriticality during reflooding of the damaged core; and (2) the impact of fission product release and transport on the distribution of decay heat in the core during the later stages of a severe core damage accident.

2.5.1. Impact of alternative core/vessel designs

As noted in the previous sections, the behaviour of the core, particularly the heating of the core due to oxidation and the melting of core materials, is very strongly dependent on the composition and configuration of the core. Since UO_2 and zirconium based cladding alloys are used in most commercial power reactors being operated around the world, the strong consequence of zircaloy oxidation will be repeated with minor variations due to the actual alloying elements present. For example, Zr–niobium alloy oxidation rates are somewhat lower than that for zircaloy. As a result, the oxidation driven heating rates at high temperatures may also be somewhat lower than those for equivalent amounts of zircaloy. The melting points and chemical interactions

between different core materials will also have a similar consequence on the changes in core geometry. The general melting of core materials will depend on the melting temperatures of each core material but will be affected by the formation of lower melting temperature alloys as different materials in the core chemically interact where the materials are in close contact. In most cases, the formation of the lower melting temperature alloys will result in the earlier and lower temperature failure of core structures, similarly to the impact of the chemical interactions between zircaloy, stainless steel/Inconel, control material structures on the early failure of Ag–In–Cd, and B₄C control structures. The relative consequence of these chemical interactions can be determined using the appropriate phase diagrams and reaction kinetics rates. In the case of zircaloy–stainless steel reactions, the reaction rates become nearly instantaneous as temperatures approach 1500 K, typically resulting in the destruction of the structures at this temperature even though lower melting point alloys are initially formed at much lower temperatures.

For other core materials, the oxidation and melting processes, although still important, may have a significantly different consequence on the behaviour of the core. For example, aluminium based fuel elements, used in many research reactors, will respond very differently from Zr–UO₂ fuel rods due to the lower melting temperature of the aluminium alloys. In this case, although these alloys can react very strongly with steam, the early melting and relocation of the cladding effectively prevents the oxidation of these materials under most conditions. A more subtle difference, although of equal importance, is the consequence of the grid spacer materials and designs used in the core. Because of the strong interaction of Inconel and stainless steel with zircaloy cladding, spacer grids composed of these materials will be destroyed at relatively low temperatures (1500–1700 K) because of the formation of lower melting point alloys. On the other hand, zircaloy spacer grids will remain in place up to much higher temperatures (2000–2100 K). However, the zircaloy spacer grids will also oxidize much like the zircaloy cladding materials. Since the intact spacer grids also act as debris catchers, the location of in-core blockages will depend on the spacer grid materials.

The design of the core will largely determine accident progression. For example, in typical PHWR designs with horizontal flow channels, the changes in fuel channel geometry at temperatures above 1000–1200 K may be somewhat different from those of typical LWRs with vertical fuel elements, as the PHWR horizontal fuel elements sag and contact the inner wall of the flow channels. In addition, molten material will tend to accumulate locally since the melt can only relocate to the bottom of the fuel channels. In this case, the formation of blockages that may restrict the flow in individual flow channels may be enhanced. Such blockages may have a beneficial effect, limiting the

total hydrogen production as steam is prevented from entering the channels. However, these blockages will also have a negative effect, reducing the local convective heat removal from the coolant channels. In this case, the initial formation of blockages may have a very strong impact on the subsequent failure of flow channels and the longer term formation of molten pools in the core.

The general impact of the natural circulation of coolant or steam in the reactor coolant system and vessel is to reduce temperature gradients in the core and vessel by moving heat from the hotter channels to the cooler channels and structures. However, the natural circulation is strongly affected by the design of the plant. Natural circulation in the primary loops results in the heating of the reactor coolant system piping and components while providing additional cooling of the core. Even in the event that the natural circulation in the loops is blocked by the presence of water in loop seals or equivalent piping configurations, the possibility of natural circulation within the piping similar to hot leg circulation noted for US PWR designs still must be considered. In all cases, natural circulation helps remove additional heat from the core and vessel structures, slowing the heat-up of the core. On the other hand, the transfer of heat to the reactor coolant system piping and components may also lead to the failure of these structures. In particular, the accelerated heating and failure of the steam generator tubes may be of concern from the viewpoint of the source term.

Although similar in design to western LWRs, WWER plants, particularly some of the older designs, may also exhibit notable differences in their overall response during a severe accident. The additional water inventory in some WWERs, relative to the total power in the core, may result in core uncover times notably longer than for otherwise equivalent LWRs. Thus the overall heating and melting rates associated with decay heat and zircaloy oxidation may be correspondingly lower. Differences in the control rod design in some WWERs, in particular, the materials used and location of those materials, will have an impact on the early failure of control rods observed in other LWR experiments and, ultimately, on the fission product retention in the system. Other notable effects are discussed in Ref. [29].

RBMK reactors with separate vertical flow channels surrounded by graphite are very different from typical LWR designs. For temperatures above 1500–1700 K, the channels are likely to fail due to interactions between the materials in the fuel bundles and channel walls, similar to the failure of grid spacer and control rods in LWRs. As a consequence, the subsequent progression of the accident will be totally different from that of LWRs because of the presence of graphite and separated fuel channels. In addition, other features of the RBMK design, including differences in core neutronics, the

limited strength of the primary cooling circuit (due to the lift-off of the upper core plate at relatively low pressures), and differences in the reactor coolant system design (locations of loop seals, for example) will also have an effect on the response of the plant.

For a gas cooled reactor, the presence of graphite will also be an important factor in the overall response of the plant. Similar to RBMKs, the thermal capacitance of the graphite will change the thermal response of the core relative to LWRs, slowing the heat-up of the core for similar power levels. At the other extreme, the oxidation of the graphite, particularly in the presence of air, may result in additional heat generation and the production of non-condensable gases similar to the oxidation of zircaloy or B_4C .

2.5.2. Recriticality

Core recriticality in a damaged core may also be an important factor in the heating of the core during reflooding and the long term management of severe accidents. As noted in a previous section, core recriticality can occur because of the difference in temperatures for the failure of control structures versus failure of the fuel. In the case of typical PWR and BWR designs, the chemical interactions between zircaloy, stainless steel, Inconel, B_4C and Ag result in regions of the core with relatively intact columns of fuel and void of any control materials. These regions can exist over a fairly wide temperature range, since the control materials are removed at temperatures between 1500 and 1700 K while the fuel may not fail until temperatures exceed 2800 K. Although these regions are not expected to become critical during the core heating and melting phase, the addition of water into such regions during initial reflooding, and the period of time following the successful termination of the accident, may result in recriticality in such a region. Compared to the initial core power for those reactor designs, the power levels in this region have been shown to be relatively small, but additional heating due to recriticality may have a bearing on the ability to remove heat from the core over the longer term.

2.5.3. Fission product release and transport

In addition to the importance of fission product release and transport with respect to the source terms associated with severe accidents, fission product release and transport can also have an influence on the progression of the accident. Depending on the reactor design and burnup history of the fuel, the release of fission products, particularly as less volatile fission products are released at higher temperatures, reduces the local decay heat contribution in the fuel. In the case of PWRs and BWRs, this release can reduce the decay heat

in the fuel by as much as 30–40% over an extended time period. However, this decay heat may still be retained in the reactor coolant system since it is carried with the fission products that are transported through the system. In some cases, the redistribution of heat has a consequence similar to that of natural circulation since the release of fission products helps reduce the heating of the hotter regions of the core while contributing to the heating of the reactor coolant system piping and components.

Fission product release and transport is also very design specific since the release of fission products and their chemical form are very much dependent on core materials and coolant conditions in the vessel and reactor coolant system. In turn, the deposition of the fission products in the system is very much dependent on the chemical form of those products.

3. IMPORTANT EX-VESSEL PHENOMENA

In the course of a severe accident, a wide spectrum of different phenomena may occur; it is useful to group these phenomena as:

- (1) Relating to thermohydraulics;
- (2) Relating to fission product and aerosol behaviour;
- (3) Relating to melt behaviour;
- (4) Processes involving phenomena related to technical systems activation.

The thermohydraulics group contains, as a special part, phenomena related to the hydrogen issue, i.e. the distribution of hydrogen and the different modes of its combustion. The fission product and aerosols group includes a consideration of iodine chemistry. The melt behaviour group includes direct containment heating, as well as molten corium concrete interaction with melt spreading and fuel coolant interactions. The various containment technical systems, which are treated in the fourth group, mainly affect containment thermohydraulics.

A subdivision of the four groups into related phenomena is shown in the following:

- (a) Thermohydraulics:
 - Sources and sinks;
 - Pressurization/depressurization;

- Transport (gas/water flows);
- Heat and mass transfer;
- Hydrogen distribution and combustion;
- (b) Fission product behaviour:
 - Aerosol behaviour;
 - Iodine behaviour (chemistry);
- (c) Melt behaviour:
 - Melt release;
 - Direct containment heating (DCH);
 - Melt coolability;
 - Fuel coolant interaction (FCI);
 - Molten corium concrete interaction (MCCI);
 - Relocation of melt and spreading;
 - Interaction with refractory and sacrificial materials;
- (d) Technical systems activation:
 - Systems impacting on gas transport (fans, doors, rupture discs);
 - Systems impacting on containment leakages (filters, valves);
 - Safety engineering systems (sprays, ice condensers, recombiners, igniters, passive heat removal systems, suppression pool).

3.1. CONTAINMENT THERMOHYDRAULICS

The containment structures of current reactors are designed to be capable of withstanding, without loss of function, the pressure and temperature conditions resulting from design basis accidents. The containment structures are also intended to maintain their functional integrity in the long term period after an accident.

The containment design basis considers the following conditions:

- (1) The temperature and pressure conditions in the containment that are due to a spectrum of postulated primary circuit ruptures or secondary side steam and feedwater line breaks;
- (2) The maximum external overpressure to which the containment may be subjected because of the inadvertent operation of containment sprays or the air fans for the ice condenser containment;
- (3) The effects of passive and active heat removal mechanisms;
- (4) The pressure conditions within subcompartments that act on systems, components and supports because of high energy line breaks;

- (5) For the ice condenser containment, the design provisions and proposed surveillance programmes that have to ensure that the ice condenser will remain operable for all plant operating conditions.

To cover various uncertainties, conservative assumptions are used in the containment design analysis, and margins between calculated values and design values are taken into account.

In the case of a severe accident, the following thermohydraulic loads must also be considered:

- (a) Pressurization caused by the presence of radioactive materials inside the containment (decay heat), non-condensable gas generation and metal–water reactions;
- (b) MCCI; molten core material may erode the containment basemat while producing hydrogen and other non-condensable gases, thereby threatening containment integrity;
- (c) Long term effects, in particular, in terms of long term temperature and humidity effects;
- (d) Pressurization caused by the continual release of steam.

The phenomena can further be classified according to the main processes occurring within the containment.

3.1.1. Sources and sinks

During an accident, the containment thermohydraulic behaviour is directly related to the mass and heat sources affecting the containment.

Mass (water, steam and hydrogen) may come from the primary circuit: it corresponds to the fluid flows at the primary break or from discharges through relief valves into the containment volume. During the accident progression in the vessel, it can be, successively: liquid flows, two phase flows (steam and liquid) and single phase flows (mixture of superheated steam and hydrogen). If core reflooding occurs, it can give rise to liquid flows at the break again (this is the case, for example, in long term primary loop recirculation due to the operation of safety engineering systems).

Mass sources may also originate in the cavity during the ex-vessel phase of the accident. DCH, MCCI and melt water interactions, including FCI in the cavity phenomena (see Section 3.3), will produce fluid flows from the cavity to other parts of the containment. These sources are essentially composed of gases (mixture of steam and non-condensable gases, such as hydrogen, carbon monoxide and carbon dioxide).

Finally, mass sources may be generated by the operation of some technical systems such as spray systems (see Section 3.4). In this case, water droplets are sprayed from nozzles in the upper part of the containment to reduce the containment internal pressure and to remove a significant part of the aerosols and iodine from the atmosphere.

Heat sources are essentially associated with the radioactive core products in the containment. These fission products exist in the form of vapours or aerosols, or core melt materials (see Section 3.3). Fission products released from the primary circuit via the break, or released from the cavity after DCH phenomena or due to MCCI, will heat up the containment atmosphere and structures. The corium spread in the cavity is also a non-negligible radiative heat source. The combustion of hydrogen and carbon monoxide will also contribute as a heat source (see Section 3.1.5).

Heat sinks are related to containment leakages. Leakages are of different forms: either normal leakages (typically about 1 vol.% per day or less), or leakages linked to accident consequences (i.e. resulting from the accident management procedures, such as filtered venting, or due to cracks in containment walls due to thermohydraulic loadings). Because of these leakages, radioactive elements may be released to the environment.

3.1.2. Pressurization and depressurization

Pressurization and depressurization are the processes causing containment pressure changes due to effects other than energy or mass exchange with structures or pools. They are related to the sources and sinks described previously. The processes are considered adiabatic. Rapid blowdown into the containment is an example of a pressurization process. In the case of a large (double ended) break in a primary circuit cold leg of a PWR, a peak pressure as high as 4 bar can be reached in the containment in less than one minute. Smaller breaks and loss of power transients will lead to containment pressurization on a longer timescale, which may be several hours.

Depressurization can occur, for example, due to the expansion of gases when the containment boundary is breached. Such a condition may be the result of a planned action in the case of containment venting schemes, or the result of the failure of a structure. Additionally, depressurization can also take place as a result of some mass and energy exchange within the atmosphere, as in the case of energy and mass exchange with the containment sprays.

3.1.3. Gas/water interflows between containment compartments (transport)

The containment is physically composed of different compartments, separated by walls and connected to each other through doors and the ventilation circuit (valves, openings). In the course of an accident, mass and energy sources appearing in a compartment will also affect other compartments. Transport is a process where fluids (and carried aerosols) move from one defined region to another. Transport usually refers to the flow between compartments, such as convection loops with the flow of gases that develop between a series of interconnected compartments, or the flow of liquids between various compartments. Transport may also occur between components within a compartment, such as between pool and atmosphere or from structures to pools.

Transport may also take place within a single compartment, as in the case of the flow of liquids along the walls.

3.1.4. Heat and mass transfer

3.1.4.1. Within the gas phase

Mixing in the gas phase is a process in which separate fluids with different characteristics tend to mix together to form a fluid with a single characteristic. Mixing is an intracompartiment process, whereas transport is an intercompartment process. Mixing includes all phenomena that affect the processes occurring within a single compartment or a room. The characteristics mentioned previously can be the temperature or the concentration. For example, if hydrogen is injected into a mixture of air and steam, the incoming hydrogen stream mixes with the surrounding atmosphere. If the mixing process proceeds to completion, a uniform composition of hydrogen, air and steam will be created. In many cases, however, the mixing process is incomplete during a substantial time period and during this period, the atmosphere is considered to be in an unmixed state. If mixing does not proceed to completion, but flows rather than stagnates, then a stratified condition will be created. The particular case of processes related to hydrogen is described in the following section.

The gas entering the containment will exchange heat with the internal structures of the containment (in a 900 MW(e) PWR, the concrete wall surface is about 20 000 m²). Convective and radiative heat transfer will occur on boundaries between the atmosphere and walls, and there will be heat conduction within the walls.

3.1.4.2. *Gas/sump interface*

Sump processes are relative to the thermohydraulic behaviour of the water collected in the sumps at the bottom of the reactor building. In an initially dry containment, this water may originate from the primary circuit break or from safety engineering systems. During the next phase of the accident, mass transfer processes, such as condensation and evaporation, will take place (in a 900 MW(e) PWR, the sump surface is about 2000 m² for a gaseous volume of 50 000 m³, leading to a surface to volume ratio of ~0.04). Due to the presence of radioactive elements deposited in the sumps, sump water is heated (liquid temperature of ~120°C) and evaporating conditions are likely to occur in the absence of any spray. In some cases, boiling processes can appear. For example, the opening of filtering systems will lead to depressurization of the containment and thus to sump boiling.

Another sump process which may occur is gas injection into a water pool, leading to bubbling and non-condensable gas cooling. This process would occur, for example, in suppression pools of the WWER-440/213.

3.1.5. **Hydrogen issues**

The possible combustion of hydrogen or carbon monoxide from MCCI (see Section 3.3.5) is a major source of heat and pressure loading of the containment. Assessment is required of: (a) the sources of hydrogen and other combustible gases; (b) the distribution of hydrogen and oxygen in the containment; (c) the potential for ignition; and (d) the combustion modes and resulting loads on the containment. An objective of the work is to study whether measures are necessary to prevent the combustion of large amounts of hydrogen that could jeopardize the containment.

3.1.5.1. *Sources of hydrogen and combustible gases*

In a severe accident, the dominant source of hydrogen is from the oxidation of metals, such as zirconium in the fuel cladding, with steam. This reaction can occur at various times and locations during the accident sequence, in particular, during:

- (a) The initial period of core degradation, while the fuel is essentially in its original geometry, once high temperatures (typically in excess of 1500 K) are reached;

- (b) Relocation of molten material following clad failure; this exposes new surfaces to the reaction and oxidation is probably limited by the steam supply;
- (c) Relocation of molten material into residual water in the lower head of the reactor vessel;
- (d) Relocation of molten material into any water beneath the reactor vessel;
- (e) A high pressure melt ejection event (see Section 3.3.2);
- (f) A molten core concrete interaction (see Section 3.3.5).

High temperature steel surfaces, or steel incorporated into the debris, will also react with steam to produce hydrogen. This is a particularly significant source of hydrogen from MCCI, where the debris may include steel structures from below the core region and from the rebar in the concrete basemat. The oxidation of B_4C by steam would provide a further source of hydrogen. In addition, there is evidence from the FARO-LWR tests (and earlier tests performed in the United Kingdom) that hydrogen can result from the additional oxidation of a stoichiometric UO_2 melt stream entering water.

The phenomena associated with the in-vessel production of hydrogen are discussed in more detail in Section 2, while an overview of hydrogen sources is provided in Ref. [30]. Additional sources of hydrogen from ex-vessel phenomena are the radiolysis of water and corrosion reactions. However, these are usually minor contributors during severe accident scenarios.

Carbon monoxide is formed by the reactions between reactive metals (Zr, Cr, Fe, etc.) in the debris with carbon dioxide released during the decomposition of concrete during an MCCI.

Combustible gases will be released into the containment building at different locations as the accident proceeds; in most cases, they will be accompanied by the release of steam from the same locations (this is not necessarily the case for an MCCI in a dry cavity).

3.1.5.2. Hydrogen and oxygen distribution

Combustion can only occur if hydrogen or other combustible gases mix with oxygen in the containment atmosphere. Mixing may occur initially through entrainment of the atmosphere in the steam/hydrogen plume. In addition, convective processes within and between compartments will contribute to mixing (see Section 3.1.5.1). On the other hand, the concurrent release of large quantities of steam may contribute to the voiding of compartments of oxygen required for the combustion of hydrogen. Recent calculations performed within the licensing procedure for the implementation of recombiner systems for German PWRs have shown that often the lack of

available oxygen limits hydrogen combustion. For certain containment designs with pressure relief to the atmosphere during the initial blowdown, it is possible to have situations where there is not sufficient oxygen to support combustion for an extended period of time. During this time in a severe accident, a significant amount of hydrogen could accumulate. An increase in oxygen concentration due to an insurgence of air from the external atmosphere may then create dangerous conditions in which an explosion is possible.

The distribution of hydrogen and oxygen will also be affected by hydrogen sinks, such as igniters and recombiners, or by spontaneous local burns. In some situations, a standing flame may be possible (e.g. the combustion of the combustible gases from MCCI at the cavity exit).

3.1.5.3. Potential for ignition

The prospects for ignition of a mixture of combustible gases and oxygen depend on the concentration of the reactants and the presence of an ignition source. Experimental data on the limits for combustion (deflagration) have been summarized in the well known Shapiro diagram. This indicates that for a dry atmosphere, combustion is possible for hydrogen volume fractions between 6 and 75%. As the steam content of the atmosphere increases, these limits narrow, so that for a temperature of 375 K, 60 vol.% steam content will prevent any combustion taking place (note that these limits do not apply to catalytic recombiners).

The likelihood of the presence of an ignition source depends on the accident sequence. Operating electrical equipment may provide sparks that act as ignition sources. In addition, hot surfaces (e.g. residuals of the reactor vessel or its internals after vessel failure) or high temperature debris ejected into the containment atmosphere at vessel failure are other possible sources of ignition. The containment may contain igniters, or under conditions of high load, the recombiners can become sufficiently hot to act as igniters themselves. Thus, due to various stochastic processes, ignition may occur anywhere in the containment at any time when there is a combustible mixture.

3.1.5.4. Hydrogen combustion modes

Hydrogen combustion may occur as a laminar flame, a turbulent flame, an accelerated flame or a detonation [31]. Laminar and turbulent flames are examples of deflagrations, where the speed of flame propagation is slow compared to the sound velocity, thus there is pressure equilibration throughout the volume in which the combustion is taking place. Turbulent flame is the expected combustion mode relevant to severe accidents. Transition to

detonation is undesirable because of the local pressure loads that would be acting on the structures; these may be considerably in excess of the pressure resulting from an adiabatic burn.

Turbulent flames evolve due to gas dynamic effects. Burn speed will be dependent on direction, particularly close to the combustion limit. It is necessary, therefore, to consider both the direction of propagation and the local flow connections that will influence the flows. The flame velocity depends both on the processes at the flame front, such as the burning velocity (i.e. the rate at which unburnt material is incorporated into the flame) and the expansion of the burnt region. Buoyancy effects are expected at low hydrogen concentrations but, in this case, the pressure buildup will be limited and not significant for safety.

Gas mixtures near the combustion limits will not burn out completely. It depends on the burning direction (upwards, downwards, horizontal). If the flame propagates downwards and the hydrogen concentration is high enough, the burnout is nearly complete. If the propagation is directed upwards, the mixture can combust at relatively low concentration, but the burnout is not complete. For the horizontal direction, no relevant measurements exist. Under some circumstances, for example, when additional turbulence is generated by obstacles, flame acceleration can occur. The flame acceleration process can possibly lead to a deflagration to detonation transition through shock ignition or an auto-amplification mechanism [31]. The final flame velocity produced by the turbulent flame acceleration process depends on a variety of parameters, including: the mixture composition; the dimensions of the enclosure; and the size, shape and distribution of the obstacles. A number of criteria have been developed to determine whether flame acceleration and deflagration to detonation transition are possible for given conditions. One approach for flame acceleration is to compare the expansion ratio (conventionally denoted by σ) with critical values obtained as functions of the Lewis and Zeldovich number. This criterion typically indicates that hydrogen concentrations of greater than 10 vol. % are necessary for flame acceleration. Detonability limits are related to the detonation cell size (λ) — detonations cannot be supported in a volume if the ‘diameter’ is less than about 7λ (the experimental support for this criterion is reviewed in Ref. [31]). The detonation cell size is a function of gas composition. For rooms with a diameter of about 10 m, detonations are possible in dry conditions with 10% of volumetric concentration of hydrogen by volume in air, however, 40 vol.% of steam in the atmosphere is sufficient to prevent detonations.

3.2. AEROSOL AND IODINE BEHAVIOURS

Failure of the engineered safety systems to provide rapid and sufficient cooling to the core leads to a severe accident, which entails partial or more extensive melting of the reactor core. The high temperatures induce failure of the fuel rods, consequently giving rise to the release of fission products and relocation of structural materials from the reactor core. The radionuclides transported through the primary system to the breach escape into the containment, where they contribute to the source term. Further sources of aerosols, later in the accident progression, originate from the MCCI process. Gases released from the basemat concrete decomposition, as they pass through the corium pool, will entrain fission products and structural material which will quickly be in the form of aerosols (about 1 t of mainly non-radioactive concrete aerosols can be expected from an MCCI). In addition, high pressure melt ejection and fuel coolant interactions will also produce small corium droplets from which fission products can be released.

The ultimate safety objective is to limit the release of fission products to the environment. An understanding of the various phenomena leading to fission products entering the containment (containment source term) and their behaviour inside the containment is important to achieve this objective. This understanding includes the timing, quantity, identity, and physical and chemical form of the released fission products, as well as their transport and retention in the containment, and the effects of their removal by any mitigating features. Among these fission products, iodine and, in particular, its short lived isotope, ^{131}I , deserve particular attention owing to their specific properties, with the primary concern of short term radiological risk. Major phenomena governing aerosol behaviour and iodine behaviour in the containment are described in the following sections.

3.2.1. Aerosol behaviour

In the containment, aerosols deposit by settling processes. The settling kinetics depend on the agglomeration processes and the thermohydraulic conditions. For example, at the beginning of the accident, the humidity is quite high (up to 100%) and the heterogeneous condensation of steam on aerosol particles occurs, leading to an increase of the particle mass and accelerated gravitational settling. Experiments indicate that it is reasonable to assume that multicomponent aerosols behave like their most hygroscopic component.

An additional deposition process is the diffusiophoresis (due to steam condensation on containment structures that have not yet been heated to the gas temperature). Other processes, such as diffusion and thermophoresis, may

also contribute to the reduction of the suspended mass of aerosols. On the contrary, the resuspension process will increase the suspended mass. This process occurs when there is a sharp variation of thermohydraulic conditions (differences in pressure, temperature and heat transfer, as expected from a hydrogen combustion or DCH). Pre-deposited aerosols on walls are mechanically swept from the surface to the gas phase. This process, along with revalorization from pools, may be important should the containment fail due to overpressure.

Transport of aerosols between the different regions of the containment follows the gas transport. When gases pass through a water pool containing aerosols, a process called pool scrubbing may remove aerosols, while additional aerosols may be generated in the gas phase due to bubble entrainment and bursting.

3.2.2. Iodine behaviour

The rather high iodine inventory in the fuel, and its fast and almost complete volatilization from the core at higher temperatures, promote the rapid transfer of a significant fraction of iodine into the containment, where it tends to form volatile species. Moreover, from a radiobiological point of view, the short lived iodine isotopes belong to the most problematic fission products due to their carcinogenic effect upon release to the environment and accumulation in the human thyroid gland after inhalation or ingestion. Once incorporated into the thyroid gland, iodine is only slowly excreted, and the short lived iodine isotopes will rather be removed through radioactive decay.

While being swept through the primary circuit by a steam hydrogen carrier gas, iodine undergoes a multitude of processes which determine its physical and chemical form, as well as the magnitude of the iodine release to the containment. The first two experiments of the PHÉBUS fission product integral test programme suggest that for the high temperatures attained in a severe accident with core meltdown, iodine is rapidly and almost completely volatilized from the molten fuel, presumably in the form of gaseous iodine. With increasing distance from the fuel bundle, and thus with decreasing temperature, metal-iodide vapours form, either by reaction with control rod material, such as silver, indium and cadmium, or with fission products, such as caesium and rubidium.

As the temperature decreases further in the primary circuit to 1000°C, reactions between aerosols originating from structural materials, fission products or fuel and metal-iodide vapours occur. These aerosols, formed by vaporization, nucleation and condensation, or by mechanical suspension, act as condensation or absorption sites for fission product vapours, thereby exerting a

significant influence on the transport and deposition properties of iodine during a severe accident. In fact, aerosol deposition in the primary circuit provides a retention mechanism that reduces the fraction of iodine eventually released into the containment.

In the cold leg of the primary circuit, at temperatures as low as 150°C, most of the iodine will be associated with aerosols, which convey the iodine fraction that passes through the circuit without being retained in the containment vessel. Henceforth, iodine behaviour in the containment atmosphere is essentially governed by aerosol physics, and mechanisms described previously, such as wall deposition or settling on the containment bottom, significantly deplete the amount of suspended iodine over a period of a few hours.

The major fraction of iodine-bearing aerosols will eventually reach the containment sump, where quite complex aqueous chemistry processes will take place. Upon contact with the sump water, soluble aerosols such as caesium iodide will dissolve in the liquid, yielding non-volatile iodide ions. Subject to high radiation fields and temperatures of up to 140°C, iodide changes its chemical form readily by thermal and radiation induced chemical reactions, ultimately giving rise to the formation of dissolved volatile iodine. Mass transfer processes through the liquid gas interface, which depend both on the mass transfer coefficient and the equilibrium partition coefficient, will eventually allow the volatile iodine species to become airborne. This process can, however, significantly be reduced if the sump contains some silver components (issued from the control rod) that can trap volatile molecular iodine by chemically producing silver iodides. Another aqueous process concerns reactions between molecular iodine and the organic solvents issued from submerged painted walls. Such processes can give rise to high volatile iodine species such as CH₃I. The partitioning of iodine from water bodies to the containment atmosphere entails the persistence of airborne iodine for many days following an accident. It is, therefore, of interest to manage the potential iodine source by suppressing the volatilization of iodine from the liquid phase (e.g. by changing the sump pH, which is known to have a great influence on chemical reactions).

In the gas phase, molecular iodine can react with air radiolysis products and can be sorbed onto painted and steel surfaces. The sorbed iodine can react with organics from paints and produce iodine volatile species such as CH₃I. These species, in turn, can also be destroyed by air radiolysis products. In the long term, it is commonly accepted that organic iodides would be the dominant species airborne in the containment.

3.3. MELT BEHAVIOUR

Ex-vessel melt behaviour affects the potential consequences of a severe accident in a number of ways. The heat accumulated in the debris, decay heat generated in the debris, and heat generated from any chemical reaction between debris and the containment atmosphere or water lead to the potential overpressurization of the containment building. The debris may erode containment structures, either directly or indirectly, thus threatening the performance of the containment. Interaction with the structures may also cause additional loading of the containment from the release of steam or gases only or carbon dioxide. Further reduction of these gases with metals contained in the debris will lead to the additional production of combustible gases (hydrogen and carbon monoxide). Long term high temperature of the debris may lead to the release of fission products into the containment atmosphere. Structural materials may also form aerosols. Interaction with water in the containment building may form coolable debris, thus terminating the erosion threat to the structures. However, the interaction with water will also be a source of steam to the containment and there may be a threat to containment structures from fuel coolant interactions (steam explosions).

In the past, the ex-vessel melt behaviour concentrated on the issues of DCH and MCCI. MCCI was studied to clarify if – and, if yes, when – the melt may penetrate through the concrete, thus opening pathways to the environment. The fission product source term to the containment was also evaluated. In addition, ex-vessel fuel coolant interactions, which may lead to damage of the containment structures or even to the containment itself, were considered for some NPPs.

Various other issues have also to be considered which are important to control the corium and mitigate severe reactor accidents, if the melt damages the reactor vessel. A substantial increase of research and design activities to control ex-vessel melt was reported in Ref. [18]. Especially in western Europe, these issues are related to higher safety requirements. These design related activities may impose additional requirements for modelling melt behaviour, including models for the interaction of melt and debris with engineered structures, such as core catchers.

3.3.1. Melt release

Melt or debris will be released into the containment following a failure of the lower part of the reactor vessel, typically of the lower head of the reactor. It is one of the objectives of modelling of in-vessel phenomena to predict the likely conditions at vessel failure, such as:

- (1) Timing of first melt release and, correspondingly, the decay heat level;
- (2) Primary system pressure at first melt release, and thus the likelihood of melt dispersal;
- (3) Mode of vessel failure, i.e. failure at a penetration, location with respect to the bottom of the vessel and height of the debris, size of initial opening and subsequent ablation;
- (4) Melt temperature, composition and mass of first release. The melt temperature will have an impact on the initial erosion of structures, while the metal content of the melt will have an impact on the potential for combustible gas generation. It is now widely recognized that in many plant designs, only a fraction of the core debris may be released immediately at vessel failure due to:
 - (i) Incomplete relocation from the core region;
 - (ii) Partial quenching of debris after relocation in-vessel;
 - (iii) Location of vessel failure above the bottom of the lower head;
 - (iv) Incoherence in core degradation processes for channel type reactors;
- (5) The period and melt conditions for any subsequent release. It is anticipated that, in most cases, any subsequent release will be a flow under gravity. This may also entail the release of structures, such as the remains of the vessel lower head into the cavity. The timescale for subsequent release is likely to be in the order of between 20 minutes and several hours, depending on the design and the sequence considered.

If the first melt release occurs when the primary circuit is at a higher pressure than the containment pressure, there is a possibility of melt dispersal beyond the reactor cavity. The main issue is the likelihood of direct containment heating, considered in the following section. However, pressure driven release of melt may also lead to a local attack on structures through jet impingement effects, and to the distribution of debris in the containment which should be considered in subsequent analyses of containment loading and debris coolability.

3.3.2. Direct containment heating

In a core melt accident, if the reactor pressure vessel fails while the reactor coolant system is at high pressure, the expulsion of molten core debris may pressurize the reactor containment building beyond its failure pressure. A failure in the bottom head of the reactor pressure vessel, followed by the melt expulsion and blowdown of the reactor coolant system, will entrain molten

core debris in the high velocity steam/water mixture. This chain of events is called a high pressure melt ejection (HPME) [32].

Three mechanisms may cause a rapid increase of pressure and temperature in the reactor containment:

- (1) Efficient debris-to-gas heat transfer;
- (2) Exothermic metal/oxygen reactions;
- (3) Hydrogen combustion.

These processes that lead to additional loads in the containment building are referred to together as DCH.

DCH was a major issue for sequences starting at a high system pressure. However, many NPPs have the capacity to reduce the system pressure prior to reactor vessel failure. Both preventive and mitigatory accident management measures implemented at NPPs should lead to pressures at vessel failure significantly below the operating pressure; this leads to a substantial reduction in the threat from DCH. In addition, DCH would be avoided, as convection of the hot gases in the primary circuit for a coolant system pressure close to operating pressure leads to failure of the primary piping prior to a release of debris into the containment.

Note that the HPME phenomenon beside the short term containment pressurization may also have an impact on other aspects, such as long term cooling of the core debris, or a partial or complete blockage of recirculation sump screens.

For the issue of DCH, the most important factors associated with debris entrainment are the geometry of the reactor cavity, impingement of the debris on containment structures immediately downstream of the reactor cavity, re-entrainment of the debris and the dispersal of the debris to other containment compartments.

The phenomena of HPME have been investigated using simulant fluids and transparent scaled models of reactor cavities. These experiments demonstrated that:

- (1) A substantial fraction of the melt dispersed from the reactor cavity configuration is not entrained in the form of fine particles and, therefore, is less effective at depositing heat instantaneously into the containment atmosphere.
- (2) The entrainment process results in larger debris sizes than would be typically evaluated through a standard Weber number representation, again limiting the efficiency of the heat transfer process.

- (3) There is substantial removal of debris from the airborne fluid stream as a result of interactions with structures in the containment subcompartments.
- (4) Only a small fraction of liquid mass simulant of the corium remains entrained in the upper containment region.

These last two observations are also consistent with the findings of integral tests.

3.3.3. Melt coolability

In some NPPs, melt released from the reactor pressure vessel will come into contact with water in the reactor cavity. Water may be present either through natural spillage, or as the result of deliberate accident management actions. The melt is expected to enter the water in the form of one or more jets. Although the term ‘jet’ is widely used, this may be a pour under gravity, or with only a small driving pressure. For a single failure of the reactor pressure vessel, a single jet is likely. The initial diameter of the jet depends on the reactor pressure vessel failure mode, but studies indicate that jets of about 0.3 m should be considered. Such jets may break up by a number of processes [33], including:

- (a) Atomization at the orifice, or splitting into a number of smaller streams;
- (b) Rayleigh-Taylor-like instabilities at the leading edge, as the leading edge is decelerated;
- (c) Stripping of the edge of the jet through Kelvin-Helmholtz-like instabilities;
- (d) Gross instability of the melt column.

The mechanisms most likely to apply to the melt jet are atomization and stripping of the edge of the jet. Both processes will produce melt ‘particles’ that may be broken up further by subsequent interactions with the coolant. Experimental data indicate that the final particle size is likely to be a few millimetres in diameter. Additional oxidation of the melt and associated hydrogen production may accompany these processes.

In order to form coolable debris, not only must the jet break up, but sufficient heat must be removed by the coolant to obtain particles that will not re-agglomerate when they reach the bottom of the cavity. At typical melt temperatures, thermal radiation is a highly effective way of cooling small particles, however, there has to be a heat sink for radiation. This implies that for an efficient cooling process, water should be retained in the mixture. Other cooling mechanisms, such as film boiling, also require the close proximity of melt and coolant. For fully liquid drops, cooling may not lead to immediate

crust formation, as there is insufficient nucleation of the solid phase, resulting in supercooling. However, once solidification starts, it may then proceed rapidly.

Solidified debris will only remain coolable if there is:

- (1) A continuing supply of coolant to the reactor cavity (or other regions to which the melt has been dispersed);
- (2) A coolant that can penetrate the debris bed.

The principal impediment to coolant ingress is the counter-current flow of the resulting steam (flooding limit). The flooding limit depends on the particle size, porosity of the debris bed and containment pressure. In addition, adverse gradients in particle size, or stratification of the debris, may limit the coolability. Coolability is enhanced if water can be supplied from underneath the debris bed (e.g. using an engineered structure).

3.3.4. Fuel coolant interactions

When liquid melt contacts water, more or less energetic reactions may occur. These are called fuel coolant interactions (FCIs). FCIs may have a number of negative effects:

- (1) Local pressure loadings can damage containment structures and systems.
- (2) Pressure loadings may generate missiles that have an impact on containment structures.
- (3) Pressure loadings may move the primary circuit sufficiently to cause leakage at containment penetrations.
- (4) Debris produced in a fuel coolant interaction is submillimetre in diameter. This has a negative impact on the coolability.
- (5) Additional releases of fission products may occur during the interaction.

For in-vessel FCI (steam explosions), most assessments have been concerned with the potential for missile generation (core slug impact on the upper head and, subsequently, the containment building), nevertheless, this is usually less important for ex-vessel considerations.

Water may contact the melt in two ways: the melt is injected into the water or water becomes an overlay of the melt (stratified FCI). Melt injection into the water is likely to be of more concern, as experimental evidence indicates that stratified FCIs in all systems are limited to the interaction of a few centimetres of melt at most. For melt injected into water, a pre-mixing

phase is anticipated. This involves jet break-up, accompanied by some break-up of the larger fluid particles, as discussed previously (Section 3.3.3).

For an FCI to develop from a pre-mixed configuration, a triggering event is required. This may be contact with the structures in the cavity, a small local melt–water interaction, or the effect of a falling structure causing an impact. The trigger causes local pressurization which drives fluid motions that enhance the fragmentation of droplets. The corresponding increase in heat transfer can then lead to the generation of a pressure wave that passes through the mixture. Pressure loadings and work on the surroundings are developed by the resulting high pressure steam–water–melt mixture.

3.3.5. Molten corium concrete interaction

In the absence of water in the cavity, or if a coolable configuration is not formed, debris will interact with the concrete basemat [34]. Melt depths of between 0.2 and 0.5 m are expected in the reactor cavity — only depths of about 0.1 m would be coolable by conduction alone (i.e. without water ingress).

Concrete consists principally of a mix of ceramic oxides (silica, calcia, alumina, magnesia, etc.), hydroxides and carbonates together with bound and free water. On heating, the water is released as steam, the hydroxides decompose, also releasing steam, and the carbonates decompose, releasing carbon dioxide. The melting temperature of concrete varies with composition, but it is usually in the range of 1400–1600 K (significantly below the melting point of the corium). Thus, if the debris remains at high temperature, the MCCI results in decomposition and melting of the concrete, accompanied by the release of large quantities of carbon dioxide and steam. A cavity forms, advancing both axially downwards and radially outwards in time. Heat transfer in the melt is driven by the flow of bubbles from the decomposition gases. The cavity grows primarily through melting of the concrete; this may be augmented by spallation. At later times, as the surface area of the cavity increases and the heat input decreases, cavity growth will be limited by conduction. Typical heat fluxes of 250 kW/m² early in the interaction give an ablation rate in the order of 0.2 m/h.

Heat transfer from the top of the melt (in the absence of water) will be by thermal radiation, with some heat taken by the off-gas flow. This heat flux will heat up structures in the vicinity of the melt to high temperatures, leading, possibly, to the addition of more material to the melt. The cooling of these structures by natural circulation flows in the containment should be considered. In some plant designs, thermal attack on structures, such as doors, may lead to a threat to the integrity of the containment.

The steam and carbon dioxide react with the ingredients of the corium to produce a variety of chemical reactions and products. For example, they oxidize part of the metal inventory and produce heat, in addition to the radioactive decay heat. These reactions lead to the production of hydrogen and carbon monoxide, which will increase the loading of combustible gases in the containment. The more reactive metals in the debris, such as zirconium, may also react with concrete decomposition oxides, particularly silica. Depending on the melt temperature, this reaction may be exothermic, resulting in silicon formation in the melt, or at higher temperatures be endothermic, resulting in the release of silicon monoxide gas. Silicon monoxide gas decomposes in the containment to form an aerosol of silicon and silica. For siliceous concretes, this may be the dominant aerosol formation process from the MCCI.

Some tellurium and most of the low volatility fission products, for example, cerium, strontium and lanthanum, would be retained within the corium and would be available for release during the ex-vessel phase. The fission products and other materials in the corium form various chemical compounds, which may vaporize and be carried away by the flowing gases. After emerging from the corium, these vaporized materials will form an aerosol source as they condense in the containment atmosphere.

Detailed MCCI models require knowledge of the distribution of the corium and the concrete oxides. At high temperatures, the concrete oxides and the oxidic components of the corium form a single liquid. On cooling, it is anticipated that crusts of the more refractory (i.e. corium) oxides will form preferentially, however, there is also experimental evidence of segregation by gravity leading to the top surface being covered by a primarily siliceous layer which may form foam. It is also anticipated that the metals will form a separate phase. This may be mixed in with the oxide (particularly when there are high gas generation rates), or form a segregated layer (particularly later in the accident when the gas generation rate is low and there is a larger density difference between the metal and the oxide material).

If the melt is not cooled, the MCCI may proceed for days, and if no heat transfer cycle is established, there is the possibility of containment overpressurization and failure. In addition, the concrete ablation may lead to basemat penetration by the melt and release of radioactive material.

Water may be present in the cavity from the start of the MCCI, or added at a later stage, through natural spillage or the restoration of reactor systems. Any water will remove the upward heat flux from the MCCI, resulting in steam generation. The water will encourage the formation of a crust on the melt. Both the crust and pool scrubbing in the water will limit the aerosol release to the containment. It has been further postulated that the presence of water may

lead, in time, to the generation of a coolable configuration. A number of processes have been identified in the MACE experimental programme:

- (1) Bulk cooling of the melt on water addition. This occurs before a stable crust forms (it may not be relevant for the late addition of water).
- (2) Formation of a porous crust. A porous crust allows a greater fraction of the material to remain below its solidus temperature.
- (3) Water ingress. As the debris cools, it contracts on freezing, allowing water to enter cracks and percolate through the debris. In addition, there may be existing porosity as a result of passages formed to vent the off-gas from the concrete decomposition.
- (4) Melt entrainment and eruptions. Gas passing through vents in the crust may carry melt with it, forming volcano-like structures or particle beds. Melt eruptions have been observed in experiments leading to the successful quenching of significant fractions of the material involved, however, it is currently uncertain to what extent these events, or their suppression in other tests, are experimental artefacts.
- (5) Crust collapse. If a crust anchors to the wall, then the melt will recede from it, due to the release of the off-gas component of the concrete. At some point, the crust is likely to become unsupported, crack and allow water ingress. However, this may also remove support from previously quenched material which then becomes re-incorporated into the melt.

3.3.6. Relocation of melt and spreading

If melt falls into a dry cavity, it is usually assumed that it will relocate to provide a layer of uniform height. This is not necessarily the case, however, if either the melt mass relocating is small (e.g. in the case of melt from a single channel in a channel reactor) or there is pre-existing water. The spreading of melt is also of importance for some engineered approaches to the retention and cooling of debris, which require the debris to be spread over a large surface area. Typically, corium depths of 0.1 m would be coolable from above by a water layer by conduction alone, without any water ingress. The spreading of melt is governed by the gravity head driving the spreading and the phenomena resisting the spreading — essentially, viscosity and yield stress, which impacts the timescale, and the freezing of the melt. In a transient pour, there will be sufficient thermal radiation from the leading edge of the melt and its upper surface to allow an incipient crust to form. By itself, this is unlikely to be strong enough to resist the motion of the melt, although this may be halted temporarily. Folding the crust material into the melt, however, will increase its effective viscosity, which may then have an impact on the amount of spreading.

Similarly, if the initial material is below its liquidus temperature, spreading may be impaired, depending on the solid fraction.

3.3.7. Interactions with refractory and sacrificial materials

The development of engineered structures to contain and cool core debris has led to the consideration of a broader group of materials that the melt may contact. These can be divided into refractory materials (designed to protect structures) and sacrificial materials. Sacrificial materials may also protect structures, but their principal goals are to dilute and condition the debris, for example, by lowering its liquidus or decreasing its solid fraction. Both heat transfer (jet impingement, natural convection) and material interaction models are required to address the performance of these materials. In general, the phenomenology is similar to that discussed for the MCCI, although it is likely that there will be a greater emphasis on material interaction aspects. In particular, the performance of refractory materials is dependent on the lack of chemical interactions with the debris which might severely degrade the proposed material's use. Furthermore, there is a desire to avoid both exothermic chemical reactions and those that release gas to the containment building.

External cooling of retaining structures will require models for heat transfer, for example, critical heat flux for cooling channels where there is no pumped coolant flow.

3.4. SELECTED ENGINEERING SYSTEMS

The containment is equipped with several engineering systems whose activation may have an impact on the containment phenomena and thus on the progression of the accident. Some of these systems will have an impact on the fluid and aerosols flows (transport and distribution) inside the containment: fans, doors, rupture discs, etc. Some others, such as filtered venting systems and atmospheric valves, will affect the containment leakages. There are also safety engineering systems whose activation serves to mitigate accident progression, such as spray systems, suppression pools, ice condensers, igniters and recombiners, and passive heat removal systems. A brief description of the phenomena involved follows.

3.4.1. Systems impacting transport

Fans and doors constitute pathways for fluids and transported aerosols. Taking into account their characteristics (e.g. sections and pressure loss

coefficients) is of prime importance for evaluating the right gas and aerosol distribution inside the containment. For example, a melt through of the cavity door due to MCCI in some PWR designs offers another pathway for burnable gases to reach the containment dome.

3.4.2. Systems impacting containment leakages

The activation of filtered venting systems and atmospheric valves constitutes a direct contribution to the source term outside the containment. Retention phenomena in filters are thus to be considered (e.g. filter efficiency as a function of particles sizes) and valve characteristics (opening/closing pressures) have to be described.

3.4.3. Safety engineering systems

Containment safety engineered systems that can significantly influence the progression of a severe accident include:

- (1) Spray systems;
- (2) Ice condensers;
- (3) Suppression pool;
- (4) Passive heat removal systems.

4. STATUS IN THE MODELLING OF IN-VESSEL PHENOMENA

The behaviour of the plant during a severe accident results from a combination of the occurrence of several physical and chemical phenomena. It is necessary to take these phenomena into account for proper modelling in the codes. The objective of this section is to give some details about the important physical phenomena that should be modelled in the codes for a severe accident analysis. Comments on the modelling are also provided to help users in their selection of a severe accident code and its modelling options. Information provided in this section was derived from Refs [5, 35–43]. To facilitate the references in Annex I, the same terminology for phenomena is used in this section.

4.1. MODELLING OF INDIVIDUAL PHENOMENA

4.1.1. Thermohydraulics

Three basic types of models are used to describe the thermohydraulic behaviour of the reactor system. As discussed in Section 4, the general types of codes, detailed system thermohydraulic codes, integrated codes and dedicated codes can be roughly characterized by the level of detail used in the thermohydraulic models used in the codes. The detailed system thermohydraulic codes typically use two phase, non-equilibrium models, sometimes referred to as six equation models because the models use a set of six conservation equations (mass, momentum and energy for each phase). These models typically describe a set of variables for each of the two phases, including void fraction, pressure, velocity, flow rate, temperature and/or enthalpy. These models also include several additional variables and conservation equations to track non-condensable gases, such as hydrogen and nitrogen. The integrated codes typically use quasi-equilibrium models where fluid momentum conservation equations are neglected or simplified. Assumptions of well mixed flow or stratified flow are commonly used to simplify the momentum conservation equations. Correlations, such as drift flux correlations, may be used to describe regions where two-phase flow conditions exist. The dedicated codes, in particular, CFD codes, may include single phase or multiphase descriptions with sophisticated models for heat or momentum transfers and detailed turbulence models. The limitations of each type of thermohydraulic model are described in Ref. [6]. It may be emphasized here that for severe accidents, due to the high temperature of materials, the assumption of thermal equilibrium may not always be valid, and strong evaporation rates may lead to high velocities and mechanical non-equilibrium, particularly under the conditions of vessel reflood. CFD codes may also be used, although they are usually not assessed for severe accident conditions.

Different approaches may also be used in severe accident codes for the definition of the modelling domain, that is, the parts of the reactor coolant system being described by the model's systems of equations. In some cases, the modelling system domain may include both the thermohydraulics in circuits and reactor pressure vessel (i.e. ATHLET-CD and SCDAP/RELAP5). In other cases, separate modelling domains may be used. For example, two separate modelling domains are used for the circuits and the reactor pressure vessel in ICARE/CATHARE (V1 version) with coupling usually in the downcomer and the upper plenum, while MELCOR uses overlapping models for the circuits, plena and core regions. The advantages and disadvantages of these different approaches relate primarily to the speed and reliability of the different

numerical schemes used in the codes, the ease of coupling different kinds of models, and the flexibility of the approaches to modelling different systems. In general terms, the modelling domains describing the overall system, including circuit and vessel response, can be more easily (a) optimized for speed and performance, and (b) applied to different plant designs, but are more difficult to develop and maintain. At the other extreme, the models for separate model domains are easier to develop and allow the code developers to optimize the models for the different regions of the system.

Although there are different ways of characterizing the thermohydraulics in the system, the discussions in the references roughly characterize the response in terms of the following: (a) regimes of core thermohydraulics, including boil off, dry core and reflood; (b) flow patterns; (c) debris coolability; and (d) hydrogen production.

Boil off

Boil off is the steady evaporation of the core coolant inventory as the core is uncovered. The heat transfer regime switches from single phase convection to liquid, through nucleate boiling and dry out to single phase convection to vapour. As a result of the decreasing convective heat removal, the core temperatures increase. Although the rate of core uncovering is strongly dependent on the type of transient that is being analysed (i.e. large break LOCAs may result in a rapid, very dynamic uncovering of the core), boil off usually refers to a relatively slow core uncovering where both the detailed non-equilibrium and quasi-equilibrium approaches work well. In some cases, the quasi-equilibrium models, in combination with options selecting stratified flows, may describe transients where there is a well developed water level more accurately than the more detailed non-equilibrium approaches, since the quasi-equilibrium models were designed for such conditions. However, most of the non-equilibrium models also have optional level tracking models that help to counter this problem. As could be anticipated from the difference in modelling approaches, the non-equilibrium models can handle a wider range of transients, particularly when level tracking or other stratification options are available, but the quasi-equilibrium approaches become more accurate as the transients become slower.

Dry core

If the liquid level approaches or falls below the lower core support plate, the core becomes totally dry and steam flow through the core mainly depends on the evaporation rate of the water in the lower plenum. In turn, the

evaporation rate in the lower plenum depends on the heat transfer from the core to the lower plenum by radiation and conduction, since there is little or no heat generation in the lower plenum (unless melt has relocated into this region). Although these heat transfer mechanisms should be modelled in the codes, in many cases, they are ignored because of the difficulty of modelling the axial heat transfer in the complex geometries of the lower core plate support structures. In some cases, the user can utilize input modelling options to describe more accurately this process. If the axial heat transfer is neglected, the heating rates in the lower portion of the core may be distorted by the underprediction of the evaporation rates in the core. If the temperatures of the lower portion of the core are relatively low, the heating rates may be overpredicted since heat losses from this region will be underpredicted (due to both the underprediction of the axial heat losses to the lower plenum structures and convective cooling from the steam produced in the lower plenum). If the temperatures are relatively high, the heating rate may be underpredicted since an underprediction of the steam flow rate will in turn limit the heat generation rate due to the oxidation of any zircaloy in this region.

However, since the relocation of melt into the lower plenum typically results in significantly more energy deposition into the lower plenum water and structures than would occur due to axial heat transfer only, the lack of such models may only have a temporary effect on the temperatures at the bottom of the core.

Reflooding of the rod-like geometry

For reflooding of a rod-like geometry, modelling approaches and correlations developed for design basis accident conditions are applicable with the following limits. Firstly, these models are typically developed for the original geometry of the core (with the possible consideration of flow blockages due to ballooning and rupture). As noted in the previous section, as temperatures above 1500 K are reached, reflooding of the core may result in the partial or total break-up of these structures as a result of the strong thermal shock associated with reflood. Secondly, the reflood can result in large increases in hydrogen production, so the flow conditions above the quench front may be altered by the presence of large concentrations of non-condensable gases, which may not have been considered in the correlations for design basis accident conditions. Thirdly, physical changes in the rod surface are apparent, as break-up of the protective oxides or the structure itself occurs. Thus, because of the strong consequence of this process on the subsequent heating and melting of the core and the production of hydrogen, it is necessary to model both the thermohydraulic and mechanical aspects of this process in some detail.

Since this is an issue that is being addressed currently, the type of models available and the accuracy of these models vary widely from one code to another.

Reflooding of debris beds

Models and correlations developed for the original geometry of the core under design basis accident conditions are not generally applicable to the flow in debris beds, particularly during reflood conditions. However, a number of correlations have been developed specifically for porous media that are, in many cases, also applicable to the flow in debris beds, as long as the flow does not disrupt or levitate the debris. In many cases, these correlations were developed to address the coolability of debris beds. That is, these correlations were used to define under what conditions it was possible to quench and cool debris beds. In general terms, these correlations indicate that debris beds with fine particles and lower porosity (or permeability) are difficult or impossible to cool (because of the internal heat generation), while beds with large particles and high porosity are easier to cool. In the case of reflooding of debris beds from above, the counter-current flow of steam acts to further reduce the coolability of a debris bed because of the reduced ability of the water to penetrate into the bed.

However, many of the correlations that were developed for porous media or debris are either zero dimensional or one dimensional. The zero dimensional correlations simply define whether the bed as a whole is coolable or not, while the one dimensional models also attempt to describe the quenching elevation within the bed. However, the debris beds that occur under severe accident conditions tend to be somewhat non-uniform and may vary axially, radially and circumferentially around the core. Thus, zero dimension or one dimension correlations that predict reflooding for uniform debris beds may be inaccurate under the conditions expected in actual conditions. In the case of reflooding from below, such correlations may not predict adequately the formation of hot spots that may ultimately melt and form local blockages. In the case of reflooding from above, the correlations may be overly conservative in terms of the limiting effects of counter-current steam flow, since water may be able to penetrate from the side of the debris even though the penetration of water from the top may be limited [43].

Although the modelling of the reflooding of debris beds varies substantially from one code to another, reflood models dependent entirely on quenching or coolability based correlations may be increasingly inaccurate as the non-uniformity of the debris beds increases. Zero dimension based correlational models are largely ineffective except in the limited situations where the

debris beds are small and uniform. One dimensional correlations are also limited but may be most accurate when predicting the reflooding of debris beds in the lower plenum where two dimensional and three dimensional effects are more limited. In some cases (uniform debris bed), since such models may overestimate the effect of counter-current steam flow, such models may provide a conservative limit on the reflooding of the debris in the lower plenum. In very general terms, the more detailed codes tend to rely less extensively on quenching or coolability correlations while the integral codes are more reliant on such correlations. However, in all cases, the accuracy of the models used to predict the reflooding of debris beds is largely dependent on the ability of the codes to accurately predict the state of the core and debris beds at the time of reflood. Thus, the ability of the codes to accurately predict the extent and timing of the break-up of the fuel and core structures, the formation of local blocked regions of previously molten material, and the characteristics of the debris bed (e.g. particle size, porosity, permeability) will ultimately determine how accurately the codes can predict the reflood of those debris beds.

Reflooding of the molten pool

The models for the reflooding of molten pools are unique to severe accident conditions, and vary widely from code to code. However, in general terms, the models are varying from user input (e.g. switches which specify whether molten pools can exist or not, user defined heat transfer coefficients in molten pool regions) to more detailed models that attempt to predict the convective and radiative heat transfer on the outside of the crust surrounding the molten pool. In general, the detailed models rely on the application of standard correlations for heat transfer on simple geometries, such as plates, spheres or cylinders in combination with a prediction of the general shape of the molten pool crust based on the history of the formation of the melt. The one important constraint that limits the accuracy of such models is the difficulty in predicting the exact shape, orientation and characteristics of the surface of the molten pool (actually, the frozen crust surrounding the molten pool). This results in significant uncertainties in the selection and application of the most applicable correlations. In general, the detailed codes can predict the general configuration of the molten pool, but there are important uncertainties on the local geometry and surface characteristics of the crust. Even the most detailed models include modelling parameters that are used to determine the consequence of significant uncertainties in the calculated reflood behaviour.

In either extreme — user defined behaviour or detailed modelling of the reflooding process — the primary issue to be addressed by the models or the

user is the mechanical stability of the molten pool during and following reflood. If the molten pool crust is mechanically stable and does not fail, the behaviour of the melt inside the crust is somewhat irrelevant while long term cooling is sufficient to remove the resulting decay heat — otherwise, the water will simply boil off again. On the other hand, as occurred in the case of TMI-2, if the crust is not stable and fails, the melt can continue to relocate downwards even if the core is completely covered with water (and perhaps much of the crust surface is adequately cooled). Thus, the ultimate consequence of the reflooding of the molten pools will be determined by either models that can successfully predict the thermal and mechanical response of the crust surrounding the molten pool or by the choices of the user.

Flow patterns

It is important that thermohydraulic models for severe accidents be able to calculate the two specific complex flow paths, as follows:

- (1) Natural convection in the reactor pressure vessel and in the reactor coolant system. This is essential to predict the temperature along the hot leg, and up to the steam generator where weak points may break due to overheating.
- (2) Flow across the partially blocked core. After substantial degradation and relocation of material, there are regions of low porosity (blockages) and regions of high porosity (voids) in the core. The flow becomes at least two dimensional, with steam being diverted from the centre where the first blockages appear and being attracted to the centre again in the upper part where void regions exist.

The early models for predicting the thermohydraulic response of the core and vessel during severe accidents were one dimensional models. As a result, these models could not predict the flow patterns in the core or vessel and the resulting heat-up and melting of the core very accurately. Most, if not all, of the commonly used codes now employ two dimensional models with varying degrees of sophistication. The integral codes generally use models that predict the flows within predefined patterns and so, as discussed in Section 2, can predict the general trends associated with the flow patterns in the vessel but have difficulty predicting the effects of change in core geometry. The detailed codes generally use models that predict the flow patterns in the vessel using a two dimensional or three dimensional nodalization of the vessel and core. Some CFD codes (TRIO, PHOENICS, FLUENT, CFX, etc.) have been used to predict three dimensional flow patterns under limited conditions (a few

elements of the circuit, with imposed boundary conditions), primarily under single phase steam flow conditions. Examples include the calculation of flow mixing in the lower plenum region of steam generators to help quantify the flow patterns during hot leg natural circulation and the heating of the upper core and upper plenum structures in the later stages of the TMI-2 accident.

Coolability of debris beds

As discussed in the previous section on the reflooding of debris beds, standard thermohydraulics correlations which have been developed for intact bundles cannot be directly applied to debris beds. As a result, either these correlations must be adapted for use in debris beds or correlations developed specifically for flow in debris beds must be utilized.

Hydrogen transport

Hydrogen enhances natural convection and heat transfer but reduces steam condensation. One of the main results of in-vessel analysis of a severe accident is the prediction of the hydrogen flow rate and the hydrogen/steam ratio at the break(s). These key parameters are then used as boundary conditions by ex-vessel codes or models to estimate the hydrogen distribution in the containment. Hydrogen is essentially a threat to the containment because of the risk of combustion. To predict this risk, the hydrogen transport to the break(s) must be properly calculated. This is obtained by including the transport of non-condensable species in the thermohydraulics model (at least one additional conservation equation).

4.1.2. Heat transfer

Radiation heat transfer

Radiation heat transfer becomes important at high temperatures (above 1000 K) and after collapse of materials, when some structures are in direct view with hot debris located below. Radiation is modelled in most of the codes, including absorption of heat by steam, but usually the models cannot deal with scattering media (e.g. water droplets) or large cavities with strong absorption by the gas. Such cases would require multidimensional models which require a lot of computation time. In any case, models for radiation heat transfer with a relevant estimate of view factors, across rod assemblies or debris and across large cavities, should be available in the code. The lack of appropriate radiative

heat transfer models will lead to an incorrect temperature distribution in the vessel.

Thermal behaviour of a debris bed

Heat conduction in a debris bed is usually solved by using an effective conductivity characterizing the complex bed made of particles, liquid melt and fluid. The type of models used varies from code to code, with the detailed codes tending to describe the temperature distributions within the debris beds while the integral codes may use lumped parameter approaches. In some cases, a porous medium description is used to characterize the heat transfer. In this case, radiation heat transfer is included in the effective conductivity.

4.1.3. Fission and decay heat

Recriticality

Recriticality situations may appear due to changes in core configuration (melting of control rods and absorber/fuel separation) or boron dilution. In such a case, fission power may become a significant heat source. In most severe accident codes, the spatial distribution of the neutron flux is not modelled — indeed, such models are not considered necessary. In a case when criticality is expected to occur, separate bounding calculations concentrating on reactor physics can be used to check what the consequence will be. In those cases where the potential consequence may be severe, accident management strategies that ensure an adequate level of reactivity control through such considerations as boron addition to water sources would be necessary, making detailed modelling of the process unnecessary.

In the context of the Fourth Framework Programme of the European Commission, a project dedicated to recriticality during a severe accident was carried out. The results are available in Ref. [44].

4.1.4. Oxidation

Zirconium oxidation

Many experiments have been performed up to 1500 K, and reliable correlations exist to reflect the kinetics of the growth of the oxide layer and the hydrogen production rate. They may be more questionable for higher temperatures, which are in the range of interest for severe accidents. Most codes use the same correlations (with options to be selected by the user), or more detailed

models including equations for the diffusion of oxygen through the different layers (zirconium, a-Zr, b-Zr). Although better accuracy of diffusion models as compared to correlations has been shown in separate effects tests, their positive effect is not so clear for large integral tests or for reactor calculations, and they require more computation time. Therefore, the use of correlations is still a good choice even for mechanistic codes.

Steel oxidation

Steel oxidation is modelled in the same way as zircaloy, but it is less exothermic compared to zircaloy oxidation. The mass of steel in the core and the surface area is small. Thus, the steel oxidation does not contribute much to the amount of hydrogen produced. An exception may be Russian PWRs of WWER type which contain a larger amount of steel than the western type PWRs.

B₄C oxidation

B₄C oxidation is very exothermic and may have a significant effect on the early phases of degradation, in particular, during the reflood. However, the complex chemistry of this reaction (production of boric acid, methane and other gases) is still under investigation and models have only been introduced into the codes recently. Boric acid and methane affect the fission product chemistry.

Oxidation by air

The consequence of air ingress is starting to receive more attention because oxidation of zircaloy by air is more exothermic than oxidation by steam. Nitrogen may also diffuse into the zircaloy, particularly if the oxygen of the air is depleted. Fuel oxidation by air results in hyperstoichiometric uranium (slightly more than two atoms of O for one atom of U) and higher release rates for several fission products. These effects are not typically modelled in severe accident codes.

Steam starvation

When the water level has dropped significantly, the oxidation of the core may be limited by the availability of steam. This leads to steam starvation zones which cannot be oxidized although they are at a high temperature. Such zones are likely to produce Zr-rich melts which will be oxidized after relocation in

another part of the core or during reflooding. Starvation may also occur before blockage formation, in the case of low steam mass flow rate, downstream of the oxidizing region. This phenomenon is modelled by a limitation of the steam diffusion mass flux available at the cladding surface. There is not much controversy about such modelling and it is available in all codes.

Several oxidation processes were studied within the framework of a European Commission project, Oxidation Phenomena in Severe Accidents (OPSA) [45].

4.1.5. Material interactions

Control rod degradation (absorber models)

Each one of the chemical reactions between control rod materials ('non-fuel dissolution') is modelled in most codes by simple 'eutectic temperature' models, or kinetic rates and/or equilibrium diagrams (B_4C oxidation and interactions with steel may not exist in all codes). Similar models are necessary for spacer grids. Models for the mechanical behaviour of claddings with internal overpressure calculate the deformation (ballooning), the possible fuel/cladding contact and the creep failure (burst or flowering).

At present, it appears that Ag-In-Cd rod degradation does not have a strong effect on fuel rod degradation and the subsequent evolution, because it relocates at a lower elevation than the oxides. As a result, simple interaction models may be sufficient (i.e. equilibrium models assuming extremely fast chemistry). For B_4C , the situation is more complex because of its very exothermic oxidation. Finite rate kinetics should be used for B_4C rod oxidation and degradation.

Fuel rod dissolution

Fuel dissolution and ZrO_2 dissolution by liquid Zr are modelled in most codes, by kinetic rates (correlations) and/or equilibrium diagrams. Some recent models are able to deal with the two simultaneous reactions. They offer a strong potential for the accurate description of complex situations, such as the dissolution of the zirconium layer in the case of steam starvation. When available, the consequence of such models should be checked. It was observed experimentally that increasing the fuel burnup increases the fuel dissolution by liquid zircaloy. However, such irradiated fuel effects are not currently modelled in severe accident codes.

Several experiments were undertaken and models were developed that related to this subject during a European Commission project, Corium Interactions and Thermochemistry (CIT). The results are available in Ref. [46].

Cladding failure

The modelling of oxide shell failure, which determines the start of relocation, is also very important. It is usually based on simple temperature and oxide thickness criteria coming from experimental observations.

After phase transition of the zircaloy (first into α phase, then into zirconium), the mechanical resistance is strongly reduced. Therefore, it is usually assumed that the cladding integrity depends essentially on the thickness of unoxidized zircaloy (β phase) and on the temperature (thermal stresses). Several experiments have shown that cladding failure occurs for temperatures in the range of 2000–2500 K and oxide thickness in the range of 200–400 μm .

In the case of reflooding, cooling of the cladding may be faster than phase change, therefore, more complex models taking into account finite rate kinetics and the relaxation of stresses across the cladding are more accurate.

Material interactions — phase diagrams

Due to the complexity of these two simultaneous reactions, it is necessary to use an up to date U–Zr–O phase diagram in the chemical interaction models to be able to predict at least the equilibrium states, the amount of liquefied materials, the relocation velocity (which depends on the solid fraction in the melt) and the freezing temperature (which will determine the location of the blockages).

This phase diagram was investigated and improved during the European Commission CIT project [47].

For other interactions, binary phase diagrams also exist, and should be used to determine the volumetric fraction and composition of the liquid mixture resulting from the interaction between two materials.

The impact of iron on the material interactions can be rather strong: when iron is in contact with a partially oxidized U–Zr–O melt, some part of the uranium contents is reduced and included in a metallic phase that also contains iron and zirconium. Such results have been confirmed recently by the OECD MASCA project performed in the Russian Federation. Therefore, the use of a proper U–Zr–O–Fe diagram may be necessary to predict the late phases of the accident, especially the behaviour of molten debris in the lower plenum.

When the phase diagram information is not incorporated in the models, it is necessary to specify the ‘melting temperature’ of the mixtures. According to

the definition of such a temperature, it may lead to a rather bad prediction of the amount of molten materials and a resulting error in the time of core slumping.

The present knowledge of phase diagrams, at least for binary diagrams and some ternary ones, is reliable enough to advise their use in chemical interaction models, especially because of the strong impact of chemical interactions on the accident evolution. However, and despite the large amount of experimental programmes throughout the world, there are still many uncertainties on material properties, especially for complex mixtures or under oxidizing atmosphere.

Kinetics of material interactions

Oxidation and dissolution processes are controlled by the diffusion of the species (especially oxygen). Diffusion coefficients are introduced in correlations or in oxygen diffusion models. They are usually described by an Arrhenius law. The growth rate of oxidized or dissolved layers is, in most cases, given by a parabolic law (except for diffusion models). The comparison between diffusion models and correlations has shown that parabolic laws are usually acceptable as long as the heat-up (or cooldown) rate is not too large. In general, this concerns only some short periods of the accident sequences.

4.1.6. Material relocation

Melt progression

The modelling of corium relocation must take into account the state of the materials but also the geometry of the solid components along which it flows (reduced cross-section, grids, debris, etc.). It may be either one dimensional if the candling along rods only is considered, or at least two dimensional for a more general description, such as horizontal spreading above crusts or plates and relocation towards the lower plenum. Several models exist to calculate the velocity of the melt: from a simple imposed velocity to a more detailed calculation using porous media theory. Validation studies have shown that simple one dimensional relocation models are acceptable for bundle calculations (integral tests) because of the fast melt relocation process. However, only two dimensional models (with radial spreading) have been able so far to reproduce melt progression in experimental debris beds. Therefore, the user should be aware of the limitations of one dimensional models. In particular, the relocation observed in TMI-2 showed a radial progression of the melt (molten pool), followed by an axial progression through the bypass, down to the lower

plenum. Such relocation processes were studied within the framework of a European Commission project, CObest estimate: Experimental and Computational Modeling of Corium Formation and Behaviour during a Severe Accident in LWRs (COBE) [47], with an emphasis on the use of relevant material properties (density, viscosity) and advanced multidimensional flow models to predict melt relocation and progression.

Early fuel pellet slumping

If the amount of fission gases inside the fuel is significant (high burnup), the fuel pellets may be subject to swelling when the temperature reaches 2700 K. This corresponds to a large volumetric expansion of the fuel and a reduced mechanical resistance. This may be a cause of fuel slumping. Such a phenomenon is not yet modelled by the codes. Another possibility is the collapse of solid fuel fragments (relocation of non-molten structures), which is already modelled by some codes.

Up to now, there has been some experimental evidence of irradiated fuel relocation at fairly low temperatures compared to the values predicted by phase diagrams. Such behaviour could not be explained in a satisfactory way (especially because it was only observed in a few experiments) and, therefore, is not currently well modelled by codes.

Behaviour of the molten pool

A natural circulation regime is established in the molten pool, and the heat fluxes at the boundaries of the pool depend on the internal Rayleigh number. This is usually modelled with standard heat transfer correlations applied at the external boundaries of the pool. It also requires the modelling of crust formation which changes significantly the heat transfers along the pool boundaries. Although this modelling may be sufficient for heat transfer, it is not sufficient for mass transfer aspects, such as phase segregation between solid and liquid or the separation of non-miscible liquids. Models exist for this problem but they require the complete resolution of Navier–Stokes equations with a very refined meshing which cannot be considered yet in severe accident codes. Dedicated codes may be used if necessary. A simple comparison between internal heat generation and maximum heat flux that may be removed (critical heat flux) at the external boundaries shows that there is a maximum size for the pool, above which it becomes impossible to cool and stop its progression. If this size is reached, the pool expands and grows, and finally reaches the external baffle or the lower core plate. This leads to relocation of corium into the lower plenum, which is a significant step in the severe accident

progression. For the majority of severe accident scenarios, there will be no water pool within the core which is in contact with a molten pool. Rather, the molten pool will be supported by non-molten structures. Consequently, the heat from the pool can only be transferred to steam or other structures and critical heat flux is not an issue.

Three relocation scenarios into the lower plenum should be mentioned:

- (1) Lateral crust failure and relocation via the core bypass;
- (2) Bottom crust failure and jet flow through the lower support plate (unlikely);
- (3) Massive relocation due to failure of the lower support plate.

Solidification

At the boundaries of the molten pool, the formation of crusts may have a strong impact on the heat transfer. It appeared clearly in the last few years (e.g. in the experimental programmes RASPLAV [48] or VULCANO [49]) that the solidification of corium mixtures may lead to material segregation, which may even result in a stratification of the pool. Such a process is related to thermochemistry: the equilibrium compositions of the solid and liquid phases are different. To calculate such complex phenomena, some models exist but they have been implemented into stand-alone codes and are not yet available in severe accident codes. However, they usually include crust formation models without phase segregation. Crust formation, especially on top of the pool, has a strong impact on the heat transfers.

4.1.7. Lower plenum behaviour

Corium/coolant interaction

For most scenarios, there will be water in the lower plenum when corium relocation occurs. The interaction of the molten corium with water has several consequences, including:

- Fragmentation of the melt jet, which leads to the formation of a debris bed mixed with possibly remaining corium. This is usually roughly modelled with correlations for the jet ablation rate and the size of particles produced. The particles are then assigned to a predefined part of the lower plenum (either above or on top of the remaining liquid corium). Even rough models are acceptable because alternative models are very

complex and require a lot of computation time for a transient phase of approximately 1 s duration.

- Vaporization of water inducing a pressure increase in the vessel and more steam available for oxidizing the remaining claddings. Correlations for this specific heat transfer between corium and fluid are used in the thermohydraulics model. Such models are simple and may be inaccurate, but alternatives are much more expensive to run in the central processing unit (CPU).

Possible steam explosion

This risk has been estimated to be very unlikely even at low pressure (according to the conclusions of several experts after FARO and other experimental programmes). The phenomenon is not modelled by severe accident codes (but dedicated codes, such as MC3D, were developed for this purpose). For the time being, dedicated codes are only able to calculate the dynamics of fragmentation; the energy in the case of a postulated steam explosion depends still on assumptions.

References about this subject include state of the art reports from the OECD and the European Commission [50]. The results of a European Commission project, Characterization of Processes, Which Govern Quenching of Molten Corium in Water, Including Steam Explosion (MFCI), are also available [51].

Gap cooling

The behaviour of the debris bed and the molten pool in the lower head is similar to the one in the core, except that there is no access for the coolant to the lower surface in contact with the wall. Assumptions have been made regarding possible access through a gap between the wall and a stable solid crust. Gap cooling is only important for reflood scenarios. Considerable heat may be removed through this gap which would have a great impact for lower head integrity. Some codes include the modelling of this process by critical heat flux correlations applied along the gap, with a user defined gap thickness. However, there are large uncertainties about the gap formation process, and there is not a consensus on the proper way to model such a process.

Focusing effect

Another specific feature of the lower head molten pool is that it may be covered by a layer of non-miscible molten metals (especially steel coming from

the melting of lower structures, but possibly mixtures containing Zr). This induces large heat fluxes to the parts of the vessel in contact with the metallic layer. This phenomenon is known as the ‘focusing effect’. It may be neglected as soon as the layer becomes thick enough (the critical thickness depends on the size and the residual power of the pool). It is generally modelled by integral codes which assume the existence of a predefined metallic layer above the oxidic debris. The mechanistic description of the oxide/metal separation is very complex and it can be hardly possible to achieve a proper modelling of the focusing effect even in mechanistic codes.

There are large uncertainties associated with this phenomenon because of the complex process of stratification in the pool. It depends on the successive arrival of materials in the lower plenum and the miscibility of the materials which may need to be investigated experimentally. Existing models may be acceptable, but the results should be analysed carefully.

Failure of the lower head

Once a large amount of debris (particles and/or molten pool) is in the lower plenum, the temperature of the lower head wall increases and several modes of failure are possible:

- (1) Failure due to heating at medium or high pressure. This may preferably occur at locations where the reactor pressure vessel is slightly thinner or weaker because of local variations in the composition of steel.
- (2) Creep rupture due to non-uniform heat flux (e.g. focusing effect).
- (3) Failure of the welds and ejection of instrumentation tubes (if any). The lower plenum debris may be poured through this hole if they are not supported by a solid crust.
- (4) Melting of some part of the wall by direct corium jet impingement. This may happen if there is not enough water or if the jet is wide.

Some of these failure modes (creep rupture and tensile failure) have been observed experimentally in the course of the lower head failure (LHF) or OECD lower head failure programmes.

The first two modes of failure are modelled with a one dimensional or two dimensional representation of the vessel in which a mechanical deformation model is applied. It includes the calculation of elastic, plastic and creep deformations, and the use of appropriate failure criteria (several options may be found in various codes). For such models, the mechanical properties of the vessel wall material must be known and introduced in the input data (this includes ultimate yield strength, creeping velocity as a function of temperature,

etc.). Conclusions of the ongoing experimental programmes are not complete up to now and they have not been used in the codes yet. However, the assessment of mechanical failure models against experiments is the best way to select a model.

If the timing of vessel failure is a key parameter for the analysis and has to be estimated accurately, the user should use a dedicated code, such as ABAQUS or CASTEM-2000 (the heat fluxes to the wall calculated by the degradation code are provided as boundary conditions for the mechanistic code).

For instrumentation tube failure, models exist and have been implemented in some codes, but they are rather difficult to assess, since not many experiments have been performed in connection with this issue (LHF, CORVIS), and the appropriate measurements may not have been carried out (welding temperature, expansion of the hole).

Jet impingement is usually modelled by heat transfer correlations, depending on the impact velocity and width of the jet.

External cooling of the reactor vessel

One possible way to avoid creep rupture is to cool the vessel wall externally. Different experiments dealing with this issue showed that the heat flux to the water may be sufficiently below the critical heat flux for downward facing walls. For large PWRs, however, the related uncertainties, mainly with respect to the molten pool behaviour inside the reactor pressure vessel (focusing effect), do not allow a proper estimate of the effectiveness of outside cooling. On the other hand, for LWRs with a lower power density, for example, BWRs or the smaller WWERs, this melt retention strategy can be regarded as sufficiently reliable. Determination of the critical heat flux is still the subject of different experiments. Once it has been demonstrated that the actual heat flux is well below the critical heat flux, a simple temperature boundary condition on the external surface of the vessel is sufficient for plant calculations.

Several European Commission projects about reactor vessel integrity during severe accidents have been undertaken within the scope of the European Commission Fourth Framework Programme, and the results are available in Refs [52–55].

4.1.8. Fission products

Fission product release

The initial inventory and distribution of fission products are usually provided as an initial condition of the calculation. They result from the power loading and operating time of the reactor. The first significant release of fission products occurs when the cladding fails. This is called 'gap release': the fission products that have migrated from the pellet to the gap between fuel and cladding are released. It is not always modelled in the codes due to its relatively low importance. The second release starts at temperatures between 1500 and 2000°C, up to the melting temperature of the pellet. At this point, the noble gases and the more volatile fission products (iodine, caesium, tellurium) are released from the pellet. From the point of view of the amount of fission product, this release is comparatively much larger than the gap release. Since there is typically ten times more caesium than iodine, usually all the iodine is released as caesium iodide and the rest of the caesium as caesium hydroxide. Tellurium is released in its elemental form but may react with zircaloy and thus be retained in the corium. It was also observed that boron and boric acid react with fission products.

Three kinds of models exist: kinetic release rate correlations (Arrhenius law); semi-empirical models which describe only limited phenomena and give a detailed description of gas behaviour (atoms and bubbles inside and outside the grain) and models of chemical behaviour of the fission products. The advantages and drawbacks of each model have not been clearly demonstrated yet, and more validation needs to be done. The vaporization of structural material (steel) and control rod materials (e.g. cadmium or silver) must also be considered because these can form the bulk of the aerosols which will subsequently carry the fission products. This is not modelled yet in all the codes. The fission product release from pellets is rather well understood, but it is not yet possible to obtain quantitative results. In particular, the effects of burnup and oxygen potential in the carrier gas are not convincingly modelled (if at all). For a debris bed or a molten pool, models have been proposed which rely on existing experiments (VERCORS, MP project in the 4th Framework Programme, PHEBUS fission product) or which will be applied to future ones (LPP project in the 5th Framework Programme).

A state of the art report about fission product release was issued by the European Commission [18].

Fission product transport

The fission products are carried by the coolant through the reactor coolant system. Noble gases move with the other gases while other fission products may be either deposited in the reactor coolant system or driven to the containment through a break in the primary circuit. As the carrier gas leaves the core, it cools down and the least volatile substances condense as aerosols, which may be deposited onto the walls (by direct impact, thermophoresis, diffusiophoresis, turbulent diffusion, etc.). The aerosols contain fission products which, after deposition, will heat up the wall and may react chemically with it.

Therefore, the behaviour of aerosols in the reactor coolant system has a major impact on fission product transport. Comprehensive models exist for these phenomena. They have been implemented into dedicated codes (VICTORIA, SOPHAEROS, etc.) which may be coupled to the thermohydraulics/degradation code for accurate calculations. SOPHAEROS is already coupled with such codes within the ASTEC integral code.

4.2. IMPLICATIONS OF MODELLING OPTIONS AND CATEGORIES OF CODES

Depending on the level of accuracy that is needed, the modelling options may be crucial for each one of the physical processes described previously. However, despite the diversity and complexity of the phenomena occurring during a severe accident progression, there are a few models that will have a much stronger impact than others on the relevance and accuracy of the calculation. Therefore, to summarize the importance of the choice of models, analysts should pay very careful attention to:

- Thermohydraulics: Mechanistic codes actually calculate the flow pattern according to the changes of geometry and porosity in the core and to the flow regime (forced convection, natural circulation), whereas integral codes usually assume the flow pattern, which may lead to inconsistent results (especially for hydrogen production). A notable exception is the hot leg circulation for detailed codes, which depends on specialized input models tuned according to hot leg natural circulation experiments.
- Melt progression and core slumping: Mechanistic codes consider several modes of material relocation (rod candling, fuel melting and collapse, relocation to the lower head) and track different phases of damage progression, whereas integral codes tend to lump zircaloy and fuel

- melting phases together, using core slumping temperature and relocation models depending only on temperature, whatever the configuration is. The modelling of cladding failure, which determines the start of relocation, is also very important, but is only considered in detailed codes.
- Significant differences in peak/average core temperatures and energies of the melt at core slumping result from these modelling differences. This potentially affects the vessel failure. In general terms, detailed codes may show delays in core slumping and much higher stored energies relative to integral codes since ceramic melting temperatures are required for core slumping.
 - Behaviour in the lower plenum: Mechanistic codes actually calculate the successive arrival of materials under various forms (particles, liquid corium, molten steel structures, etc.), and the resulting thermal and mechanical changes in the lower head wall, whereas integral codes assume the configuration of the debris in the lower plenum and use steady state assumptions to calculate the material inventory and the resulting heat fluxes to the vessel wall. Such assumptions may not be conservative since they do not allow for transient situations that may result in higher heat transfer rates than the steady state configuration (e.g. a temporary thin metallic layer).
 - Reflooding: It has been noticed in the past that simplified thermohydraulics models may predict quenching in almost any case. This transient physical process involves, in most cases, thermal and mechanical non-equilibrium which has to be taken into account in the modelling. Integral codes use quasi-equilibrium thermohydraulics models, whereas detailed codes use non-equilibrium models. For this reason, integral codes (but to some degree detailed codes, too) may not model all of the features of reflooding of damaged cores very well. Current research programmes in Europe try to address the remaining uncertainties. An international standard problem (ISP) started, in late 2000, to look at QUENCH modelling with widely available codes. It should be noted that a substantial amount of hydrogen may be produced during reflooding.

Finally, there are significant differences in user effects since integral codes rely heavily on user input to define model parameters, whereas detailed codes usually offer default options that were optimized from validation results in small scale tests.

4.3. UNCERTAINTIES IN MODELLING SEVERE ACCIDENT PHENOMENA

Although progress has been made in the modelling of relevant severe accident phenomena, there are still significant uncertainties, mainly in the late phase (onset of melt relocation, formation and behaviour of a molten pool, relocation into the lower head, heat-up and failure mode of the lower head). This is mainly caused by the lack of experimental data or, more specifically, the absence of large scale experiments. A general discussion of the relevant phenomena and the state of their physical understanding is given in Ref. [5]. More detailed publications are available for many of the severe accident codes, including more detailed discussions of the uncertainties in the models and, in some cases, independent peer review and assessment of modelling uncertainties. The different phenomena as discussed in Ref. [5] are classified into three levels of knowledge: high, medium and low. In the following discussion, a short overview is given.

4.3.1. Well understood phenomena (high level of knowledge)

For these phenomena, the processes are adequately modelled and, in general, well validated.

The majority of phenomena involved in the early phase of core degradation are well known. This concerns boil off, recriticality in case of intact geometry, boron dilution, absorber–fuel separation, reflooding of the core before onset of significant hydrogen production, fuel cladding contact, ballooning, dissolution of fuel and non-fuel core materials, oxidation of zirconium and steel, release of volatile fission products, and elastic deformation of the lower head wall.

4.3.2. Phenomena not fully understood (medium level of knowledge)

The phenomena are understood on the whole, but uncertainties remain for unexplored parameter ranges or extrapolation to reactor scale. The main processes are described by adequate models but the validation of the models may be limited due to the limited database.

Not all phenomena related to the early phase have achieved a sufficiently high level of knowledge. That concerns the failure of an oxide shell, oxide flowering in the case of high thermal stress, and interaction of molten absorber material with its cladding as well as with the cladding of the fuel rods and potential canister walls.

With respect to oxidation, there is insufficient knowledge about the behaviour of UO_2 under oxidizing conditions (steam or air). A possibly important deficiency is also the behaviour of the reaction products of the oxidation of B_4C within the reactor coolant system (production of methane).

For some scenarios, the heat transfer to the steam generator secondary side significantly influences the overall timing of the scenario. In the case of non-condensable gases, the used heat transfer correlations are not sufficiently validated and potential stratification of steam and non-condensable gases is not treated explicitly.

Higher uncertainties also exist for the release of less volatile fission products. With respect to the deposition of fission products and their resuspension, both volatile and less volatile ones, the models may not be good enough for containment bypass scenarios (e.g. steam generator tube rupture or, more importantly, for interfacing LOCAs).

The phenomena involved in melt relocation, such as candling, impact of spacer grids and the formation of metallic blockages, are known in principle and adequately modelled.

The behaviour of a molten ceramic pool is described usually by empirical correlations and compared with deficiencies related to the formation of a molten pool sufficiently exactly.

With respect to the phenomena related to the behaviour of a debris bed or molten pool in the lower plenum, the following ones are related with only medium knowledge: heat transfer within and from a debris bed, heat transfer from a molten pool to the lower head wall.

4.3.3. Phenomena only partially understood (low level of knowledge)

Although there has been enormous progress since the late 1970s, in both understanding and the ability to analyse severe accidents, there are still several technical issues that have not yet been resolved which may have an important impact on future analysis activities, particularly in terms of successfully managing severe accidents.

Phenomena listed here are characterized by parametric models and an insufficient state of validation.

The reflooding of a hot core is well understood with respect to thermohydraulic behaviour. In contrast to it, there are still open questions with respect to the hydrogen production (e.g. loss of protective oxide shell) and additional R&D is necessary. The more the core is degraded, the less reliable data are available with respect to the thermohydraulics. Of course, if the thermohydraulics during reflood of a degraded core is not sufficiently known, one cannot expect a reliable simulation of the related hydrogen production. For the time

being, the user is forced to assess the uncertainties based on engineering judgement. A further phenomenon which may also become important during reflood is a potential recriticality of a partly degraded core (i.e. a core with fuel rods but no control rods due to early meltdown of the latter one). The uncertainties lie in the knowledge about the state of the core at the beginning of the reflood as well as in the behaviour of the fuel rods during quenching.

The flow behaviour of the fluid (steam) during the degradation of the core has an important impact on the availability of steam for the oxidation of zircaloy and steel. After the formation of blockages or the failure of the core baffle, flow diversion occurs and leads probably to locally steam-starved conditions. A proper nodalization (cross-flow) is strongly recommended.

Due to the lack of adequate large scale experiments, knowledge about the formation of a debris bed and a molten pool (e.g. collapse of fuel rods, radial spreading, size of particles, porosity of particulate debris bed, steam flow through a debris bed, relocation of upper core structure) is very low. Therefore, even detailed codes must use some parameters to enable sensitivity studies.

Another weak point in the late phase core degradation is the behaviour of a molten pool (e.g. stability of the crust, potential break of the crust by relocation of the upper core structure) in the core region. Significant uncertainties also exist with respect to the relocation mode, for example, whether there is initially a localized crust failure or failure of the lowest support plate; and the interaction of the molten pool with massive core shrouds (e.g. heavy reflector).

The formation and behaviour of a molten pool in the lower head is possibly the weakest point for in-vessel analysis, because more or less all previous uncertainties have been accumulated. Therefore, for any melt stabilization measure (in-vessel or ex-vessel), parametric studies must be performed to obtain suitable boundary conditions for the design.

5. STATUS IN THE MODELLING OF EX-VESSEL PHENOMENA

5.1. CONTAINMENT THERMOHYDRAULICS

The phenomena associated with local compartment pressurization as well as with global containment pressurization are sufficiently well understood to allow the safe design of the containment. A comparison of pre-test predictions with large scale test data indicates that safety margins required by the

regulatory guidelines are, in general, sufficient to warrant a reliable design of the containment systems. Code validation work and, in particular, results of the ISP activities [56] allow this qualitative conclusion to be made.

On the other hand, long lasting processes, which dominate the long term containment behaviour after termination of a blowdown, are less understood [57]. Phenomena such as natural convection, heat exchange with structures, and the formation of temperature stratification inside the containment are generally predicted with large uncertainty margins. This problem has not been too much of a concern for the design and licensing of plants. However, it is important for the assessment of phenomena dominating the results of risk analyses. For this area, additional research has been considered necessary to improve the basis for predicting long lasting containment internal processes and phenomena, in particular, the hydrogen distribution.

The containment is typically modelled as a number of interconnected control volumes or compartments. Within a compartment, the atmosphere is generally assumed to be well mixed. Flows between compartments are driven by the pressure differences. Generally, the flow inertia within a compartment is considered negligible. This is referred to as the ‘lumped parameter’ approach, discussed in more detail in this section. In addition, CFD techniques may be applied to aspects of containment modelling. Alternatively, hybrid models may be used that combine a general lumped parameter treatment with detailed CFD nodalization of specific parts of the containment.

A ‘component’ is a generalized type of a containment subvolume (node) which is used in the modelling of containment phenomena. A component is characterized by its volume and boundaries (surfaces) across which the exchange of mass and energy occurs between volumes and by the composition of the constituents in it. The constituents within the components are gases, liquids and solids. Energy and mass exchange can take place inside a volume (as a source or sink, or as an exchange between the constituents within a volume), at the surfaces between volumes, or between the depth of a volume and a surface or the depth of another volume (emitting or absorbing thermal and gamma radiation).

There are three key components considered in a PWR dry containment: atmosphere, structure and pool. All containment computer codes have models to represent these basic components, and most of the experimental and validation efforts described in this report investigate phenomena associated with these components. Usually, describing an atmosphere refers to a region inside the containment building, however, it can also refer to the normal atmosphere of Earth, external to the containment. The constituents of an atmosphere are predominantly gases, although two phase mixtures, liquid droplets and solid particles, may be present during a transient. The constituents

of a pool are predominantly liquids, although two-phase mixtures, gas bubbles and solid particles, may be present during a transient. In certain cases, one component may transform into another component, for example, water runs onto a structure (dry floor) forming a pool, or a pool is drained away leaving a structure.

The three key components are defined as follows:

- (a) Atmosphere: The open volume or free flow volume for gases. It excludes an originally existing pool of water or a pool of water that may form during an accident.
- (b) Structure: A solid material that communicates with the containment atmosphere or pool through a surface. It may be an external wall or floor that forms the containment system boundary, or an internal wall that subdivides the containment into subcompartments. The structure represents a barrier for the flow of gases.
- (c) Pool: A volume of water that lies on a floor.

Communication between components is through their surfaces. A surface is an interface between the containment atmosphere and a structure, between the containment atmosphere and a pool, or between a pool and a structure. A surface includes the boundary layers of air and water that condense on a solid surface, and through which heat and mass transfer occurs.

5.1.1. Sources and sinks

Sources of mass and energy are defined either externally from user input, or internally through processes modelled in the integral or containment code. Consistent properties are required to ensure energy conservation. Modern containment codes use internal energy as the primary variable considered in an energy conservation equation. Direct sources of heat then increase the internal energy by the amount of heat input. However, when gases are channelled through the model boundaries, work is done on the gas already in the compartment. In this case, the internal energy of the system is changed by the enthalpy of the discharged, or transferred, fluid. Care is also needed to ensure that energy transferred between different systems is correctly accounted for, for example, any heat losses from the primary circuit should be accounted for as heat input into the containment. The radiation heat flux from MCCI should appear as an input for other structures or, if it contains sufficient absorbers, for the atmosphere.

5.1.2. Pressurization and depressurization

The calculation of pressure in a compartment is straightforward if the internal energy and the composition of the atmosphere are known. However, an accurate prediction of the containment pressure requires sufficient nodalization of the containment to account for possible stratification effects, and to ensure that the heat sinks are properly distributed in the (sub-)compartments.

5.1.3. Gas/water cell interflows

The control volumes in a lumped parameter code are connected by junctions. Junctions are used to simulate mass flow between these volumes.

For the description of flow between atmospheres in control volumes, atmospheric junctions have to be defined between these volumes. These junctions can represent either real openings between the rooms (control volumes) or so-called ‘virtual junctions’ between the control volumes subdividing a real physical volume. For each atmospheric junction, different flow models can be chosen for modelling, for example, models based on an incompressible transient momentum equation, an incompressible steady state momentum equation, or an orifice flow model.

For the simulation of the liquid flow from one control volume to another, drainage junctions are needed. For the description of a downward flow, the drainage via an opening in the bottom of a volume and the drainage along a wall considering the interaction between water flow and structure surface have to be modelled. The latter one is needed, since during severe accidents a large amount of water flows down along wall structures, resulting in a possibly strong interaction between the existing water film and the structure surface, for example, if a part of spray water reaches more or less directly structured surfaces. Furthermore, the sump mass balance has to be considered.

5.1.4. Heat and mass transfer

The most commonly investigated processes within the containment are those involving heat and mass transfer. The resulting energy exchange between the atmosphere, the pool and the structures controls both the pressurization of the system and the resulting flows which will contribute to the mixing of the atmosphere (or the partial displacement of the existing atmosphere). This exchange takes place both within and at the boundaries of components. For a solid component, the interior process is conduction. As solid components form a major heat sink, it is important that structures be sufficiently discretized to account for the developing thermal profile.

For a fluid component, the interior processes usually are convection but they can also include conduction and diffusion under certain circumstances. Suitable correlations are required for both forced and natural convection. Models should account for condensing conditions on structures.

Aerosols and sprays can exchange energy and mass with the atmosphere through evaporation or condensation or through sensible heat transfer. Condensation and evaporation also are important processes at the interface between the atmosphere and other types of components: structure and pool. Condensation and evaporation represent a combination of mass and latent energy transfer processes. The exchange of energy without an accompanying exchange of mass is classified as a sensible energy transfer process.

Thermal radiation may also be a significant heat transfer process, particularly when there is hot debris in the compartment or there is a hydrogen deflagration. In addition, radiative cooling may be important in aerosol processes; aerosols also absorb and scatter thermal radiation. Models of various levels of complexity are available. Where radiative heat transfer is a significant process (e.g. in the reactor cavity during MCCI), the use of a net enclosure model should be considered.

5.1.5. Hydrogen issues

5.1.5.1. Overview

One of the objectives of analyses for non-inerted containments is to address the risk posed by the burning of hydrogen and other combustible gases generated in the severe accident. Codes may also be used to assess relevant mitigation strategies, such as the installation of passive autocatalytic recombiners or post-accident inerting. The demands for addressing these issues require the complexity of the containment model, as the combustion process depends on the local concentrations of the gases. There may be the need to supplement analyses performed using lumped parameter codes with more detailed CFD models for deflagrations. In addition, if the potential for a hydrogen detonation is established, there may be a requirement to address the consequences using a combination of CFD and structural analysis tools.

5.1.5.2. Sources of hydrogen and combustible gases

As discussed in Section 2.2.1, hydrogen is generated both inside and outside the reactor vessel. If an integral code is used, this should include models for all important hydrogen sources. If separate codes are used for in-vessel and

ex-vessel processes, there is a need to ensure that there is a consistency of treatment. Care is required to ensure that all sources of hydrogen are accounted for, as some codes have typically omitted hydrogen production during melt relocation passing through steam or water. In the absence of sufficiently validated models, these processes may need to be treated parametrically. Concurrent steam release to the containment should be treated in a consistent manner. It is particularly important to ensure that reinforcing steel in the concrete basemat is properly accounted for as, during an MCCI, this provides a continuing source of steel that will then convert steam and carbon dioxide into combustible gases.

The long term source of hydrogen from radiolysis is omitted in many codes. This may not be significant compared with the other sources of hydrogen, however, it is also a means of supplying oxygen into the containment. It is, therefore, desirable to include models; radiolysis can be estimated by considering the activity in the sump.

5.1.5.3. Hydrogen and oxygen distribution

The distribution of hydrogen and oxygen in the containment is determined by the location of the sources and by the transport processes discussed in Sections 3.1.4 and 3.1.5. For a realistic assessment, it is important to: (i) minimize the effects of numerical diffusion; and (ii) consider plume effects that may lead to incomplete mixing near the source. Attention should be given to the possibility of recirculation flows in a series of linked volumes that will increase the mixing. In the past, for example, in some ISPs, it became obvious that lumped parameter models may have problems in predicting the timing and location of atmospheric and temperature stratification. Though it is not a general problem of lumped parameter models, it should be clearly stated that some experience in handling the code and detailed knowledge of the specifics of the containment are necessary, especially in elaborating an adequate nodalization. Here, support from the use of CFD models may be helpful. CFD, or more general fluid dynamic concepts, may be useful in addressing issues of plume behaviour and associated entrainment. The CFD models should account for the proper geometry of the containment volumes, including obstacles and, therefore, should preferably be fully three dimensional. The use of CFD to address combustion issues is discussed further in Section 5.1.5.5.

Combustion and recombiners will reduce the hydrogen inventory. Note that after combustion, the fractional oxygen content of air will be decreased and this should be reflected in the modelling.

5.1.5.4. *Potential for ignition*

In general, limiting conditions for the possibility to burn mixtures of hydrogen, oxygen and steam as reactants and other arbitrary admixtures of nitrogen or other gas components are important. Some measurements related to these conditions exist, but not for all the required range of concentrations. Existing measurements in the literature have to be adjusted in a form that can be used in a code. Additionally, it has to be considered that the conditions (temperature, pressure, gas composition) may be very different from the experiments. Therefore, it is necessary to define some safety margins (e.g. use of margins for the activation of igniters) within the framework of severe accident studies.

The code user may be given the choice as to whether to allow mixtures to burn when the flammability limits are reached, or whether to allow hydrogen to accumulate, posing a greater threat to the containment should ignition occur at a later time. If ignition sources (e.g. operating electrical equipment, high temperature debris) can be identified in compartments with combustible mixtures, it is reasonable to assume that local combustion will occur, with the possibility of then igniting any combustible mixtures in neighbouring compartments. The likelihood of effective ignition sources may be considered as part of a Level 2 probabilistic safety analysis (PSA), and if the containment analysis is performed to support the PSA, consistent assumptions should be used. On the other hand, if the purpose of the calculations is to justify a hydrogen management system, then it may be appropriate to neglect spontaneous ignitions in the analysis.

5.1.5.5. *Hydrogen combustion processes*

Different containment codes model hydrogen combustion with different levels of sophistication. At one extreme, an adiabatic burn model can be used for a containment volume (typically, when an integral code is used). At the other extreme, detailed CFD calculations may be performed. More detailed models for turbulent deflagration can be included in a lumped parameter code using the following approach:

- (a) The combustion model assumes a flame front, which separates the burnt from the unburnt gas. The flame front penetrates the unburnt region; the burning velocity is calculated using an empirically based model.
- (b) The burnt and unburnt regions are assumed to be in different thermodynamic equilibrium states. The combustion heat is released into the burnt part. During combustion, heat transfer to the walls occurs by radiation

from the hot steam and other polyatomic species on the burnt side; convection is also considered. Mass and energy flows across the room boundaries can take place at any time from both parts. As the deflagration processes to be investigated are slow compared to the sound velocity, complete pressure equalization between the two varying parts (burnt and unburnt region) is assumed.

- (c) The model takes into account only the net changes in the masses of hydrogen, oxygen and water on both sides of the flame front. Diluent portions of other materials remain unaffected by the chemical reaction.
- (d) Buoyancy effects are not explicitly modelled, but they are considered via so-called stretching factors. A major influence due to buoyancy can be expected only for low hydrogen concentration. In this case, the effect on pressure buildup is relatively low and not relevant to safety.
- (e) In combination with H_2 , CO will also be burned.
- (f) The system of differential equations for the temperature and volume in the two parts of the room can be solved explicitly for the volume change. This volume change represents a total volume change composed of burning progress and subsequent thermal expansion. In older models, the gas expansion was either neglected or treated as a constant (density ratio), leading to a considerable underestimation of the resulting flame velocity and to a loss of predictability.
- (g) The total volume change can be understood as the displacement of the flame front acting on a representative cross-section along the actual burning axis. With this assumption, the set of differential equations is complete and can be submitted to the solver. Compared to the situation without combustion, only one new variable — the flame front location — has to be solved and the number of equations increases to two times plus one. The flame front position itself is used to determine the propagation into neighbouring rooms.

The objective of the model is not to represent the processes in detail. The model considers estimates for the total and for the dynamic pressure buildup during deflagration and energy release to the combustion chamber.

The limitations of the lumped parameter concept in terms of combustion are:

- (a) It cannot provide detailed flow field predictions. All processes that depend on these may be restricted in their results. These can be high momentum gas mixing phenomena, combustion, particle flows and others.

- (b) Lumped parameter combustion models, therefore, are only applicable to slow combustion (flame acceleration and deflagration to detonation transition criteria are not fulfilled), with flame speeds not exceeding 200–300 m/s. It may be hard to decide if this condition is fulfilled prior to carrying out a simulation. Special care should be taken during the validation process of the model to fix the application limits.
- (c) Combustion as a very fast and short term process cannot be described in great detail. It is worthwhile simulating combustion with a lumped parameter code, whenever the impact within a large system such as containment is of interest and to get a first idea of the pressure increase and energy input.

A coupling between the simpler lumped parameter concept and complex CFD codes appears to be a very promising way of addressing combustion issues in more detail.

5.2. AEROSOL AND IODINE BEHAVIOURS

As indicated in Section 3, fission products will enter into the containment from the primary circuit break or from the cavity in the case of MCCI, mainly in the form of aerosols. Some of them exiting the primary circuit will, however, be in a gaseous form (i.e. noble gases, such as Xe and Kr), and those which are in vapour form in the primary circuit are supposed to rapidly condense in aerosol form in the containment. Once they reach the containment, they will be transported to different regions of the containment and deposited by different processes, as illustrated in Fig. 1. Modelling behaviour of aerosols thus consists of modelling the evolution of their mass, size distribution, composition (agglomeration and condensation processes), as well as their location (sources, transport and retention mechanisms). Such models, described in the following section, have been originally implemented in MAEROS software and are still used in the majority of existing codes (ASTEC, COCOSYS, CONTAIN, MELCOR).

However, it is important to follow the fission product inventory within these aerosols. Indeed, these aerosols are significantly radioactive and an evaluation of the source term to the environment requires knowledge of their composition (i.e. ^{131}I , ^{137}Cs). Moreover, an evaluation of the heat released by these aerosols (decay heat of fission products) in the different containment locations also requires knowledge of their composition. This decay heat has an important role, as it affects:

- (a) Natural convection and hydrogen distribution;
- (b) Relative humidity and bulk condensation on aerosols;
- (c) Wall surface temperature, wall condensation and total pressure.

Besides the modelling of aerosol behaviour in the different zones of the reactor containment, modelling of the time dependent fission product inventories is usually considered. Decay chains of isotopes are usually calculated, allowing the calculation of a fission product elements inventory for the different 'hosts' of aerosols. These hosts (or media) are usually the gaseous phase (suspended aerosols and fission product noble gases), the aqueous phase (containment sumps), and the walls (deposited aerosols), either immersed or not. Additionally, deposits of fission product on recombiners and filters may be considered.

Precise decay heat and activity is usually calculated by a dedicated module of the system of codes, dealing with the isotope inventory. From these calculations, α , β and γ radiations for fission product elements, as well as fission product element masses, are known and transferred to modules in charge of calculating the thermohydraulic and aerosol behaviour in the containment. This process supposes some grouping from isotopes to fission product elements, and allows exact decay heat released from aerosols in the different 'hosts' to be taken into account.

5.2.1. Aerosol behaviour

5.2.1.1. Aerosol agglomeration

Models usually consider a homogeneously mixed polydisperse aerosol system inside a control volume. The system may be composed of chemically different aerosol components of different sizes. The particle size range is discretized into particle size classes (typically 20). Each size class may be differently composed of the various chemical components. However, all particles of one category have the same component composition.

The process referred to as agglomeration or coagulation describes what happens when two or more particles collide, stick to each other and form a larger particle. The agglomeration rate rises quadratically with the particle number concentration.

In LWR containment, significant agglomeration rates can be expected from about 1 g/m^3 of aerosol mass concentration. Different aerosol agglomeration processes are usually taken into account, including the following processes:

- (1) Brownian;
- (2) Gravitation;

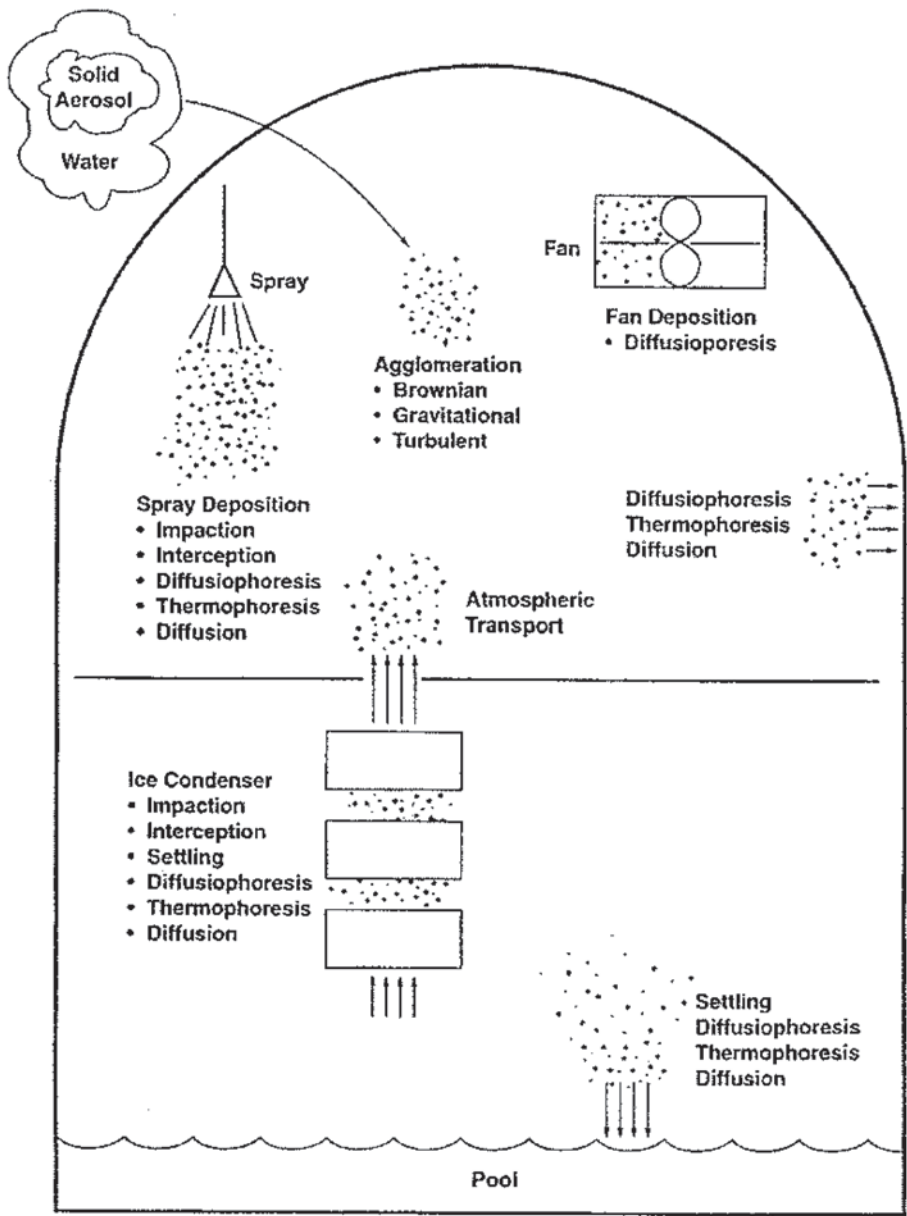


FIG. 1. Aerosol behaviour considered in containment analyses.

- (3) Turbulent shear;
- (4) Turbulent inertial.

The agglomeration processes depend on the physical properties of the gas and of the particles. Because the particles can be highly irregular, it is customary to base the agglomeration modelling on the compact spherical equivalent particle diameter, the agglomeration form factor and the dynamic shape factor.

Particle Brownian diffusion takes place through the Brownian motion of the aerosol particles in the gas atmosphere. The deviation of the particles from spherical form is taken into account with the agglomeration form factor and the dynamic shape factor; for spherical particles, both of them have the value of one. Brown's motion is proportional to the agglomeration form factor and inversely proportional to the dynamic shape factor. The gravitational settling takes into account the collision of large, faster falling particles with smaller, and thus slower, ones. The agglomeration rate increases collision efficiency. The size-class dependent agglomeration and deposition coefficients are obtained by integration across each size category range.

5.2.1.2. Condensation on aerosols

There are two methods for calculating the condensation on the particles: the fixed grid and the moving grid. The latter reduces calculation times and the 'numerical diffusion' compared to the fixed grid method. During the calculation, the grid of the particle size categories apparently moves. In the case of the conventional fixed grid method, growing particles pass through the grid. 'Numerical diffusion' describes the uncontrolled smearing of aerosol mass over several particle size classes in an aerosol calculation. It occurs when a particle size distribution moves in the grid by the growing or shrinking of particles due to the condensation or evaporation of water, and aerosol mass is lost numerically.

In the moving grid model, the 'stiffness' of the equation system is bypassed by the separation of the condensation calculations for the different particle size classes, which is done by keeping the steam concentration in the atmosphere at a constant level throughout the entire time step, the level being represented by the predicted value at the end of the time step. This is possible by the applied iteration procedure. In this way, the thermohydraulic, condensation and aerosol calculations can also be separated.

The moving grid method has models for the hygroscopic and Kelvin effects that are not available for the fixed grid method.

Some aerosols can be hygroscopic, that is, they have the ability to absorb steam molecules of the surrounding atmosphere. When this is sufficient, the aerosol is transformed into a solution whose solute concentration corresponds to the saturation (solubility limit of the solute). The hygroscopic effect is modelled by the chemical activity of the solution, which is determined by the van't Hoff factor. It corresponds to the number of ions, i , into which a molecule of the salt dissociates in an ideal solution (e.g. $i = 2$ for NaOH; for insoluble substances, $i = 0$). Thus, a particle with soluble material will grow faster than a particle with insoluble material. It may absorb water from the atmosphere even if the atmosphere is superheated. Particle growth will continue until the water vapour pressure above the particle surface is equal to that of the atmosphere.

The Kelvin effect considers the effect of the surface tension, which increases the water vapour pressure in the particle over that of a flat surface. The smaller the particle, the greater the surface area to volume ratio of the particle and, hence, the greater the effect of surface tension. For particles of pure water or with water and insoluble material, the increase in water vapour pressure because of the Kelvin effect will result in water evaporating from small particles in saturated environments. For particles with soluble material, the Kelvin effect increases the water vapour pressure in solution over that of a flat surface or solution. Thus, if a flat surface of a solution is in equilibrium with the atmosphere, the Kelvin effect would result in water vaporizing from a particle of the same composition as that of the solution.

With the surface tension, the influence of the Kelvin effect on the particle growth is taken into account. The Kelvin effect depends strongly on the particle size.

5.2.1.3. *Aerosol retention*

Different processes lead to aerosol deposition:

- (a) Settling;
- (b) Diffusive deposition;
- (c) Thermophoresis;
- (d) Diffusiophoresis.

Settling is the deposition of particles on floor surfaces by gravity. As the sedimentation process in a well mixed volume takes place in a thin boundary layer along the surface, all horizontal surfaces serve as sedimentation surfaces. In an LWR containment, sedimentation is generally the most effective deposition process.

Separation through diffusion takes place in the form of Brownian's movement in the concentration gradient on the surface. It is mainly relevant for small particles.

The thermophoretic separation of aerosol particles takes place in the temperature gradient of a boundary layer on a cold wall. In an LWR containment, it only plays a subordinate role since there are no great temperature differences between the dry atmosphere and the wall.

Diffusiophoretic deposition takes place through steam condensation on a cold wall caused by the aerodynamic Stefan flow. This deposition phenomenon can notably contribute to the depletion of suspended aerosols in scenarios where steam condensation on containment walls occurs.

Some aerosol retention may take place in leakage paths of containment penetrations. Under severe accident conditions, containment penetrations might be damaged and aerosols might be released into the environment. In Japan, tests have been carried out to investigate the failure temperature of containment penetrations and aerosol trapping effects along the leakage paths of the degraded penetrations. These tests were carried out using actual containment penetrations in a BWR plant with CsI as a representative aerosol. Aerosol retention along the leakage path was evaluated as a decontamination factor with values from 10 to 1000, depending on the size of the damage. Additional work is needed to assess the leakage and retention through different types of paths, such as containment cracks, and to incorporate adequate models in severe accident containment codes.

Finally, it is noted that when the carrier flow encounters obstacles or channel direction changes, some retention by impaction may arise. Although this mechanism essentially occurs in primary circuit geometries, it may apply to large particles (having larger inertial characteristics) for some thermohydraulic transient where the gas velocity is increased. Such deposition is inefficient for small particles (diameter less than $0.1 \mu\text{m}$). However, a thermohydraulic transient leading to a strong increase of carrier gases may give rise to some mechanical resuspension (e.g. in the case of H_2 combustion). Models used to calculate this resuspension essentially come from resuspension experiments performed for primary circuit wall geometry, not containment walls.

5.2.2. Iodine behaviour

As discussed in Section 3, all fission products which reach the containment are essentially in the form of aerosols, with the exception of noble gases Kr and Xe. Of the condensed fission products, iodine has the potential to form volatile compounds at the containment temperature ($\sim 150^\circ\text{C}$). The extent to which any of the other fission products would be released to the

environment through any containment leakage or failure is, therefore, determined only by the physical behaviour described previously; for iodine, chemistry is of equal or even greater importance. The following aspects have to be considered in an iodine chemistry model [58]:

- (a) Aqueous phase chemistry;
- (b) Interfacial mass transfer;
- (c) Gaseous phase chemistry;
- (d) Surface effects.

5.2.2.1. *Aqueous chemistry*

Iodide aerosols entering the sumps will be dissolved, producing I^- ions in solutions. The chemical reactions which contribute to produce molecular iodine in the sump are thermal reactions and radiation induced reactions.

One very important thermal reaction is the hydrolysis of iodine and its inverse reaction: $I_2 + H_2O = HOI + I^- + H^+$. Under most circumstances, this equilibrium is obtained rapidly, and the equilibrium constant is quite well established and is sufficient to predict the speciation. Iodide may also be thermally oxidized to iodine in the presence of oxygen: $2I^- + 2H^+ + 1/2O_2 \rightarrow I_2 + H_2O$; however, since the counterpart radiation induced oxidation of I^- to I_2 is much faster (see the following discussion), thermal oxidation is unlikely to be important under radiolysis conditions. A similar statement can be formulated for the disproportionation of HOI and the Dushman reaction ($3HOI \rightarrow IO_3^- + 2I^- + 3H^+$ and $IO_3^- + 5I^- + 6H^+ = 3I_2 + 3H_2O$): they are generally too slow to have a significant effect on iodine volatility under radiolysis conditions. So the radiolytic oxidation of I^- is an important process. The extent of this oxidation depends on a number of factors — temperature, dose rate, etc. — the most important of which is the pH of the solution: I_2 production is favoured in acidic conditions.

The I_2 concentration is highly dependent of the presence of silver in the aqueous solution. It has been observed in the PHÉBUS experimental programme that iodine can be trapped in the sump by the heterogeneous formation of silver iodide ($I_2 + 2Ag \rightarrow 2AgI$).

The kinetics database for aqueous iodine chemistry is relatively well established. A few areas exist where there are uncertainties and essentially concerning organic radiolytic decomposition, ‘managing’ the pH behaviour.

5.2.2.2. *Interfacial mass transfer*

I₂ is reasonably volatile and can pass from the aqueous phase into the containment atmosphere. The rate of mass transfer is usually expressed from the theory of boundary layers ('double film theory'), introducing gas phase resistance, k_g, liquid phase resistance, k_l, and the overall mass transfer coefficient, k_m:

$$\frac{1}{k_m} = \frac{H}{k_g} + \frac{1}{k_l}$$

where H is the partition coefficient between aqueous and gas phase, specific for each species.

k_m shows a small dependence on the nature of the species and depends more strongly on thermohydraulic conditions within the stagnant boundary layers at the interface. Over the course of the accident, the aqueous–gas mass transfer is likely to evolve. There are uncertainties in evaluating these mass transfer rates and one practical solution to dealing with this is to assume rapid interfacial mass transfer. This assumption is valid under the conditions employed in intermediate scale studies because this rate is, in general, faster than the rate of change of iodine in the aqueous phase and, therefore, is not rate determining.

5.2.2.3. *Gaseous phase chemistry*

The main chemical forms of iodine that are likely to exist in the gas phase are molecular iodine and organic iodides. Although some suggest that the volatility of iodine will be determined primarily by aqueous phase chemistry and by surface effects, gas phase reactions may have an impact on the behaviour of iodine in some circumstances. The main reactions in this phase are those with products of air radiolysis (OH radicals or ozone) and the creation of organic free radicals, which react with airborne I₂ to produce organic iodides. The thermal reactions are the thermal organic iodide formation from I₂. There are still some uncertainties regarding these gas phase reactions.

5.2.2.4. *Surface reactions*

The interaction of iodine species with surfaces can also play a role in the determination of iodine volatility (adsorption/desorption processes). Adsorption of iodine on surfaces may significantly deplete both gas and

aqueous iodine concentrations ('passive iodine sinks'). However, despite a large body of literature on iodine adsorption, there are still large uncertainties in modelling these processes. The actual models remain quite empirical: an integral first-order rate is usually deduced from the overall observed adsorption, taking into account the nature of the surface (steel or paintings). Moreover, there is no rigorous consideration of the surface temperature evolution and relative humidity (including condensing conditions) in the adsorption/desorption models.

Another surface effect is the formation of organic iodides from surfaces by direct interaction of sorbed iodine species with painted surfaces in the gas phase. In the aqueous phase, in a radiation field, heterogeneous organic iodide formation can also occur if organic radicals are formed from radiolytic decomposition of the organic coating. These can react with molecular iodine to form organic iodides. The process of understanding these processes is still under way and although some semi-empirical models exist (e.g. the Funke model for the gas phase), they still need extended qualification.

The parameter used to express the overall iodine volatility in reactor safety studies is the iodine partition coefficient defined by the ratio between total iodine concentration in the aqueous phase to total iodine concentration in the gas phase. The models used to evaluate the iodine partition coefficient include all the processes described previously: thermal and radiation induced aqueous chemistry, liquid-gas mass transfer, surface reactions and gaseous reactions. Many of the reactions involved are slow, so the models have to be based on kinetics rather than equilibrium thermochemistry. There are two basic types of model, which differ mainly in their approaches to modelling the radiolytic reactions: mechanistic and semi-empirical.

Mechanistic models, such as INSPECT (United Kingdom) and LIRIC (Canada), include a large number of reactions (several hundreds) to describe the radiolysis of water and the interactions of radiolysis products with iodine species. Radical and intermediate species are included, and the reaction rates are mostly taken from fundamental studies.

Semi-empirical models, such as IODE (France), IMOD (Canada) and IMPAIR (Germany), model the radiation effects with a small number of reactions (~20) which aim to describe the most important effects without considering intermediate species. The rate constants are derived from experimental studies.

In the frame of an ISP 41, there was an opportunity for code users to assess their codes over a wide range of accident conditions, such as pH, dose rate, initial iodine concentration, temperature, the effect of condensing or non-condensing atmosphere, the presence of organic impurities, the presence of painted surfaces and the presence of silver. The parametric study identified

several areas of discrepancy between the various codes. Most of the discrepancies are quantitative in nature, that is, the codes agree regarding the trends, but the actual amount of volatile iodine predicted by each of the codes varies considerably. The largest source of the discrepancies between code predictions appears to be the differences in modelling the formation and destruction of organic iodides in each code. Another major actual uncertainty is the importance of the ozone strongly influencing the type of iodine species in the gas phase.

5.3. MELT BEHAVIOUR

Melt behaviour in the containment can be very complex. Integrated severe accident and containment codes have concentrated on molten corium concrete interactions. In addition, some have included models for high pressure melt ejection and direct containment heating. Although parametric type models have been included to address issues such as melt coolability, such assessments have typically been based on separate effects analysis or engineering judgement. Melt spreading has also been addressed primarily by stand-alone models.

Codes should model both the thermohydraulic aspects of the melt behaviour and the fission product behaviour, as the latter determines the heat source for long term ablation and provides input into the potential release to the environment.

5.3.1. Melt release

Melt release characteristics are to be determined by the detailed in-vessel codes, or the in-vessel parts of the integral codes. As some of the debris may remain in the reactor vessel after failure of the lower head, it should be possible to continue the in-vessel calculation beyond vessel failure. Feedbacks from containment phenomena should be considered as appropriate, for example, the effect of containment (cavity) pressure on the discharge, external heat-up of the lower head, flows of air and off-gas through the failed vessel.

Where it is a requirement to consider the survivability of a structure at vessel failure, specific models can be developed to consider the thermal loading from jet impingement and the estimate of blowdown forces. Validated models for jet impingement heat transfer, which may be incorporated with material interaction models have been developed by the Royal Institute of Technology, Stockholm [59].

5.3.2. Direct containment heating

The first models for DCH were of the bounding type. The intention was to delineate that part of parameter space (melt mass, metal content, melt temperature and failure pressure) where a threat of containment failure might exist. The specified conditions are equivalent to a certain level of energy injection into the containment atmosphere. The response of the containment was then evaluated, taking account of previous pressurization and the possible contribution of hydrogen burns. For some plants this approach, either by itself or coupled with a probabilistic approach for the input variables, was sufficient for resolution of the DCH issue. However, this approach proved to be too conservative for most applications and there was a need to develop more representative models. These require a more mechanistic approach to the HPME phase of the accident.

Following vessel failure, depressurization occurs in two phases:

- (1) Liquid melt is ejected. There is little reduction in pressure during this phase.
- (2) When the level of liquid melt above the failure site has fallen sufficiently, the steam/hydrogen mix from the primary circuit will be discharged. If the system pressure has remained above the accumulators' set point, water may be discharged into the vessel during this phase, producing more steam (in most cases, accident management actions will have already been taken to bring the system pressure below the set point prior to vessel failure) increases. Blowthrough will precede the single phase gas discharge.

Although there is some uncertainty on the blowthrough condition, the depressurization transient can be calculated straightforwardly, provided the initial condition and hole size are known. Although the initial hole size is likely to be uncertain, some of this uncertainty will be removed by hole ablation. Well established models are now available for hole ablation based on experimental work at the Royal Institute of Technology, Stockholm [59]. The gas blowdown will be through the final diameter hole (typically 0.3 m).

Very complex flows are likely to develop, depending on the discharge location and the geometry of the cavity, and adjacent subcompartments. In some plants, the debris is expected to be blown along the instrument tunnel and then entrained; where there is no instrument or inspection tunnel, venting is likely to be through the annular space around the vessel itself. In principle, multiphase CFD codes, similar to those developed for pre-mixing studies (see Section 5.3.4) could be used to predict the gas flow and the entrainment of melt. However, given the lack of validation of codes for this purpose, and the

uncertainties in failure location, efforts have concentrated on using the experimental database to support and benchmark relatively simple models.

Even though blowdown times are longer with small exit holes and the velocity on the cavity floor is governed by the exit velocity out of the reactor pressure vessel hole, the velocity in the lower cavity does not change much because a recirculating flow occurs. Therefore, the entrainment rate of melt from the lower cavity to the annular space will not differ greatly for different hole sizes. The debris entrainment time is expected to be in the order of 0.1 s or less, as seen in the CE test series with much longer blowdown times. A longer gas blowdown does not increase the dispersal out of the lower cavity into the annular space. The velocity in the annular space around the reactor pressure vessel, however, will be larger given a larger hole diameter.

The threshold for particle levitation up the annulus is based on the Kutateladze number with the limiting value of 14 for levitation.

The so-called two cell equilibrium model assumes that debris–gas interactions in the cavity are limited to that portion of the blowdown gas that is coherent with the dispersal process. The ratio of the characteristic dispersal time to the characteristic time constant of blowdown is termed the coherence ratio. The coherence ratio determines how much blowdown gas has been vented from the reactor coolant system on the same timescale as debris dispersal. Smaller values of the coherence ratio mean that the primary heat sink for debris–gas thermal interactions is smaller and that metal–steam reactions are more likely to be steam limited.

Pilch developed a correlation for the coherence ratio based on momentum considerations. The constant factor in the coherence correlation takes on different values for different cavity designs. The fraction of blowdown gas that is coherent with debris dispersal can be estimated for an isentropic blowdown of the reactor coolant system.

The two-cell equilibrium model can also be used to estimate hydrogen production for the high pressure melt part of the sequence. Firstly, hydrogen is produced from the dispersed reactive metals, subject to a possible steam limitation. However, the possibility of atmospheric steam interacting with the molten debris droplets as they are ejected out of the cavity and also during the fallback should be considered. Another potential source for hydrogen production is iron oxidation. Further possible sources of hydrogen production are cavity condensate water, hygroscopic parts of the melt, and concrete decomposition. The melt remaining in the cavity can contribute to long term hydrogen production.

The pressure increase caused by the primary system blowdown, the heating of the discharged gas by the debris, and the chemical energy from oxidation of the dispersed debris can be estimated using the two-cell

equilibrium model. Alternatively, containment codes can include models that account for the input of hot gas and the effects of particles injected into the containment atmosphere [60]. In experiments, the difference between this pressure rise and the measured peak pressure rise must be due to hydrogen combustion. If a complete and adiabatic burn of the hydrogen is assumed to produce the pressure difference previously mentioned, lower and upper bounds of the number of hydrogen moles burned during the event can be estimated. Equilibrium calculations performed with the two-cell equilibrium model essentially assume an instantaneous production, but additional hydrogen production probably occurs during the interval that molten debris is suspended in the atmosphere.

In some cavity geometries, the mitigating processes resulting from debris trapping in subcompartments will not apply and most of the melt will be dispersed directly to the upper dome of the containment. Thus, there is the need to consider the specifics of the plant design, preferably using scaled model tests.

Two potential processes used in the two-cell equilibrium model have been identified which yield non-conservative results, both related to hydrogen combustion. If the ratio of the energy release rate caused by hydrogen combustion to the energy loss rate caused by heat transfer from the atmosphere to containment structures is less than unity, hydrogen combustion (even if it occurs) will not contribute to peak containment pressures. In two-cell equilibrium, the hydrogen combustion energy release rate is essentially a function of the amount of hydrogen predicted to combust and the predicted effective flame speed. The effective flame speed may be based on debris to dome time of flight to obtain a conservative overprediction of the pressurization.

5.3.3. Coolability

Coolability, if treated at all in system codes, tends to be assessed in a parametric manner. For example, the analyst may invoke a heat removal rate equivalent to a fraction of the critical heat flux for the relevant geometry. Melt-water interactions have been mainly treated by separate effect codes developed for the pre-mixing stage of fuel coolant interactions. Examples of such codes are IFCI, PM-ALPHA, TEXAS, COMETA, IVA-KA, JASMINE, MC3D and CHYMES. Some of these codes are restricted to the pre-mixing phase, others attempt an integrated treatment of the whole fuel coolant interaction.

Most of the codes mentioned solve the multiphase equations in two spatial dimensions for a minimum of three phases: water, steam (including non-condensable gases) and melt. The melt is usually assumed to be present as a particle field, although some codes also treat a continuous 'jet' phase. The

phases are not assumed to be in mechanical or thermal equilibrium with each other, so there is the need to incorporate models for the constitutive physics, such as heat transfer coefficients and drag coefficients. The relations used for the constitutive physics depend on the volume fractions of each phase, either in a continuous manner or through the use of flow regime maps. Although significant efforts have been undertaken to validate the constitutive physics in the codes, this effort is incomplete. The codes have been applied with some success to the modelling of the FARO-LWR melt–water interaction experiments. However, even knowing the results beforehand, there has been considerable variation in predictions.

Separate efforts have concentrated on the stability of jets, taking linear stability theory as a starting point. Critical wavelength and energy based methods are then used to estimate the resulting particle size. An example of this approach is the IKEJET model. Although reasonable agreement with experimental data has been obtained by invoking an effective medium around the jet that includes debris fragments, this approach is still primarily a research tool.

There have been attempts to include jet break-up in the CFD multiphase codes. However, special techniques are required to track the jet interface with the other components.

The actual status of such codes is demonstrated by the results of ISP 39, which was an ‘open’ exercise based on FARO Test L-14 on Fuel Coolant Interaction and Quenching. Particular emphasis was given to vessel pressurization, pre-mixing, debris formation and cooling, quenching and steam production rates, and quantification of the hydrogen formation rate. Major findings of the ISP benchmark were:

- (1) In view of the ‘open’ nature of the exercise and the considerable scatter of the calculated results, it was concluded that the codes had not yet demonstrated acceptable accuracy.
- (2) The released energy and resulting vessel pressure is, in general, too low, a result attributed to energy partitioning between steam/water phases in non-equilibrium, which indicates that the codes were conservative with respect to coolability.
- (3) The origin and impact of hydrogen production on the quenching phase are unclear.
- (4) There are great differences in calculated vapour void fraction and melt particle distribution at a given point in time (typically 0.9 s).
- (5) Code user effects on calculated results were evident from multiple use of the same code and from supplementary sensitivity analyses on effects of ‘tunable’ parameters.

The analyst may avert the difficulties of the jet break-up phase by referring directly to the FARO-LWR data, which indicate a substantial increase in the surface area available for interaction between the melt and the coolant as melt is poured into the water. However, this is limited to pours of a maximum nominal diameter of 0.1 m; and only pours with a diameter of 0.05 m lasted sufficiently long to be sure that the results were not dominated by leading edge effects.

Once solid debris forms, the prospects of it remaining coolable can be estimated by a number of models. Those based on the theory of two-phase flow in a porous medium, for example, as developed by Lipinski, offer the best physical basis, and have substantial validation for well mixed debris beds.

5.3.4. Fuel coolant interactions

Although extended experimental as well as analytical programmes were performed over about 25 years, the capability of the present analytical models to predict fuel coolant interactions is very limited. None of the numerous models is part of any comprehensive containment code, but they are used as stand-alone codes, to obtain information about the magnitude of the possible energetic event and thereby estimate the extent of the possible damage inside or to the containment. Such codes have to simulate pre-mixing of the melt and the coolant, triggering, propagation, etc., and the hydrogen generated in the course of the interaction. The pre-mixing codes have been discussed above. In some cases (IFCI, TEXAS, IVA, MC3D), the pre-mixing codes also have capabilities to model the propagation phase. Alternatively, separate models have been developed for the propagation phase, including ESPROSE-M, CULDESAC and IDEMO. There is no physically based treatment of a spontaneous trigger, so the proto-explosions have to be triggered by artificial increases in fragmentation. Code results can be highly dependent on the constitutive physics, particularly the amount of coolant that is associated with the debris. Typically, detailed models have been used to study the propagation phase of the FCI. Following the passage of the pressure wave through the mixture, work on the surroundings is performed by expansion of the mixture. Experimental data suggest that this conversion of released thermal energy to work is inefficient, indicating that non-equilibrium processes should be modelled.

If there is an intention to combine an FCI model with a comprehensive containment code, it is recommended to incorporate one of the present FCI models not in a fixed way, but in a loose one, so that the FCI model could be improved with a limited effort, whenever it seems advantageous.

5.3.5. Molten corium concrete interaction

Models for MCCI were included in the first severe accident codes, for example, MARCH. The models were subsequently developed taking account of results from tests with prototypic concrete, but mainly simulant melts performed at Sandia National Laboratories, USA, and the Best Estimate Programme at Karlsruhe, Germany. Subsequently, the ACE and MACE consortia have supported MCCI tests with prototypic melts at Argonne National Laboratories, USA. Examples of current MCCI codes are CORCON-Mod3 (also incorporated into CONTAIN and MELCOR), WECHSL, COSACO, the DECOMP module of MAAP and CORQUENCH .

There have been a number of benchmarks performed to assess code performance. For example, in simulating the German best estimate TA V3.3 experiment, the available codes produced significantly different results for concrete ablation: versions of the CORCON code calculated 27–42 cm of vertical concrete ablation, WECHSL 36 cm, but MAAP-DECOMP only 13 cm. Melt temperature predictions for the ACE Phase C experiments show a similar diversity.

The MCCI codes have, in general, been developed from the mechanistic viewpoint. Subprocesses have been identified (e.g. bubble induced convective heat transfer), with attempts to quantify them in separate effects and integral experiments. An alternative approach has been used to consider the impact of uncertainties on containment loading — a basic heat balance was used to partition heat input between concrete ablation and containment heating. The partition was treated in a parametric manner, to demonstrate that claims for containment robustness were not dependent on the details of a specific MCCI model [61].

A reliable MCCI code/model has to address the overall phenomenology of MCCI, including the corium coolability issue in various geometries, for example, reactor pit and neighbouring rooms, and with any substrate material; such a code will be composed of the following submodules or models:

- (a) Cavity evolution model;
- (b) Ablation of a substrate of any composition, i.e. concrete, zirconium or multilayer;
- (c) Relocation and/or spreading of melt;
- (d) Handling more than one (in different geometries) in parallel but without any interaction between pools;
- (e) Pool heat transfer and swelling models;
- (f) Building the crusts at the interfaces with liquid/solid segregation;
- (g) Solid, liquid and gas chemistry;

- (h) Gas release model for combustible (H_2 , CO) and non-combustible gases;
- (i) Influence of the water;
- (j) At the top by injection;
- (k) Molten pool stratification and layer mixing;
- (l) Convective and radiative (with absorbing media) heat exchange with the water pool or cavity structures;
- (m) Heat conduction through the basemat;
- (n) Models related to the coolability issue: treatment of upper crust thermo-mechanical behaviour and water into the crust, melt eruption phenomena, debris cooling;
- (o) Aerosol release model, which could predict the heat exchanged by the corium with the cavity and have an impact on the aerosol behaviour in the containment.

Moreover, an assessment of fission product release during MCCI could be obtained indirectly using a thermochemistry code which should be coupled with the thermohydraulics code. Although it has a consequence for the MCCI phenomenon, it is mentioned here because its impact on the source term may be significant.

The current status of MCCI codes is considered broadly acceptable for the initial stages of the interaction in dry conditions. However, the long term predictions for dry conditions are considered less reliable because of uncertainties in the partition of the heat flux between the downward and radial directions. Current MCCI models concentrate on the interaction with the concrete in contact with the melt. There is a need to consider the effect of radiation from the top surface of the melt on concrete or steel structures above the top of the melt. This may be achieved by the use of view factors for radiation transport, together with thermal penetration modelling of the walls.

Differences between code predictions are much more striking for wet cavity conditions — reflecting fundamental differences in the views of the code authors. At one extreme, it is assumed in models such as CORCON and WECHSL that an impervious crust forms across the top of the melt. The main role of water is then to provide a guaranteed heat sink; if a crust would form anyway (e.g. because of radiative cooling to colder structures), the presence of water would have a negligible effect on ablation. At the other extreme are models such as DECOMP, where it is normally assumed that the overlying water will remove a fixed heat flux from the melt. Once the upward heat flux generated by the MCCI is less than this value, quenching of the debris will start. The MACE experiments were intended to resolve this issue, but although they show aspects of cooling not captured in codes such as CORCON, it was not conclusive and their interpretation remains a matter of debate.

5.3.6. Relocation of melt and spreading

As melt relocation and spreading has been studied as part of the debris retention strategy for proposed future reactors, there has been a significant effort to develop detailed models of the processes. The resulting codes have been validated using experiments in a number of facilities, including FARO and COMAS experiments with real materials. A number of approaches have been used for the development of the spreading codes:

- (a) LAVA and THEMA solve the mass, momentum and energy balance equations integrated over the flow height, reducing the dimensionality of the problem.
- (b) CROCO solves the two dimensional Navier-Stokes equation in one horizontal (Cartesian or axisymmetric) direction and the vertical direction with a free surface; a thin film approximation may be used.
- (c) CORFLOW solves the two dimensional or three dimensional Navier-Stokes equation with a free surface.

Models are required for the immobilization of material by crust formation and for the increase in viscosity as the melt freezes. Some codes allow a non-Newtonian flow model (Bingham fluid) in addition to the usual Newtonian treatment.

The general performance of these codes is considered satisfactory, and some discrepancies with experimental results may be partly attributed to experimental uncertainties. The actual understanding of the melt stabilization process is that the stopping might be due to the growth of a low temperature, highly viscous boundary layer at the leading edge. None of the codes presently simulates the mechanical stability of the front crust, but all of them take credit from the increase in viscosity or the yield stress near the freezing temperature [58].

Melt spreading under dry conditions is well understood. There are only a few experiments considering spreading under pre-flooded conditions. It has been found that shallow water (typically 10 mm deep) had only a minor influence on the spreading. In this case, the models for spreading in dry conditions can be adapted. Currently, there are few relevant data for deep water pools. It may be possible to predict the initial spreading, but subsequent behaviour if melt continued to accumulate is less certain. Tests with a binary oxide ($\text{CaO} + \text{B}_2\text{O}_3$) spreading under water show that the upper surface of the spread melt was a fragmented structure, and that spreading was predictable, provided the upward heat removal rate was estimated correctly. It is still a

matter of judgement as to what height corium would respread under water (e.g. after a partial quench); estimates are from 0.2 m to in excess of 0.6 m.

5.3.7. Interactions with refractory and sacrificial materials

Models for the interaction of melt with refractory and sacrificial materials are required to assess the performance of core retention concepts. In principle, MCCI models may be appropriate, provided that they contain the full range of heat transfer processes (including natural convection) and that they fully represent possible chemical interactions between materials. However, it has been recognized that MCCI codes have typically only treated the condensed phase chemistry in a simplistic manner. This shortcoming has been addressed by the work of Seiler and Froment [59], who have considered the quasi-equilibrium conditions for a melt pool enclosed by a cool boundary. In this quasi-equilibrium, the interface temperature between any crust and the liquid pool is the liquidus of the remaining liquid. The concept of the chemical equilibrium of solid and liquid phases at interfaces can also be applied to the interaction of melts with refractory or sacrificial materials. It should be noted that the formation of eutectics or low melting point compounds may reduce the effectiveness of refractory materials as a thermal barrier.

Validated phase diagrams are required to apply the methods of Froment and Seiler. Phase diagrams may be constructed from thermochemical models of the melt. These are optimized using existing data for binary and more complex systems. The phase diagrams can then be used to estimate properties, such as density, which will have an impact on melt segregation, and thus heat transfer from the debris to the containing structures.

It is also necessary in some circumstances to consider whether full chemical equilibrium is established in a stratified system (e.g. where a refractory ceramic liner is protected from a ceramic melt by a metal layer). In these cases, consideration of the diffusion of species through the intervening layer is necessary.

Models for the external cooling of structures may also be required. Correlations for critical heat flux that exist are derived from studies of in-vessel retention. There is a need to consider whether these are applicable to the geometry under consideration.

5.4. MODELLING OF SELECTED ENGINEERING SYSTEMS

5.4.1. General description

As discussed in Section 3, activation of containment engineering systems may have an impact on the containment phenomena: their modelling is of prime importance to simulate the accident progression and accident management procedure.

5.4.2. Systems impacting transport

Fan systems, flaps and doors are equipments which influence the transport in the containment. Their modelling can be as crude as user defined parameters (e.g. time dependent volume flow rate for fans) or can take into account the characteristics of the systems. For fan systems, for example, the model may distinguish between outlet fan systems, where the gas mixture is taken from the different specified containment regions to the environment, and inlet fan systems, where the gas mixture is distributed from the environment to the different specified containment regions. Such system modelling is not handled as a junction model because the flow can be distributed to a lot of regions, usually discretized in 'zones'. Especially for low leakage flow rates, the influence of an inlet or outlet fan system becomes important.

Inside the containment, many different types of flaps and doors exist with very different characteristics. Due to this fact, care should be taken to perform exact simulations of these kinds of technical systems, although simplifications are necessary. The influence of a simulation with doors open and doors closed can be seen from a COCOSYS calculation (influence of doors). The characteristic values for the movement of flaps and doors and the flow through them are:

- (1) Inertia of flap or door given by area, thickness and density;
- (2) Free cross-section as a function of angle;
- (3) Opening pressure difference.

Special attention should be given to the flaps of the WWER-440 reactor type. The confinement of NPPs with WWER-440/230 reactors is equipped with safety flaps working as pressure relief valves to limit the maximum confinement pressure in the case of loss of coolant accidents. These safety flaps (in general, different number and size of the flaps in different units) have an opening characteristic determined by their special damping mechanism.

5.4.3. Systems impacting containment leakages

As activation of filtered venting systems and atmospheric valves constitutes a direct contribution of source term outside the containment, their modelling is of great importance in any source term evaluation calculation.

Simple filter models exist to calculate the removal of aerosols and vapours transported with the bulk fluid flow through filter flow paths. The efficiency of the filters is user defined through the decontamination factor function of aerosol classes. The effect of the filter loading on the flow resistance of the associated flow path can also be accounted for by modifying the laminar loss coefficient, and a maximum loading may also be specified. When this loading is reached, no further aerosols will be removed.

To simulate flow paths controlled by atmospheric valves, a classical junction model may be used, the valve being controlled by the external control conditions. Models also give the possibility to define time periods for opening and for closing the valve, simulating operator actions. For the simulation of a ruptured disc, the spontaneous opening of a flow path by transgressing a failure pressure difference is necessary.

5.4.4. Safety engineering systems

5.4.4.1. *Spray systems*

Different types of models may be used for simulating spray thermohydraulic phenomena:

- (a) A very simple model where constant 'thermal' spray efficiency is assumed: the spray droplet temperature at the end of the path section is calculated proportionally to this efficiency. If the spray path consists of several path sections, this given efficiency is subdivided relative to their height of path zones. In such a crude model, neither droplet size nor velocity are calculated along the falling path.
- (b) A semi-empirical model where the droplet/atmosphere heat transfer equation (condensation/evaporation processes) uses empirical heat transfer coefficients; the advantage of such a model is its low CPU time consumption (from the droplet relaxation expression, analytical expressions are deduced for the droplet falling time and droplet size evolution).
- (c) Mechanistic models which describe the spatial evolution of the droplets (a function of their containment height location), together with heat/mass transfer with the local atmosphere. A temperature and a velocity are thus

calculated for each droplet size class in each mesh. Droplet relaxation is obtained from the resolution of mass, energy and momentum balance equations for each droplet size class within an implicit scheme, while the gravitational agglomeration formulation is issued from the collision efficiency theory. Validation of such a model on analytical single sized droplet experiments gives good results. Although such a model is more CPU time consuming than the two previous ones, it ensures more reliable results.

Similarly to spray thermohydraulic phenomena, different types of models may be used for simulating aerosol and the fission product vapour removal by spray, including:

- (a) A very simple model where a constant 'removal' spray efficiency is assumed: default values of removal rates are provided for direct and recirculation spray modes. However, as capture efficiency depends both on water droplet sizes and aerosol sizes, such a model may be not reliable. Inertial effects are predominant during the first spray period (so not dependent on droplet size), but as aerosol size distribution tends to smaller sizes in a longer period, diffusiophoresis and diffusion processes become dominant. Such processes need a good description of droplet sizes.
- (b) A model which takes into account both mechanical processes (impaction, interception, diffusion) and thermal processes (thermophoresis, diffusio-phoresis) in the removal rate efficiency.

Validation of such models is difficult as there is a lack of large scale experiments.

Concerning gaseous species, some model accounting for droplet relaxation, volatile iodine/droplet mass transfer and iodine species hydrolysis inside the droplet exists. However, uncertainties in mass transfer and kinetic reactions inside the droplet have still to be reduced. Validation work shows that the model does not give good results for acidic pH in droplets combined with high gaseous iodine concentrations.

5.4.4.2. *Suppression pool*

Modelling of such passive systems is essential, for example, for the WWER-440 containment. One of the most used models is the DRASYS model, implemented in COCOSYS and ASTEC codes, which will be described as an example for the simulation of pressure suppression systems.

This model considers three parts: the vent pipe (PIPE), the atmosphere upper pool (GASROOM) and the water pool (POOL). The separate analytical simulation of the three zone parts leads to different zone part behaviour — a quasi-thermodynamic non-equilibrium. The main point of this model is a one dimensional, rotational symmetric fluid dynamic model describing the motion of the water inside and outside of the vent pipe. Water motion initiates a change of volume of the zone parts PIPE and GASROOM. Furthermore, the condensation of steam that flows into the vent pipe in the case of a LOCA increases the water mass and temperature in the water pool and also causes a volume rise. These changes of zone part volumes are used as boundary conditions for the calculation of the thermohydraulic zone part behaviour.

Several models may be used to describe the motion of the vent pipe atmosphere–water pool interface:

- (a) Clearing of the initial water leg in the vent pipe driven by a steam/gas mixture from the pressurized zone in front of the PIPE part;
- (b) Formation of a large subpool bubble at the vent pipe exit filled with non-condensable gas;
- (c) Steady state steam condensation with a small and further decreasing gas content;
- (d) Quasi-steady state steam condensation and the movement of the steam/water interface from inside the pipe to outside (bubble) and back.

The change of motion models depends on the position of the interface automatically. Internal mass and energy flows are considered, i.e. the condensation of steam (from the vent pipe) in pool water, the carry-over of non-condensable gases from PIPE into GASROOM and the flow of incoming water into the pool. Water flow is calculated taking account of flow velocity and gravity.

6. USE OF COMPUTER CODES FOR THE ANALYSIS OF SEVERE ACCIDENTS

6.1. CLASSIFICATION OF SEVERE ACCIDENT COMPUTER CODES

Computer codes used for beyond design basis accidents are often classified into mechanistic codes and parametric ones [6]. Mechanistic codes

are characterized by best estimate phenomenological models to enable, as far as possible, an accurate simulation of the behaviour of an NPP in the case of a severe accident. Parametric codes include a combination of phenomenological and user defined parametric models to simulate the integral behaviour of the whole plant (reactor coolant system, containment, fission product behaviour).

Within the VASA project of the Fourth Framework Programme of the European Union, the classification of severe accident codes was discussed extensively [62]. The participants recognized that the rapid increase of computer performance increasingly enables the replacement of parametric models by mechanistically based ones in the parametric codes. Therefore, the distinction between parametric and mechanistic codes became questionable. It became apparent that a classification based on requirements for different applications would be more appropriate. From the point of view of real application, existing severe accident codes can be classified into three classes: fast running integral codes, detailed codes and special (dedicated) codes.

6.1.1. Fast running integral codes

These codes should be characterized by a well balanced combination of detailed and simplified models for the simulation of the relevant phenomena within an NPP in the case of a severe accident. 'Fast running' may have different meanings but it should be close to real time (on workstations or personal computers), and the analyses of typical scenarios should not last longer than 12 hours.

Fast running codes are primarily not designed to perform best estimate simulations; the objective is rather to allow the user to bound important processes or phenomena by numerous user defined parameters.

Integral codes are usually used to support PSA Level 2 analyses and for the development and validation of accident management programmes. Their models are less mechanistically based but more of a parametric character, i.e. model parameters allow the user to investigate the consequences of uncertainties on key results. These kinds of codes may also have been used for the design and validation of severe accident prevention and mitigation systems, however, to obtain realistic results, a deep knowledge of the involved physical phenomena as well as user experience in performing severe accident analysis is required. Benchmark exercises with mechanistic codes may support the justification. Simplification of the models aims to reduce computation time.

Some examples of fast running integral codes are MAAP, MELCOR and ASTEC.

6.1.2. Detailed codes

In contrast to the integral codes, the strategy for detailed codes is to model as far as possible all relevant phenomena in detail by mechanistic models. Basic requirements for detailed codes are that the modelling uncertainties are comparable with (i.e. not higher than) the uncertainties in the experimental data used to validate the code and that user defined parameters are only necessary for phenomena which are not well understood due to insufficient experimental data (including scaling problems).

Using detailed codes, best estimate analysis can be performed, however, uncertainties also exist and must be consequently quantified. Since, as a principle, they should not have user options, existing uncertainties in the simulation of the different phenomena must be specified to enable the definition of the uncertainties of the key results.

The main advantages of detailed codes in combination with best estimate analyses are to:

- (1) Allow a better insight into the progress of a severe accident;
- (2) Support the selection of appropriate severe accident mitigation;
- (3) Allow the design and optimization of mitigation measures.

Due to the high demand on computation time, mechanistically based codes typically simulate only either the reactor coolant system or the containment. The acceptable computation time depends on the scope of the application but it normally does not exceed 10 times the real time on workstations or personal computers. Another limitation can be deduced from the requirement that computation time should not be a dominant part of the overall project timescale: analysis of a particular scenario should not last longer than one week. The disadvantage of a high demand on computer time decreases continuously with the rapidly increasing performance of computers. ATHLET-CD, ICARE/CATHARE, SCDAP/RELAP5, COCOSYS and CONTAIN are examples of detailed codes. In addition, ASTEC and MELCOR can be considered detailed codes, if the calculation is based on extensive nodalization and detailed model options.

6.1.3. Special (dedicated) codes

In addition to the system codes, other codes dealing with single phenomena have become important in context with the requirements of the regulatory authorities to take into account severe accidents in the design of new NPPs and to reduce uncertainties of risk-relevant phenomena (more

reliable likelihoods for the branches in an accident progression event tree). Depending on their task, they may be simple and consequently fast running, or very complex with the drawback of large calculation time.

Typical issues for which special codes are required include:

- (a) Steam explosion and melt dispersal (e.g. MC3-D);
- (b) Molten pool behaviour (e.g. ADINA-F [63]);
- (c) Heat-up of reactor coolant system structures (e.g. COMMIX [64]);
- (d) Structural mechanics;
- (e) Recriticality;
- (f) Lower head melt retention;
- (g) Hydrogen distribution (local effects);
- (h) Hydrogen deflagration (risk of flame acceleration) and detonation;
- (i) Melt spreading.

6.1.4. Capability assessment of present generation computer codes

For deterministic analyses of severe accidents, different computer codes have been developed in the USA, France, Germany and Japan. Whereas the basic model development of the US codes MAAP [36, 37], MELCOR [38, 39] and SCDAP/RELAP5 [42, 65] was more or less finished a few years ago, the European codes ATHLET-CD [40], ICARE/CATHARE [35, 66, 67] and ASTEC [41] have only recently reached a similar level of development, and are still subject to further developments and improvements to incorporate the recent findings of experimental programmes (PHÉBUS, QUENCH, RASPLAV, etc.).

Besides these codes there are many others (e.g. BISTRO [68], ESCADRE [69], ESTER [70, 71], MARCH-3 [72], MELPROG [73], STCP [74], THALES-2 [75], SAMPSON [76]), however, due to their limited spreading or their replacement by successors, they do not have a comparable international acceptance.

Recently, extensive R&D has been initiated in the Russian Federation to develop severe accident codes (KIT [77], RATEG/SVECHA [77]). Due to their early developmental stage, they are currently not sufficiently validated for full plant analysis.

It is recognizable that partially the same modelling basis is used inside different codes. Regarding in-vessel codes, phenomena-like cladding oxidation as well as chemical interactions are calculated using the same rate equations. Several ex-vessel codes under consideration apply the same modelling basis as the stand-alone modules WECHSL, MAEROS and SPARC, calculating molten corium concrete interaction, aerosol behaviour inside the containment

and pool scrubbing. In addition, the SOPHAEROS module for fission product transport in the primary circuit is implemented in several codes.

Existing stand-alone modules or derived simplified models of them could build the basis for the extension of the system codes under consideration. System codes are codes representing either the reactor coolant system, or the containment, or both.

Furthermore, the experiences from the use of system codes show that for an exact evaluation of the source term inside the containment, detailed calculations of core degradation processes are necessary in order to evaluate the initial conditions for ex-vessel calculations with good accuracy. Thus, the application of mechanistically based in-vessel codes is necessary.

The containment code system COCOSYS represents a coupling of mechanistically based modules describing different ex-vessel phenomena occurring during severe accident sequences. The present extent of modelling covers the determination of the main ex-vessel phenomena. Nevertheless, the implementation of several modules into COCOSYS, calculating phenomena such as ex-vessel spreading and coolability, DCH and deflagration to detonation transition, are on the way. The extent of modelling of the CONTAIN code is comparable to that of COCOSYS, but actually with a much higher degree in validation. Unfortunately, its development was stopped some time ago.

Besides the modelling of in-vessel phenomena, the integral codes ASTEC, MAAP4 and MELCOR are also able to cover ex-vessel severe accident sequences. The ex-vessel part of ASTEC contains equivalent thermo-hydraulic and aerosol models to the containment code COCOSYS.

6.2. REQUIREMENTS FOR MODELLING SEVERE ACCIDENT PHENOMENA

6.2.1. General requirements

The simulation of severe accident propagation in NNPs is required for an analysis of the potential consequences of severe accidents and possible countermeasures (severe accident management measures). Such simulation should be performed in a way that is as reliable as possible; such calculations are referred to as ‘best estimate calculations’.

The first essential requirement is the appropriate choice of physical models and model parameters, for example, heat transfer correlations or type of zone model. Severe accident analyses are best estimate ones only if complete with respect to energy and mass sources and sinks, including fission products in

the form of gases and aerosols and their local distributions. Beyond completeness in the different sources, accurate timing is important. With respect to plant specific thermohydraulics, this means starting the calculation with normal operational conditions. One has to anticipate that thermohydraulic plant analyses will be more burdened with uncertain boundary conditions than analyses of experimental tests.

To be complete means to simulate all phenomena involved in the course of the accident, but also to simulate the interactions between these phenomena. As it is, the objective of installed technical systems — for example, spray systems, catalytic and thermal H₂ recombiners or venting systems — and in order to prevent the progression of an accident or to mitigate its consequences, their adequate simulation is necessary, too.

Another aspect is the material properties. Of course, the code developers should only incorporate well known material properties based on adequate experiments, but the application range must be documented and it has to be ensured by warnings in the code output and careful user checks that the application ranges are not exceeded.

Best estimate calculations need a problem oriented nodalization. The code user has to choose a structural nodalization representing the geometry of the simulated object, for example, the containment with its internals. Although the great influence of the nodalization on containment calculation is well known, there is a trend to minimize the number of nodes of lumped parameter codes or cells of CFD codes, because with an increasing number of nodes or cells, the computation time increases dramatically.

The basis for a best estimate containment calculation is sound thermohydraulics; this means that mixing processes and the timing of formation and elimination of atmospheric stratification have to be handled in the correct way. Simulation of stratification may give rise to problems in lumped parameter approaches; in any case, a good knowledge of the plant or the facility is necessary for the elaboration of an appropriate nodalization. In the future, CFD codes may give some support in this direction. The behaviour of water pools should be included in the thermohydraulics.

Sound thermohydraulics are necessary for a reliable prediction of hydrogen distribution and aerosol behaviour. Hydrogen combustion needs models both for deflagration, and for detonation and deflagration to detonation transient criteria. For source term calculations, not only is it necessary to calculate the aerosol behaviour but also the aerosol sources from the primary circuit/reactor pressure vessel and from the molten corium concrete interaction, the iodine chemistry, and the fission product distribution. It is important to note that beyond sound models for the processes mentioned, the interactions between them have to be considered if best estimate

calculations are to be performed. Some examples of such interactions are the influence of:

- (1) Decay heat on thermohydraulics;
- (2) Humidity on aerosol depletion;
- (3) Atmospheric conditions on iodine chemistry;
- (4) H₂ combustion on CsI decomposition.

Currently, all existing codes suffer on account of the lack of knowledge about resuspension effects from walls as well as from water pools.

The application of the severe accident codes to real accident sequences requires that the risk relevant phenomena for an individual NPP should be identified and the corresponding models in the code should give reasonably accurate estimates of the consequences and the timing of events. In general, there are recognized pros and cons in many accident management issues. Knowledge of the phenomenology during the core melt accident is important, but it is equally important to know the physical phenomena involved in mitigation measures. The measures must be quantified, especially in the timing of their initialization, on a plant specific basis.

Other phenomena (or procedures), such as fuel coolant interactions, DCH, spreading and/or relocation of melt, may have great importance for special questions. It is also necessary to model technical systems, such as spray systems, filters or recombiners, taking into account relevant emergency operating procedures and accident management guidelines.

6.2.2. Required level of sophistication of models for different applications

Based on the character of the envisaged severe accident analyses, a different accuracy in the simulation of the involved phenomena by the corresponding numerical model is required. The following tables provide an indication of the required sophistication (i.e. low, medium and high) of the modelling of the relevant in-vessel phenomena for different applications. Table 1 deals with in-vessel analysis models, whereas Table 2 covers ex-vessel. Table 2 focuses on the use of accident analysis in accident management, and indicates that a required level of accuracy is not higher than for DSAM. By a cross-check of these requirements with the features of the particular codes, it should be possible to select (and to justify) an appropriate code for the particular applications.

It should be mentioned that even for PSA, the use of sophisticated models may be necessary to justify some assumptions or to clarify a specific issue, before using intensively and confidently simpler models.

TABLE 1. MODEL SOPHISTICATION REQUIREMENTS FOR DIFFERENT APPLICATIONS OF IN-VESSEL SEVERE ACCIDENT ANALYSIS

	PSA ^a	AM ^b	DSAM ^c
(1) Thermohydraulics:			
(a) Fluid conditions	L ^d	L	M ^e
(b) Momentum equation	L	M ^f	M
(c) Nodalization	L	M	H ^g
(d) Reflood model	L	M	H
(2) Heat transfer to reactor coolant system structure and steam generator:			
(a) Reflux condenser mode	L	M	M
(b) Natural circulation within RPV	L	M	M
(c) Natural circulation within reactor coolant system loops	M	M	H
(3) Core heat transfer			
(a) Radiation radial	M	M	M
(b) Radiation axial	L	L	L
(c) Radiation from molten pool	L	L	L
(4) Oxidation			
(a) During heat-up	M	M	H
(b) During quenching of a hot-rod-like geometry	L	M	H
(c) Cladding failure	M	M	M
(d) Oxidation during relocation of U-Zr-O	L	L	L
(e) Oxidation during melt/coolant interaction	L	L	L
(f) Oxidation of a particulate debris bed	L	L	M
(g) Oxidation of steel	L	L	L
(h) Oxidation of B ₄ C	L	M	M
(5) Core heat-up and melting			
(a) Ballooning	M	M	M
(b) Formation of eutectics	M	M	H
(c) Dissolution of UO ₂ by Zry	M	M	H
(d) UO ₂ /ZrO ₂ melting	L	L	L
(e) Impact of fuel burnup	M	M	H
(6) Relocation and pool formation			
(a) Cladding failure	M	M	M
(b) Relocation velocity	L	L	M
(c) Heat transfer to cladding	M	M	H
(d) Formation of particulate debris, coolability	L	M	H
(e) Formation of metallic and ceramic blockages, radial spreading, supporting crusts	L	M	H

TABLE 1. MODEL SOPHISTICATION REQUIREMENTS FOR DIFFERENT APPLICATIONS OF IN-VESSEL SEVERE ACCIDENT ANALYSIS (cont.)

	PSA ^a	AM ^b	DSAM ^c
(7) Molten pool behaviour within the core			
(a) Stratification	L ^d	L	M ^e
(b) Heat transfer	L	L	M
(c) Interaction with supporting structures	L	M	H ^g
(d) Melting of structures above the core	L	L	L
(e) Failure criteria for crusts and structures	L	L	M
(f) Relocation of non-molten structures	L	L	L
(8) Fuel coolant interaction			
(a) Melt fragmentation	L	M	H
(b) Melt dispersal	L	L	L
(c) Reactor coolant system pressurization	L	M	M
(d) Steam explosion	L	L	L
(9) Lower head behaviour			
(a) State of the metallic and oxidic melt	L	M	M
(b) Heat transfer mechanisms	L	M	M
(c) Coolability	L	H	H
(d) Lower head failure mode	L	M	H
(10) Fission product release from fuel			
(a) High volatile fission products	L	L	L
(b) Medium and low volatile	L	M	M
(c) Release from molten pool	L	M	M
(11) Fission product transport in the reactor coolant system or connecting lines			
(a) Deposition in main coolant lines	L	M	M
(b) Revolatilization in main coolant lines	L	M	M
(c) Deposition in connecting lines	L	M	M
(d) Revolatilization in connecting lines	L	M	M
(e) Pool scrubbing	L	L	M
(f) Deposition in dry steam generator	L	M	M

^a PSA: supporting PSA Level 2.

^b AM: analysis models.

^c DSAM: design and capability demonstration of severe accident mitigatory and preventive systems.

^d L: low.

^e M: medium.

^f For scenarios with an impact of counter-current flow on timing.

^g H: high.

TABLE 2. MODEL SOPHISTICATION REQUIREMENTS FOR DIFFERENT APPLICATIONS OF EX-VESSEL SEVERE ACCIDENT ANALYSIS

	PSA ^a	DSAM ^b	ST ^c
(1) Thermohydraulics			
(a) Sources and sinks	L ^d	M ^e	M
(b) Pressurization/depressurization	M	M	M
(c) Gas and water flows between cells	M	H ^f	M
(d) Heat and mass transfer			
• In the gas phase	M	M	M
• At the interface between gas and sump	M	M	M
(e) Hydrogen distribution and combustion			
• Sources	M	H	M
• Distribution			
• Deflagration	L	M	L
• Deflagration to detonation transition	L	L	L
• Detonation	L	L	L
(f) Pyrolysis	L	L	*g
(g) Momentum equation	L	L	L
(h) Nodalization	M	H	M
(2) Fission product behaviour			
(a) Aerosol behaviour:			
• Agglomeration processes	L	L	M
• Deposition processes	L	L	M
• Resuspension			
— From walls	L	L	L
— From water pools	L	L	M
• Retention in leakage paths	L	L	M
(b) Fission product transport	L	L	M
(c) Iodine behaviour			
• Gas phase			
— Homogenous reactions	L	L	L
— Surface effects	L	L	M
• Mass transfer between sump and atmosphere	L	L	M
• Liquid phase			
— Homogenous reactions	L	L	H
— Surface effects (including Ag reactions)	L	L	H
• Pool scrubbing	L	L	M

TABLE 2. MODEL SOPHISTICATION REQUIREMENTS FOR DIFFERENT APPLICATIONS OF EX-VESSEL SEVERE ACCIDENT ANALYSIS (cont.)

	PSA ^a	DSAM ^b	ST ^c
(3) Melt behaviour			
(a) Melt release	L ^d	H ^f	L
(b) Direct containment heating	L	M ^e	L
(c) Coolability	M	M	L
(d) Fuel coolant interaction	L	M	L
(e) Molten corium concrete interaction			
• Ablation of concrete	M	M	M
• Behaviour of the corium/concrete pool	M	M	M
• Influence of water	M	H	M
• Gas release	M	M	L
• Aerosol release	L	L	M
(f) Relocation of melt and spreading	L	H	L
(g) Interaction with refractory and sacrificial material	(generally the same as (e))		
(4) Technical systems			
(a) Systems impacting gas transport (fans, doors, rupture discs)	M	M	L
(b) Systems impacting containment leakages (filters, valves)	L	M	M
(c) Safety engineering systems (mainly spray system)	M	M	M
(d) Ice condensers	M	M	L
(e) Recombiners	L	M	L
(f) Igniters	L	M	L
(g) Passive heat removal systems	M	M	L
(h) Suppression pools	M	M	L

^a PSA: supporting PSA Level 2.

^b DSAM: design and capability demonstration of severe accident mitigatory and preventive systems.

^c ST: source term calculation.

^d L: low.

^e M: medium.

^f H: high.

^g The impact of pyrolysis on source term calculation is not known, but it is considered that the iodine chemistry and, to a lesser degree, the aerosol behaviour are affected.

6.3. VERIFICATION AND VALIDATION OF COMPUTER CODES

Once the objective of the severe accident analysis is established, one of the three categories of codes mentioned previously should be identified. Whatever the

selected code is, the user of the codes always has the responsibility to ensure that the codes are appropriate for their use. According to Ref. [6], this includes defining the appropriate levels of modelling detail, documentation, verification, validation and accuracy required for the intended use of the codes.

The documentation for the beyond design basis code usually includes, apart from regular manuals containing user instructions and features of the models of the theory, some manuals for material properties, code developer assessment and validation, and user guidelines.

Code verification is defined as the review of the source coding relative to its description in the document. Since the line by line verification of these large codes is a time consuming and expensive process, this process is limited to those codes which are relatively static and not subject to continued change.

With respect to code validation, all the requirements mentioned previously for a best estimate severe accident code depend on the requirement that the codes and models incorporated in them be well validated. Well validated means:

- (1) Each phenomenon should be addressed in test facilities of different scales;
- (2) Each single model within the code should be validated in separate effects tests, if possible, on different scales;
- (3) The models should be validated in coupled effects tests with regard to their complex interactions and scaling aspects;
- (4) The overall capability of the code should be demonstrated by means of numerous 'blind' pre-test calculations for different types of experiments.

The present status of severe accident codes, including integral codes, is that none of them — not even the leading ones — have the capability to perform best estimate calculations with respect to the overall aspects addressed in the wide spectrum of severe accident scenarios. Nevertheless, there is the possibility to perform best estimate analyses with most of the codes for parts of this spectrum using their specific strengths. Best estimate analysis, in any case, needs the support of appropriate sensitivity analyses for major code applications, thus helping to quantify the variance of code results for particular scenarios.

Interactions and feedback between separate phenomena play an important role in severe accident sequences. This means that validation of models against separate effects tests is not sufficient, and integral experiments benchmarking is also required. Finally, the code must be tested for particular accident sequences for assessment (comparison with plant data from selected transients or accidents). This is especially important when thinking about the living PSA needs, possible needs for equipment qualification under abnormal conditions and needs for accident management evaluations. All these capabil-

ities should be periodically tested in a structured manner and ensure that the code capabilities are maintained for new versions and revisions.

Four sources of data are generally used to validate the codes: phenomenological data, separate effects (component) data, integral data and plant operational data. Since for severe accident conditions, the availability of data is much more limited, phenomenological data are used more extensively to help develop models while integral data are used more for code validation.

Integral data are available for the early phase of severe accidents, but data for the late phase of severe accidents are obtained primarily from separate effects experimental facilities using stimulant materials in many cases. ISPs [56] provide a particularly valuable source of information for code validation, since the experiments are well documented and extensive code to code and code to data comparisons are performed. With the exception of TMI-2 and Chernobyl, plant data are not available for the validation of severe accident models. Because of limited experimental data, code to code comparison and benchmark calculations are also used sometimes as an only option for validation of the codes. For example, as discussed in Volume 5 of Ref. [65], where SCDAP/RELAP5 results were compared to FIDAP, a commercially available CFD code, and ABAQUS, a commercial structural analysis code, comparison of a code to other more specialized codes can be used where limited experimental results are available.

For validation, certain quantities are selected for a comparison of calculations with experimental data. These quantities serve as ‘indicators’ for determining whether or not a code provides satisfactory results, that is, indicators that can be used to measure the ‘level of validation’ of a code. The identification or choice of indicators is, therefore, a crucial step in the validation. The indicators are directly related to the physical driving phenomena of the accident response and are usually those code output quantities which are compared with acceptance criteria in accident analysis.

The problem of scaling of experiments used either for the development or validation of models should be mentioned. Although the experiments use prototypic fuel rods (with a length typically ranging from 0.25 m to full length), most of the experiments in the field of severe accidents use a small number of fuel rods and are thus small scale from a thermohydraulic point of view. Therefore, effects such as natural circulation or radial heat losses are distorted. Only a few experiments, such as LOFT-FP2, which was a scaled PWR, are medium scale experiments. TMI-2 was, of course, full scale, providing insights into the behaviour of a plant during a severe accident, particularly during the late stage of the accident during and following the formation of a large ceramic molten pool. However, the available measurements from TMI-2 gave only a few indications about the accident progression, and an extensive analysis with the support of codes was necessary for a good understanding of what happened during the accident.

The boundary conditions of the small scale experiments are not typical for plant conditions. In addition to the distortion of thermohydraulic conditions, such as natural circulation and flow distributions, for example, the heat losses from small rod bundles to the environment are high and contribute to relatively large uncertainties in the overall energy balance in the experiments. The method of heating of the smaller scale bundles also introduces uncertainties into the results. For example, the axial and radial power profiles can shift unrealistically as control materials and fuel are relocated in the fission heated tests. The power profiles can also shift unrealistically in electrically heated tests. In addition, the feedback between heat element resistivity and temperature result in distorted power peaking. Electrical heater rods can also stabilize the fuel columns and prevent the formation of debris. However, the comparison of results from different experimental facilities and types of experiments, and the use of the codes provide a way of scaling experimental findings up to plant level and of transferring existing physical knowledge to safety analysis and risk reduction.

For validation purposes, the ISPs make basic experiments available to the nuclear community or at least to organizations from OECD member States.

Over the last 25 years, the OECD/NEA Committee on the Safety of Nuclear Installations (CSNI) has sponsored a considerable number of international activities to promote the exchange of experience between its member States in the use of nuclear safety codes and testing materials. A primary goal of these activities is to increase confidence in the validity and accuracy of analytical tools, which are needed for warranting the safety of nuclear installations, and to demonstrate the competence of involved institutions.

ISP exercises are comparative exercises in which predictions or recalculations of a given physical problem with different best estimate computer codes are compared with each other and, above all, with the results of a carefully specified experimental study. ISP exercises are performed as 'open' or 'blind' problems. In an open standard problem exercise, the results of the experiment are available to the participants before performing the calculations, while in a blind standard problem exercise, the experimental results are locked until the calculation results are made available for comparison. Especially the following more recent ISPs should be mentioned here which, on the one hand, should be used for validation but, on the other, also enable code users to improve their ability, to gain experience and to demonstrate their competence:

- (1) ISP 37: VANAM M3: A Multi Compartment Aerosol Depletion Test with Hygroscopic Aerosol Material (influence of thermohydraulics variables, such as humidity and volume condensation on aerosol behaviour);

- (2) ISP 41: Experiments in the RTF and CAIMAN Test Facilities on Iodine Behaviour in Containment and Benchmark Calculations (adsorption/desorption, mass transfer);
- (3) ISP 44: Different KAEVER tests: different types of aerosols and mixtures under saturated thermohydraulic conditions with slight volume condensation (special emphasis on the mixture of Ag–CsI–CsOH aerosols);
- (4) ISP 47: Thermohydraulics tests in the French TOSQAN and MISTRA facilities and the German ThAI facility.

Further ISPs that might be of interest for specific validation efforts are:

- (1) ISP 16: Rupture of a Steam Line within the HDR Containment leading to an Early Two-Phase Flow (HDR V.44);
- (2) ISP 17: Marviken: Pressure Suppression Containment-Blowdown Experiment No. 18;
- (3) ISP 23: Rupture of a Large Diameter Pipe in the HDR Containment (HDR T 31.5);
- (4) ISP 24: SURC-4 Experiment on Core Concrete Interactions;
- (5) ISP 29: Distribution of Hydrogen within the HDR Containment under Severe Accident Conditions;
- (6) ISP 30: Best estimate TA V5.1 Experiment on Melt–Concrete Interaction;
- (7) ISP 35: NUPEC Hydrogen Mixing and Distribution Test (Test M-7-1);
- (8) ISP 39: FARO-Test L-14 on Fuel Coolant Interaction and Quenching (this test was performed at high system pressure, but tested models of the fragmentation of a melt pour through water);
- (9) ISP 42: PANDA Test ‘TEPPS’ (at least some phases of this test);
- (10) ISP 46: PHÉBUS-FPT1 (integral test, but with a not very representative 10 m³).

The status of the validation differs for the different severe accident codes. Within the group of integral codes, MELCOR is used worldwide by many organizations not only for validation work but also for plant analyses. The information exchange between the different users is managed annually by user group meetings. It can be concluded that the uncertainties of the code for analyses of different severe accident scenarios in LWRs are known within the user group, and based on this knowledge, experienced users are able to perform reliable plant analyses and to give an indication of the related uncertainties.

MAAP is extensively used by utilities for PSA Level 2 analyses. There are also regular user group meetings aiming at the exchange of information. However, compared to MELCOR and the other more detailed codes, MAAP

has not been used so extensively to analyse experiments and is thus validated to a lesser extent. The limited application of the code to experiments is caused primarily by the proprietary nature of the code, which has limited availability for use by research or regulatory organizations that have been most extensively involved in international experimental research programmes. In addition, the application of the code to experiments is also limited by the fixed nodalization of the reactor coolant system of standard LWR plants, which makes it more difficult to perform calculations of experimental facilities with different geometries.

The detailed codes ATHLET-CD, ICARE/CATHARE and SCDAP/RELAP5 have been extensively used by international research and regulatory organizations to support experimental programmes and have received extensive validation by their developers as well as other independent organizations. SCDAP/RELAP5 has been extensively used to support the analysis of small scale and medium scale experiments in the USA, Europe and Japan. It was also used to support the TMI-2 accident evaluation. ATHLET-CD and ICARE/CATHARE have been extensively used in Europe, ICARE particularly to support the PHÉBUS programme.

The integral code MELCOR and the detailed codes ATHLET-CD, ICARE/CATHARE and SCDAP/RELAP5 have also been used by different organizations for benchmark exercises in the framework of ISPs. MAAP has been used on a very limited basis, however, it is being used in some of the more recent ISPs. These exercises have provided further information about both code deficiencies and user effects. In Appendix II, the relevant ISPs and the main outcomes are listed. More comprehensive information is given in Ref. [56].

For several of the codes, formal and independent peer review of the models has also been an important part of their early validation. Independent peer reviews of SCDAP/RELAP5 [78], MELCOR [79] and ICARE2 [80] have been performed, resulting in detailed in-depth assessment of the models. Although the formal peer reviews noted in the references occurred in the middle stages of the code development cycles, in most cases, these peer reviews have continued on an individual model basis and have been used by the sponsoring agencies to focus efforts on the most important models. These peer reviews, along with an assessment of the uncertainties of the models by the developers and the independent organization, have been significant factors in the validation of these codes.

Validation of these codes, and other newer codes, such as ASTEC, is still continuing as the last remaining technical issues are resolved. Additional ISPs are currently under way or are planned. In the case of the new code ASTEC, the first step of validation of ASTEC V0.2 has been performed by the code co-developers, the Institut de protection et de sûreté nucléaire (IPSN) and Gesellschaft für Anlagen- und Reaktorsicherheit (GRS), in 1999–2000, using

several international programmes including PHÉBUS (SFD, FP). In addition, within the Fifth European Framework Programme (FWP), the EVITA [16] project was initiated, which deals with validation of the code by many different organizations. Therefore, at the end of the project (01/2003), significant progress in this area can be expected.

An overview of the validation of the latest publicly available versions of different severe accident codes (only the most well known codes are considered) for selected key tests [5] is shown in Annex II. For detailed information about relevant experiments and their ranking, see Refs [6, 7], which contain a very comprehensive description of the different experiments as well as a justification of their ranking. Another well justified validation matrix is included in Volume 5 of Ref. [65]. Reference to the document available for each of the major codes provides a more detailed description of these and other validation activities that have been performed for each of the codes.

Summarizing the results of the validation work, it can be stated that the early phase of core degradation (before losing the rod-like geometry) can be described satisfactorily with the detailed codes. However, quenching phenomena are still not well understood and are being addressed in ongoing experimental and theoretical efforts. For the late in-vessel phase, there are still significant uncertainties, mainly related to the following phenomena:

- (a) Relocation of molten material;
- (b) Formation and stability of metallic and/or ceramic crusts;
- (c) Interaction of the molten pool with surrounding structures;
- (d) Debris bed and pool coolability;
- (e) Failure mode of the reactor pressure vessel.

With the exception of the latter two phenomena, which are being addressed in ongoing experimental programmes, it is not expected that the uncertainties associated with these late phase phenomena will be reduced significantly in the future because of the cost of appropriate experiments for this stage of the accident.

6.4. USER QUALIFICATION AND USER EFFECT ON ACCIDENT ANALYSIS

As discussed in Ref. [6], qualification of the user is another important factor significantly affecting the results of analysis. Qualification of the user may involve several activities:

- (1) User training;
- (2) Participation in technical exchange/user groups;
- (3) Review of user guidelines and documentation;
- (4) Testing of the code for the intended application;
- (5) Uncertainty analysis.

In addition, the development of quality assurance procedures or standard practices for each application may be appropriate.

For severe accident codes, as compared to design basis accident codes, the user effects may be increased for two primary reasons. Firstly, the user must select additional modelling parameters because of the large number of physical models required to represent severe accident behaviour. This is particularly true for the use of the integral codes which rely extensively on user defined modelling parameters to control the calculations. This is less of a factor for the mechanistic codes, since user defined modelling parameters are avoided or used in a limited way. Secondly, an analysis of severe accidents requires a fundamental understanding of severe accident phenomena that is rarely included at the university level. Thus, users must not only be trained in the codes but receive training in the fundamentals of severe accident phenomena.

Because of the strong impact of the user on the results of a severe accident analysis, user training is the fundamental component of user qualification. Reference [6] recommends the following minimum requirements for any code user:

- (1) Analysts should have at least a basic understanding of important phenomena, including reactor physics, thermohydraulics and fuel behaviour.
- (2) Analysts should have a basic understanding of the plant and its performance.

To achieve an adequate qualification, the user should start with a literature survey of existing similar analyses. After implementation of the code, the proper installation must be checked by the recalculation of test cases, which should be transmitted by the supplier of the code. Sensitivity studies should then be performed with respect to the nodalization of the system. In addition, if there is no clear recommendation in the user guidelines, the impact of the maximum time step must be analysed. The user should select a code for which the supplier has already performed an extensive validation work, which must be documented in a validation manual.

Additionally, for an effective severe accident analyst, the training should cover the following subjects:

- (a) Fuel and other core material behaviour, including the metallurgy of reactor core materials, chemical interactions, release and transport of fission products;
- (b) Review of relevant experiments;
- (c) Review of relevant calculations.

Where possible, the beginning users should work with more experienced users. For severe accident analysts, this may involve working with experienced system thermohydraulic analysts and PSA analysts. The beginning users should participate in code specific training, typically offered by the code developers or other experienced code users. Users should also participate in code user and technical exchange meetings. Engineering plant simulators are also useful tools for user training.

An analysis of experiments is another efficient way to train the code user. By applying the code and comparing the code results to the experiment, the user gains a fundamental understanding of the different phenomena occurring during a severe accident, their importance and their interactions.

Other important factors in user training include the review of code user guidelines and input manuals, testing of the code, and uncertainty analysis. Most of the widely used codes have extensive user guideline publications that have been prepared by the code development staff and, in some cases, by other experienced code users. Testing of the code, in many cases using the representative sample problems provided by the code developers or code trainers, is particularly important where the calculated results can be compared to results obtained by other analysts. Uncertainty analysis, which may involve nodalization studies and the systematic variation of modelling parameters, helps the user to understand the impact of their modelling choices on their calculation results. In many cases, user uncertainty studies can be compared with similar studies prepared by the code developers or other users of the code.

Another potential source of (indirectly) user-caused uncertainties is the ‘compiler’ effect, which means that different compilers, levels of optimization and/or platforms lead to different results [81]. To minimize this effect, the user should validate the implementation of a code by benchmarking the results for relevant cases (scenarios) with reference results transmitted by the supplier of the code.

More extended information about user effects and recommendations for their minimization are included in Ref. [6], as well as in dedicated reports [81–83].

7. USES OF SEVERE ACCIDENT ANALYSIS AND BASIC APPROACHES

7.1. APPLICATION OF SEVERE ACCIDENT ANALYSIS AND CODES

Historically, severe accident analysis has been used to support PSAs, help resolve specific severe accident issues, and support severe accident research programmes. However, with the rapid progress in computer technology and maturation of severe accident codes, severe accident analysis has increasingly focused on the use of these codes for:

- (a) Training purposes;
- (b) Development and validation of accident management programmes;
- (c) Design and validation of severe accident mitigation systems;
- (d) Most recently, plant simulators.

In addition, these codes — although developed primarily for commercial western LWR designs — are being used for the analysis of a wider range of different reactor designs, including WWERs, RBMKs, research reactors and heavy water reactors.

Severe accident analysis has not been used in the past for the licensing or operation of current power plants. However, as the design of new plants has progressed, there has been an increasing tendency to incorporate the analysis of severe accidents into the design and operation of these plants. In some countries, such as Germany or France, severe accident analysis is required for the design of new NPPs. Similar requirements are also incorporated in a new set of IAEA safety standards. Such applications may require significant improvements in the accuracy and scope of applicability of existing severe accident codes, as well as increased attention to more formal quality assurance programmes.

It is important to note the clear distinction between the use of severe accident analysis and the use of severe accident codes. Severe accident analysis is concerned primarily with those accidents that result in loss of the original geometry of the core. However, codes must also be able to calculate the behaviour of the plant up to and including loss of the core geometry, thus, these codes have been used for design basis as well as severe accident analysis. In particular, the more mechanistic severe accident codes can be used for the full range of design basis accident and beyond design basis accident analysis. In these codes, the severe accident models, that is, fuel liquefaction or melting models, are only invoked when such models are needed.

Severe accident analysis can draw on tools and techniques used for probabilistic as well as deterministic analysis. However, in the context of this publication, severe accident analysis refers to deterministic models or techniques. In particular, severe accident codes utilize deterministic models. In addition, severe accident analysis can involve both best estimate and conservative calculations. However, most generally used detailed severe accident codes are designed as best estimate tools. These codes include modelling options that may provide both conservative and non-conservative results. Such modelling options are used for sensitivity studies where the uncertainties in important models may not be clearly understood.

7.1.1. Support for PSA

As discussed in more detail in an IAEA report on modelling in-vessel phenomena under severe accident conditions [24], one of the earliest uses of the integral codes was to support PSA activities. Much of the earlier work was performed by the STCP code and the MAAP code [36, 37]. These codes and their successors, MELCOR [38, 39] in the case of STCP, were used to perform a large number of calculations for those groups of sequences that would be expected to have similar effects on the release of fission products to the environment.

Plant specific calculations were performed using the integral codes for representative groups of sequences to establish the: (a) results for important variables as a function of time; and (b) timing of major events. These calculations were supported by sensitivity studies, expert opinion and, in selected cases, mechanistic code calculations, to estimate the overall uncertainties of the results. These results are then combined to determine the accident progression event trees and associated probabilities for different branch points. Additional plant specific calculations were also performed using the integral codes and, in limited cases, a combination of mechanistic codes, to determine source terms for high frequency release sequences or those sequences that were expected to include relatively large releases of fission products. These results were then combined as part of a Level 2 PSA.

In these earlier studies, as noted in the IAEA report on PSAs [24], the uncertainties in the calculated source terms and accident event trees were large, overshadowing any variations associated with plant specific results. Although the reduction in uncertainties in ongoing and future PSA studies is probably due to the resolution of key phenomenological issues, such as DCH and the introduction of more advanced severe accident codes, the modelling accuracy required for PSA studies will continue to be relatively low compared to the modelling accuracy required for other severe accident applications. As a

result, it is anticipated that fast running integral codes will remain the preferred option for PSA calculations. However, mechanistic codes may play an increasing role by reducing the uncertainties in the analysis of risk dominant accidents.

7.1.2. Resolution of severe accident issues/severe accident research

The mechanistic codes and more specialized codes and models have played a key role in helping to resolve important severe accident issues. For example, the plant specific calculations of representative plants in the USA [84], along with experiments on hot leg natural circulation and high pressure melt ejection, were instrumental in helping resolve the issue of DCH in the USA [85, 86]. These calculations, using models developed and validated with natural circulation data, were able to show that the likelihood of lower head failure, prior to the heating and failure of reactor coolant system piping due to natural circulation flows, was very low for high pressure scenarios. As a result, when this information was combined with the research on high pressure melt ejection and DCH, it was concluded that an early containment failure due to reactor pressure vessel originated missile or DCH is unlikely.

Most of the internationally recognized codes, including MELCOR [38, 39], ASTEC [41], ATHLET-CD [40], SCDAP/RELAP5 [42, 65] and ICARE/CATHARE [35], have been fundamental components of international research programmes, since their development has been sponsored by regulatory organizations in the USA, Germany and France. These codes have been used to design and analyse severe accident experiments, or were used in developing the TMI-2 accident scenario, and have been used widely by the international community for plant studies. Most recently, these codes have been used to support the analysis of plants in eastern Europe as part of the research activities to improve reactor safety for WWER and RBMK reactor designs. MAAP, although widely used by utilities around the world, has had less impact on international research programmes.

It is anticipated that most regulatory sponsored codes will continue to support international research programmes, as well as help resolve any outstanding technical issues (such as reflooding and ex-vessel cooling). In some cases, these applications may result in additional modelling improvements and the release of new versions of the severe accident codes. For example, improvements in models to treat the reflooding of a damaged core, cooling of the debris and vessel during the later stages of the accident, and the formation and slumping of molten fuel, are likely. In other cases, this research will be used to reduce the uncertainties in plant calculations. All these activities will help to develop improved user guidelines for these codes.

7.1.3. Development of training programmes

Severe accident codes have been valuable aids for training for severe accidents, since the codes embody the results of more than two decades of severe accident research. As a result, the codes, particularly the detailed mechanistic codes, can directly demonstrate the key features of severe accidents using a variety of representative input models and accident sequences. The impact of general design features, such as PWR or BWR core designs, heating rates and core mass flow rates on the heat-up and melting of the core, have been defined through an extensive series of experiments and are rather well predicted by the mechanistic codes. For example, all of the mechanistic codes have been shown to predict such behaviour through a series of blind and open calculations [87–89]. The important trends and phenomena described in Section 2 are also well represented in the mechanistic codes and can be seen clearly in the code calculations. However, significant uncertainties remain for hydrogen production in the late and even early phases of the accident sequence, reflooding is not well calculated in many cases, and melt relocation is also predicted with large uncertainties (material properties are not well known, nor are the impacts of multidimensional effects). The codes, used in combination with graphic based nuclear plant analyser displays, can also provide a realistic training environment with a minimum effort.

Although such training programmes and activities are just beginning, mechanistic severe accident codes, using plant specific input models, can also be used for training for severe accidents with or without plant specific accident management activities. In most cases, a limited number of modelling options, which have been added for sensitivity studies by severe accident researchers, can be used to help evaluate the impact of the most important modelling uncertainties. Although most of the mechanistic codes do not typically run these calculations in real time, techniques using the playback of plot files using nuclear plant analyser displays allow the user to play the calculations back at any speed. In addition, because of the rapid advances in computer technology and improvements in numerical and programme techniques, real time calculations using optimized input models and optimized versions of the codes will rapidly become routine, even using relatively inexpensive personal computers and engineering workstations.

Code specific user training in combination with generalized training on severe accident phenomena and research can also be an effective way to train technical support staff and engineering analysts. In particular, engineering analysts familiar with system thermohydraulic codes used for design basis analysis can be relatively quickly trained to use mechanistic codes for severe accident conditions. In addition, since most plant models developed for system

thermohydraulic design basis accident analysis can easily be extended for use in the mechanistic codes, experienced thermohydraulic analysts can quickly swap between data for design basis and severe accident calculations. For experienced analysts of system thermohydraulic codes, modifying the plant models to include core degradation aspects takes generally only a few days. Training for the integrated codes is somewhat more involved since these codes cannot use input models developed for design basis accident analysis, and thus require training programmes different from training for design basis accident system thermohydraulic analysis. However, generalized training in severe accident phenomena can apply equally well to analysts using either the mechanistic or integral codes.

7.1.4. Analytical support for accident management programmes

The development of accident management programmes is one of the most frequent applications of severe accident analysis. Obviously, the first priority for reactor safety has always been to prevent any accident from occurring, in line with the aim to achieve very low core melt probabilities. Should the accident progress into a severe condition despite all preventive measures, then the priority is to arrest or slow accident progression and to attenuate or mitigate the releases of radioactive material by utilizing all means of accident management available at the site.

In the hypothetical case that the prevention measures would fail during the progression of a severe accident, the ultimate safety goal is to maximize the grace period while mitigating all consequences of the severe accident. The understanding, therefore, of the mode and timing of the failure mechanisms of the various barriers is particularly crucial to designing appropriate accident management strategies, taking into account the time available for intervention, whether active or passive. It is crucial, in particular, to obtain an estimate of the time between the detection of the severe accident event and the failure of the barrier, as well as to predict 'realistic' initial or boundary conditions at the time of failure. Many research efforts, therefore, have been focusing on the aspects of mode and timing of failure of barriers.

Thus, the accident management objectives aim at the prevention of severe accidents and the mitigation of their consequences in both current and next generations of reactors. These objectives can be specified in a general wide approach, such as prevention of a degraded core becoming critical; assurance of the coolability and stabilization of the molten core for both in-vessel and ex-vessel scenarios; mitigation and quantification of the release to the containment of fission products and aerosols; prevention of explosive phenomena associated with hydrogen released through the quenching of an

overheated core; as well as the optimization of severe accident management measures and signal validation techniques under harsh conditions.

There are specific IAEA publications devoted to the accident management programme and to its review [5, 8]. These publications also include basic requirements on how to perform an analysis of severe accidents needed to support the preparation, development and implementation of the accident management programme. Basic characteristics of analytical support for accident management and emergency planning are also covered by Ref. [6]. The most important conclusions are presented here in a summary form.

Accident analysis related to the accident management programme is important in order to understand plant response to beyond design basis accidents and severe accidents, to understand which accident phenomena are important for the plant in question, to understand and rank challenges to fission product boundaries, and to provide a sound basis for the investigation of preventive and mitigatory measures of the accident management programme. The analysis should be done with a suitable and reasonably validated code and, as for other kinds of severe accident analysis, should be performed on a best estimate basis. It should be noted, however, that accident analysis is only one part, albeit important, of the development of accident management programmes. Incomplete analyses do not prohibit initial phases of accident management programmes being developed.

Three categories of analysis are identified in Ref. [21]:

- (1) Preliminary analyses which are informative in nature and provide an understanding of the response of the plant to various types of accidents and the basis for selection of recovery strategies. In particular, an analysis should be made of sequences that, without operator intervention, would lead to core damage, core melt, vessel failure and the release of fission products.
- (2) Procedure and guideline development analyses: these are needed for detailed confirmation of the choice of recovery strategies adopted, to provide necessary input to set point calculations (where appropriate), and to resolve any other open items identified during the previous step. Recovery strategies include preventive measures to halt or to delay the onset of core damage and measures to mitigate the consequences of core damage.
- (3) Validation analyses for procedures and guidelines: they are performed in order to demonstrate the capabilities and choice of appropriate strategies and optimize some aspects of these.

Since the number of sequences for analysis leading to core damage and eventually to the release of fission products to the environment is virtually infinite, a method to select a reasonable number of accident sequences, or classes of sequences, should be chosen. The selection of accident sequences to be analysed should reflect:

- (1) Adequate use of results of PSA focusing on risk significant accidents;
- (2) Additional information available, such as design specifications, equipment technical specifications, operating experience, accident precursors, design specific experimental results, severe accident research, information from similar plants;
- (3) Consideration of all specific severe accident phenomena and plant damage states.

Categorization is typically based on several state designators, such as initiating event, shutdown state and emergency core cooling state. Since accident management programme measures should also be applicable to highly improbable accident sequences, not only sequences with the highest probability of occurrence are to be selected.

The assessment of core melt risk addressed basically the integrity of the first two barriers: fuel cladding and reactor pressure vessel, with emphasis on corium formation and behaviour. Consolidated knowledge is needed, covering the influence of core degradation on various items, such as coolability, and on the release of fission products, the relocation of large masses of molten core to the lower head involving steam explosion risks, and the hydrogen kinetics due to the hydrogen combustion risk, which together with high temperature creep phenomena are challenging the vessel integrity. Conclusive statements should be discussed, in particular for the in-vessel steam explosion issue. To ensure melt retention in the vessel, mitigating strategies might be further investigated on the basis of separate effect and large scale experiments.

To assess the risk resulting from containment failure, consolidated knowledge is needed covering the influence of ex-vessel melt behaviour on various items, such as its coolability and the release of fission products, including aerosol behaviour and iodine chemistry, hydrogen sources and the distribution within different parts of the containment due to the combustion risk, and the risks due to fuel-coolant interactions. Conclusive statements should be discussed, in particular, for the ex-vessel steam explosion and HPME/DCH issues. To ensure melt retention inside the containment, mitigation strategies might be further investigated on the basis of separate effect and large scale experiments.

The source term assessment is linked to the release of fission products and other radioactive materials from the degrading core into the cooling circuits and, finally, into the containment, from where they could hypothetically leak into the plant environment. Consolidated knowledge is needed, covering chemical studies of core degradation phenomena; prediction of quantities, speciation and physical forms of the materials released; evaluation of their behaviour along the release paths; and discussions with plant personnel responsible for plant management and emergency preparedness in local organizations. In this context, the PHÉBUS FP Programme carried out in Cadarache, France, within the framework of broad international cooperation, is valuable.

Different accident management measures (e.g. dedicated safety systems, I&C, and prevention or mitigation strategies) for both present and future LWRs have been and are being developed in order to respond to the challenges of hypothetical severe accidents. Methods and tools also need to be developed for dealing with uncertainties regarding phenomena, possible adverse effects of operator actions, improved instrument survival and reduced error, equipment performance and human error under stress. Use of modern information technology systems should be carefully addressed.

Specific requirements on performing severe accident analysis which support an accident management programme include:

- (a) Analysis for mitigatory accident management programme measures should reflect the findings of accident sequence analyses without operator intervention and with preventive measures;
- (b) All identified important accident phenomena should be considered in the analysis;
- (c) Capabilities of all available equipment to perform, under accident conditions, as required for individual strategies, should be considered; depending on the accident management approach, use of existing equipment outside its design range and margins or new equipment should be considered;
- (d) The same input deck and version of computer codes should be used as for all relevant analyses, for example, for analyses with and without operator interventions; changes, if any, in the plant's database and the use of different versions of a code, should be justified;
- (e) Analysis should be performed to determine that symptom(s) selected for activating measures in key areas of mitigatory accident management can be used for the whole range of accident sequences chosen for analysis;
- (f) Sensitivity studies should be performed with varying values of the symptom(s) that indicate accidents occurring outside the design range;
- (g) Sensitivity studies should be performed and published with varying time windows for initiating (and stopping) mitigatory actions.

Uncertainties have to be considered in the evaluation of analysis results for both the in-vessel and ex-vessel phases of the accident.

7.1.5. Support for new designs

For new designs, reactor designers are contemplating the possibility of developing mitigatory measures to cope with severe accidents. Such measures have also been the subject of many international research programmes.

In this regard, many activities are being performed to gain an understanding of the main phenomenological aspects and to develop the most appropriate severe accident management, both of the preventive and of the mitigatory type. For this reason, many research projects in this area have a strong 'evolutionary' flavour, based on the consensus around the safety approach of evolutionary reactors, such as EPR, AP 1000, ESBWR, APR 1400 and ACR 1000. Reference [90] reviewed the measures which are being incorporated into evolutionary reactor designs for preventing and mitigating severe accidents. To different extents, some of the evolutionary designs incorporate severe accidents into their design and licensing approach.

Achieving the 'practical elimination' of events liable to cause early containment failure, as well as the 'control' of events liable to cause major radioactive releases to the environment, which could result from an unlikely core melt accident (achievable through, for example, the design of corium catchers) are evolutionary safety recommendations for ultimate severe accident situations, which are underlying many research projects in the area of severe accidents. As a consequence, mitigation measures against risks to corium, hydrogen and source term are under development and even already installed in some NPPs.

Consequently, specific design capabilities to be analysed in connection with an in-vessel phase of a severe accident are as follows:

- (a) Hydrogen production in the vessel and its release as input information for the design of a hydrogen treatment system;
- (b) In-vessel melt retention both by internal and external vessel cooling;
- (c) Melt composition and configuration, and reactor pressure vessel failure as an input for the core catcher design;
- (d) Reliable depressurization of the primary system to avoid high pressure vessel failure;
- (e) Long term fission product release from the reactor core;

Similarly, for the ex-vessel phase, design capabilities to be analysed include:

- (a) Reliable depressurization of the containment to avoid high pressure containment failure;
- (b) Hydrogen sources and distribution as input information for the design of a hydrogen treatment system;
- (c) Ex-vessel steam explosion and HPME/DCH issues;
- (d) Melt composition and configuration as input for ex-vessel melt retention devices;
- (e) Fission product sources and distribution within the containment with special attention to the long term behaviour.

A combination of calculations by means of mechanistic system computer codes with detailed CFD codes is typically needed. Calculations often have to be complemented by special experiments. Large uncertainties in calculations should be compensated for by more robust design.

7.1.6. Use of computer codes in simulators for severe accidents

The application of simulators and simulation techniques, in general, in accident management training is described in Ref. [91]. In this report, a simulator is characterized as:

“a computer-based assembly of software and hardware, which is capable of presenting the physical behaviour of the whole NPP or the part of it during various operational states and malfunctions. The simulators are typically equipped with an advanced user interface (graphical or hardware interface) suitable for interactive operation and particularly suitable for training purposes.”

Generally, the simulators are subdivided into engineering simulators (used for design purposes and, in particular, for justification of the design) and training simulators. There are several types of simulators recognized according to their complexity and application purpose, referred to as, for example, compact simulators, plant analysers, full scope training simulators, multifunctional simulators, severe accident simulators and accident management support tools. The terminology is not yet formally systematized. The simulators can work both as tracking or predictive simulators. The tracking simulators monitor the NPP status and provide the personnel with calculated information also of those parameters that are not directly monitored by the NPP systems. The

predictive simulator should be a fast running tool used for predicting the paths of accident progression. Simulators can be used at different training levels, such as classroom training, training in the use of procedures and guidelines, and emergency drills.

Present simulators have the capability to simulate NPP conditions starting from the initiating event through the initial core degradation up to the full severe accident phenomenology. Both integral and mechanistic advanced computer codes, the same as for other applications, are used as software for the simulators. The basic requirement is the ability of the software to simulate severe accident progression to the degree necessary for the effectiveness of the training. The crucial ability is to simulate reliably the expected accident progression, to allow operator interventions during that progression and to present the result in a user friendly graphical form, even though the accuracy of simulation is certainly limited.

Due to the complexity of the simulated phenomena and difficulties in the validation of simulators, users should be aware of limitations and uncertainties, and of how to handle them appropriately in training. In particular, so-called bifurcation points, where the further accident progression depends on the outcome of some energetic phenomena and may be developed in different ways, should be taken into account.

7.2. SELECTION OF SEVERE ACCIDENT CODES

Since for the time being there is no requirement in any country for a licensing procedure for beyond design basis accidents, no certification of severe accident codes exists or is planned in the near future. There are three important factors which should be considered in the selection of the code(s):

- (1) Identification of the potential uses of the severe accident code(s);
- (2) Definition of pertinent acceptance criteria for each application;
- (3) Ranking and final selection of potential codes.

The identification of potential uses of severe accident codes will establish the types of codes or models that would be required. Integral codes would commonly be applied to PSA support activities or source term calculations. Although a combination of mechanistic codes could be used, the current generation of mechanistic codes is not designed to conveniently run the large number of calculations typically required in PSA or source term calculations. Mechanistic codes would be required where modelling accuracy is of primary concern. Such applications would include:

- (a) Severe accident management and mitigation;
- (b) System design and operation;
- (c) The more historical roles of severe accident issue resolution or research.

Both integral and mechanistic codes could be used to support training applications, although the mechanistic codes may be the most appropriate because of their more accurate representation of important severe accident phenomena. Plant simulators would also require the use of mechanistic codes if realistic simulations were to be expected. However, advanced versions of the mechanistic codes which have been optimized for speed and reliability and/or specialized computer equipment may be required to support real time plant simulations.

The definition of pertinent acceptance criteria for each application would also help define the need for specialized codes or models. Such specialized codes or models would only be required where modelling uncertainties are the most crucial. Examples of specialized codes or models would include steam explosion models, detailed chemistry or fission product transport models and CFD codes. The identification of pertinent acceptance criteria would also be useful in determining the level of modelling detail required when developing input models for the mechanistic codes. For example, more detailed input models may be used for the design and validation of accident management procedures (and other design and operation related activities), while simple input models may be appropriate for training or plant simulator applications.

Once the level of modelling detail and potential application of the codes has been identified, the final ranking and selection criteria should include the availability of technical support and training for the code(s) and other factors related to the overall reliability, and usability of the code(s). The other factors include:

- (a) Use of internationally recognized and accepted codes to provide some assurance about the adequacy of the code(s);
- (b) Comprehensive publication to facilitate the review of the models and correlations;
- (c) Pre-existing or ongoing validation programmes to help qualify the code for its intended application;
- (d) Ready availability and unrestricted use of the code (the distribution of some of the codes is limited, or restrictions may be placed on the regulatory sponsored versions of the codes);
- (e) Availability of strong user group and training programmes;

- (f) Availability of representative input models for use in training or the development of plant specific input models;
- (g) Future development and maintenance programmes to ensure continued improvement and user support for the code(s).

7.3. SELECTION OF ACCEPTANCE CRITERIA

Acceptance criteria as a quantitative limitation of selected parameters or qualitative requirements set up for the results of accident analysis are most commonly applied to licensing calculations to prove the acceptability of the design. Since, for existing plants, severe accidents typically do not form part of the design basis for licensing, acceptance criteria for severe accidents are applicable mostly to future reactors. Moreover, these criteria are usually formulated in terms of risk probabilistic criteria, or in terms of containment integrity or in terms of acceptable radiological consequences of the accident.

A discussion of probabilistic safety criteria is provided in Ref. [92], which defines a ‘threshold of tolerability’ above which the level of risk would be intolerable, and a ‘design target’ below which the risk would be broadly acceptable. Although this approach has been adopted in some countries, there is no international consensus on its application. Often, probabilistic safety criteria are defined by reference values which serve as orientation for the levels of risk which are acceptable. However, there is also no international consensus on the numerical values. Numerical values for the levels of risk, based on experience with the design and operation of NPPs, were given by INSAG [9]. These values can be achieved by current designs of NPPs and should be achieved by future designs. The reference values for the acceptable level of risk for the core damage frequency are as follows:

- (1) 10^{-4} per reactor year for current designs of NPPs;
- (2) 10^{-5} per reactor year for future designs of NPPs.

The reference values of INSAG for the acceptable level of risk for large off-site release of radioactive materials compared to core damage frequency are one order of magnitude lower.

Although there is no consensus on what constitutes a large off-site release, similar numerical criteria have been specified in a number of countries. For example, the limit for a large off-site release of radioactive materials is set in the Finnish regulatory guide [93] to 5×10^{-7} per reactor year, and the limit for release of radioactive materials is set to 100 TBq for ^{137}Cs .

Deterministic acceptance criteria for severe accidents have also been specified in a number of countries. In addition, criteria listed previously as closely related to the results of the PSA study (e.g. specification of large off-site releases) can be considered as deterministic ones. For example, the following requirements were defined in the Finnish regulatory guide [94]:

- (1) The pressure and temperature created inside the containment as a consequence of a severe accident should not result in its uncontrollable failure;
- (2) No acute harmful health effects to the population in the vicinity of an NPP should occur;
- (3) No long term restriction of extensive areas of land and water should occur;
- (4) The atmospheric release of ^{137}Cs should be less than 100 TBq.

A more detailed discussion on acceptance criteria can be found in the Ref. [6].

The examples of acceptance criteria given previously are only partially relevant for this report, since it deals with the in-vessel phase of a severe accident. Examples of specific deterministic acceptance criteria applicable to the in-vessel phase of a severe accident can be found, for example, in the Finnish regulatory guide [95] as follows:

- (a) The reactivity control systems shall be so designed that a reactor which has sustained damage in a severe accident, or its debris, are maintained subcritical.
- (b) Pressure reduction shall be planned so that a severe accident at high pressure can be reliably prevented.

German requirements of the Atomic Energy Act for the next generation of plants state that:

- (a) Accident situations with core melt which would lead to large early releases have to be ‘practically eliminated’; when they cannot be considered as physically impossible, design provisions have to be taken to design them out.
- (b) Low pressure core melt sequences have to be dealt with such that no permanent relocation and no emergency evacuation are required.

Similar requirements are made in the technical guidelines for future PWRs prepared in the framework of the new European EPR reactor design.

In the case of using severe accident analysis for plant design, acceptance criteria can be deduced from the design objectives, that is, reactor pressure vessel failure should be prevented if the design objective is to retain the molten corium of the core in the vessel.

8. SPECIFIC SUGGESTIONS FOR PERFORMING AN ANALYSIS OF SEVERE ACCIDENTS

Design basis accident analysis and beyond design basis accident analysis are based on different approaches. Design basis accident analysis is based on a deterministic approach, where proof is given that the plant is safe in a comprehensive set of accident sequences defined on the basis of conceivable initiating events, conservative assumptions and the single failure criterion. Acceptance criteria in the form of limits on physical parameters are defined that should be met in all accident sequences. In general, there are different acceptance criteria for different types of sequences. The conservative approach is used for all the input parameters. Another approach to design basis accident analyses is the use of best estimate analyses, involving no conservatism in the initial and boundary conditions, but with an uncertainty evaluation of the analysis.

The beyond design basis accident is to a large extent based on the probabilistic approach, with the aim of demonstrating that the total risk to the environment and the public due to the plant operation is acceptably small. The acceptance of beyond design basis accident is based on the acceptance of the plant risk function that combines probability and radiological consequences. Generally, the selection of a limited number of sequences to be analysed in detail by a complex severe accident code is based on the results of PSA Level 1. The severe accident analysis methodology does not use conservative assumptions, the reason being that determining which assumption is conservative cannot be done in advance. In addition, a conservative assumption related to a particular phenomenon may not be conservative to another severe accident phenomenon. Therefore, beyond design basis accident analyses rely on best estimate data. However, this does not exclude the performance of bounding analyses for a particular analysis application.

The intention of this section is to provide the user and reviewer involved in the analysis of severe accidents for NPPs with specific suggestions about how to perform the analysis. The basic steps discussed in a general way are illustrated using an example: the analysis of severe accident transients in the

Surry NPP, USA, using the detailed code SCDAP/RELAP5. The example is presented in Appendix III of this report.

8.1. BASIC STEPS IN DEVELOPING INPUT DATA AND PERFORMING CALCULATIONS

The procedure presented for performing accident analysis presented in Ref. [6] also applies to the analysis of severe accidents. The following steps are explained further in this section with respect to the particularities of severe accident analysis.

First steps of the procedure are:

- (1) Specification of the facility and the objectives of the accident analysis;
- (2) Selection of the approach to be used;
- (3) Selection of the appropriate computer code (see Section 6.1);
- (4) Determination of the methodology.

An important part of the analysis work is spent for the input data preparation if plant models have to be developed from scratch. This comprises:

- (1) Collection of plant data and the establishment of a plant database;
- (2) Development of an engineering handbook which deals with the conversion from plant data into input data;
- (3) Verification of the input data by reviewing and cross-checking them independently;
- (4) Validation of the input data.

Further steps in a severe accident analysis process are:

- (a) Preparation of the scenario;
- (b) Execution of the calculation;
- (c) Checking the results;
- (d) Assessment of uncertainties;
- (e) Presentation and documentation of the results.

All of the steps mentioned should be subject to quality assurance procedures [6].

The amount of work necessary for the preparation of input data can be reduced considerably if qualified thermohydraulic plant models already exist for the analysis of design basis accidents. Then, only an extension (if the same

code is used) or conversion (if the input deck is prepared for another code) of the existing thermohydraulic input data is necessary. In addition, input related to the severe accident phenomena is required to be developed for the new input deck.

The thermohydraulic input model has to be adapted to the needs of specific severe accident analysis, that is, time consuming nodalizations can be simplified and the modelling of certain thermohydraulic phenomena can be suppressed if they are not necessary for the analysis. On the contrary, a refinement of the nodalization can be necessary in order to take into account phenomena of interest during a severe accident, for example, natural circulation in the upper plenum, failure of the hot leg, the surge line or the steam generator tubes due to high temperatures, corium in the lower plenum, natural convection paths in the containment, hydrogen distribution inside the containment compartments, corium in the reactor cavity and MCCI.

The input data have to be extended by the severe accident models. These usually imply, among other things, the core, the lower plenum and the upper plenum, the reactor cavity, a detailed model of the engineered safety systems, and more detailed nodalization of the containment compartments. The recommendations in the user guidelines of the codes, for example, concerning noding rules or default data for models, should be considered. For example, the core meshing must be fine enough to have a sufficient resolution of temperature profiles and material distribution. Similarly, the heat structures meshing must be fine enough to provide sufficient resolution. The nodalization of the containment compartments into control volumes and junctions may also play a significant role on the predicted long term post-accident containment response. Major undesirable influences of the noding on the results should be excluded. This should be checked by performing sensitivity calculations. However, the meshing depends also on the type of code used. Fast running codes generally use a coarse meshing for the reactor coolant system and reactor pressure vessel (in the case of MAAP, the mesh is even fixed) and containment. The adaptation to different reactor types then requires modifications in the source of the code (examples are MAAP versions for WWER and PHWR). Detailed codes generally allow a flexible representation of the core, primary circuit and containment, and thus of different types of reactors, but at the cost of a finer meshing. Further suggestions regarding essential design characteristics are given in Appendix III.

Special attention in severe accident input models has to be paid also to the properties of the core materials, such as fuel, cladding and absorber, and those of structural materials in the primary system and containment — conductivity, heat capacity, chemical composition, etc. They must be either available in the code for the materials used in the NPP to be analysed or they must be

modelled accordingly. Furthermore, they must be available up to high temperatures. It is important to take into account that the uncertainties in the material properties become large for high temperatures.

In addition, the expected material interactions have to be taken into account correctly. This can be done by either providing the respective phase diagrams and modelling the reaction kinetics or, as is usual in most of the codes, by providing the temperatures for the onset of the relocation of core materials by user input. They have to be set according to the expected failure temperatures of the core components and to take into account the possible formation of eutectic mixtures. Here, the feedback from experiments such as PHÉBUS-FP is extremely important in defining the appropriate values for some input parameters.

8.2. INPUT DATA PREPARATION

The quality of an analysis is mostly determined by the features and correctness in the input for a given computer code. If possible, it should begin from an already existing input which is familiar to the user, and from which he or she knows is leading to reliable results.

8.2.1. Input data sources

Input data sources should be plant specific and provided with a reference to the exact sources of the data used (e.g. publication title numbers and drawing numbers). The reference nuclear unit of the input deck and the state reflected by the input deck (e.g. current status and after future backfitting) should be clearly defined.

In some cases, when there are several plants of the same design, it may be useful to use a generic database for a reference plant and perform only a verification/update for credibility of the input data for a particular nuclear unit, reflecting the plant specific deviations towards the reference plant.

8.2.2. Documentation of input data preparation

The conversion of the plant data into an input deck for a particular code should be properly documented, for example, in the form of calculation notes. The major features of the publication should be:

- Sufficiently descriptive;
- Sufficiently illustrative;

- Readily reproducible calculations included in the calculation nodes.

The publication should also contain:

- Major assumptions;
- Simplifications;
- Neglected features;
- Initial conditions;
- Boundary conditions.

Initial conditions may specify whether the input refers, for example, to nominal operating or degraded conditions. At normal operating conditions, some parameters, such as humidity and temperature, may deviate within the range of the parameter, as given in the technical specifications of the plant, based on the purpose of the analysis.

Boundary conditions and sources during a transient should be clearly identified. For example, the availability of certain safety or operational systems should be properly modelled according to the scenario of the accident analysed.

The input data description should refer to a properly identified input deck (e.g. name and date of creation). A system of keeping track of changes in the input deck and the relevant document (part of the quality assurance plan) should be elaborated and operated.

It is advisable to provide comments for the input decks, to ease interpretation, handling and identification. An input deck can be considered well commented if the comment lines are about 30% of the total input deck.

8.2.3. Input deck qualification

The quality of the input can be enhanced by an internal or external review process, when different reviewers either from the same or from a different organization check the correctness of the input.

An input deck has a higher qualification if it is universal, that is, if it can be applied to different accident processes with minimal changes, providing that this is permitted for the code.

For time dependent (transient) simulations, the input deck is qualified if steady state conditions are easily achievable and it is able to keep these conditions before the beginning of the transient. Unphysical oscillations may often be attributed to a poor balance of physical quantities: temperature and pressure distribution, mass flow rates, junction form loss coefficients, boundary

conditions, etc. It should be noted that also for containment analyses, there are required stable initial conditions before starting the transient analysis.

Input decks for real plants can be qualified by comparison to relevant calculations of transients, which have happened in the particular or in a similar plant.

The quality of the input deck is also greatly enhanced if the possible range of the input parameters is identified (e.g. by operating states or known measurement errors) and if their influence on the predicted results is quantified. This approach is especially recommended if uncertainty in the input parameters is significant.

Remaining unresolved issues should be clearly identified by the input deck developers.

8.3. VALIDATION OF INPUT MODELS

The purpose of the validation of the input model is to demonstrate that the input model adequately represents the behaviour and the functions of the modelled system. Recommended steps for the validation of an input model for design basis accident analysis are described in Ref. [6].

If the severe accident input model has been derived from a qualified input model for design basis accident analysis, the results of the initial transient of both models should be checked against each other to validate the thermohydraulic part of the severe accident input model.

Furthermore, checks should be performed for:

- (a) Steady state response;
- (b) Mass and energy balances;
- (c) Time step convergence (sensitivity calculations with variation of the time step size) and spatial convergence (sensitivity calculations with variation of the core/primary system/containment meshing);
- (d) Behaviour and function of system components;
- (e) Timing of events (i.e. cladding rupture, onset of zirconium oxidation, beginning of fuel melting, relocation of fuel to the lower plenum, vessel failure);
- (f) Timing of some key events and key parameters (integral hydrogen generation, fission product release fractions, peak temperatures and pressure response, cavity ablation, etc.).

The predicted plant behaviour should be consistent with the expected plant behaviour. The timing of events in the accident sequence and key

parameters, such as the hydrogen generation and peak temperatures, should be checked by engineering judgement, taking into account the experience from integral experiments as well as the results of other available severe accident analyses. This requires a detailed knowledge about the phenomena occurring during a severe accident.

8.4. ESSENTIAL DESIGN CHARACTERISTICS INFLUENCING THE RESULTS OF ANALYSIS

The impact of different reactor designs is an important concern, since the vast majority of the experimental programmes and model development activities around the world have focused on PWR and BWR designs originating in the USA or in Europe. The lack of experiments for other reactor materials and designs results in increased uncertainties for those designs.

The core design, in particular, has an important impact on the progression of damage during a severe accident. The differences may be somewhat subtle if the core design utilizes different alloys of zirconium or different structural materials for grid spacers. Often, these differences can be handled by the use of appropriate material property correlations without significant changes in the models or modelling options used. The differences will be much greater for altogether different core materials, such as a U–Al plate, or the annular fuel elements used in many research reactor designs, or graphite moderators as in the case of RBMKs. In either of the two latter cases, alternative models as well as the use of appropriate properties would be required and may be a determining factor in the specific code that can be used.

The design of the structures surrounding the core can also have a significant impact in the latter stages of the severe accident. For example, the use of heavy reflectors on the periphery of the core may have a strong impact on the relocation of molten material from the core to the lower plenum, since the heavy reflectors may eliminate or at least reduce the likelihood of a sideways relocation of melt into the bypass region. The design of the lower core support plate and lower plenum structures can also have an impact on the relocation of core materials into the lower plenum and on the cooling of the lower head. For example, some research activities have been looking at the impact of control rod drive structures and cooling systems in many BWR designs on the cooling of debris in the lower plenum. The lower plenum structures and core plate design may also have an impact on the formation of gaps between the debris and lower head, and on the ability of in-vessel reflooding to cool the lower head. The detailed codes may have general enough models to address the impact of these structural design features in most cases,

however, even the detailed models in these codes may be based on assumptions that are not consistent with all of these design features. Thus the user should review the basic model assumptions to determine whether modelling changes are necessary. In most cases, the integral codes have predefined structures and so the user has a limited ability to make changes in the way these structures are modelled.

The design of the remainder of the reactor coolant system will also be a significant factor in the analysis of severe accidents. For example, leakage paths in the vessel upper plenum region may have an impact on the natural circulation patterns in the vessel. The design of the hot leg piping and the balance of the reactor coolant system piping will also have an impact on natural circulation in the hot legs or loop, and may ultimately determine the nature of the heating and failure of reactor coolant system structures, including the vessel. In this case, the detailed codes should be capable of modelling such features of the design, the most critical factor being the development of a realistic and accurate input nodalization for the system. In many cases, in addition to the review of code specific input guidelines, it is also good practice to review the input models that have been developed for plants of a similar design in order to determine what design features may be the most significant. With the integral codes, since the nodalization of the reactor coolant system is much less flexible and significantly less detailed in most instances, it may or may not be possible to represent the different features of the reactor coolant system. In this case, it is particularly important to use a version of the code that has been specifically designed for the plant.

The availability and capacity of safety systems, such as a high pressure safety injection system, low pressure injection system, accumulators and pressurizer valves for the primary circuit, may also be important design features in determining the nature of the accident. However, since it is necessary to assume the failure of one or several safety systems for the primary circuit in order that a design basis accident develops to a severe accident, modelling of the failed systems may be unnecessary. Furthermore, it is unlikely that the failed systems can be recovered by repair during the short time span of the in-vessel phase of an accident (generally only several hours from the initiating event up to vessel failure). However, in the event that the system was off because of operator error or because of loss of off-site power, recovery is possible so these systems may have to be modelled. Much as in the case of the balance of the reactor coolant system, the detailed codes should be able to model these systems adequately while the integral codes will depend very much on the design of the system and version of the code used.

The design and the concrete composition of the reactor cavity, as well as the compartmentalization of the containment, in particular, have an important

impact on the progression of damage during the late phases of a severe accident progression. In many cases, these differences can be handled by the use of appropriate material property correlations, appropriate containment models and proper modelling options. Alternative models as well as the use of appropriate properties would be required and may be a determining factor in the choice of a specific code that can be used for the analyses.

For some cavity designs, it may be necessary to model more than one location for MCCI. The reason may be either the real plant design, for example, a metal door that may be penetrated by the corium, spreading it outside the reactor cavity, or to allow modelling of a complicated structure of layers of concrete with different chemical compositions at the bottom of the reactor cavity. More than one location may also be necessary if a side wall structure fails and part of the molten pool is relocated.

Detailed codes may have sufficiently general models to address the impact of these structural design features. However, even the detailed models in these codes may be based on assumptions that are not consistent with all of these design features. Thus the user should review the basic model assumptions to determine what kind of modelling approach may best represent the specific features of the plant. In many cases, the integral codes have predefined (fixed) models and the user has a limited ability to go beyond the initially intended model capabilities.

The detailed codes should be capable of modelling the design features, the most critical factor being the development of a realistic and accurate input nodalization for the system. In many cases, in addition to the review of code specific input guidelines, it is also good practice to review the input models that have been developed for plants of a similar design to determine what design features may be the most significant. With the integral codes, since the nodalization of the containment may be less flexible and significantly less detailed, it may or may not be possible to represent the different features of the containment system. In this case, it is particularly important to use a version of the code that has been specifically designed for the plant.

The availability and capacity of safety systems, such as spray, flap valves, fans and fan coolers, and filtered venting systems, may also be important for determining the nature of the accident and obtaining a realistic prediction of the plant response.

Since it is necessary to assume a failure of one or several safety systems in the case of a severe accident, modelling of the failed systems may be unnecessary. Furthermore, it is unlikely that the failed systems can be recovered by repair at harsh post-accident conditions. However, in the event that the system was off because of operator error or because of loss of off-site power, recovery is possible.

Therefore, these systems may have to be modelled. This is particularly true for analyses related to the development of severe accident management guidelines.

The detailed codes generally are able to model the containment safety systems adequately, while some integral codes depend very much on the design of the system and version of the code used.

As stated previously, most codes include results and knowledge from experimental studies of US or western European designs. Therefore, when analysing other designs (among them, PHWRs, WWERs and RBMKs are the most frequently encountered), a code user is faced with several problems:

- (a) Whether it is possible to represent all the core, vessel and reactor coolant system elements with the code (e.g. absorber tubes in WWER-440).
- (b) Whether it is possible to extrapolate experimental results or modelling assumptions to a specific reactor feature which was never or scarcely studied experimentally (e.g. what the impact is of niobium on zircaloy oxidation and cladding mechanical behaviour in WWERs).
- (c) The need to model complex systems that are not available in a standard PWR (e.g. jet vortex condensers, installed on some WWER-440 reactors).
- (d) The possibility of extrapolating experimental results or modelling assumptions to a specific plant feature, which was never or scarcely studied experimentally, for example, the impact of the less compartmentalized containments of WWERs on hydrogen distribution.

A significant amount of applications have been performed for WWERs and, in general, the internationally widespread codes are easily applicable for analyses of the ex-vessel phenomena of WWERs.

Up to now, only a limited number of applications have been performed with internationally widespread codes for PHWR or RBMK designs and, therefore, no general conclusions can be drawn. However, it must be kept in mind that for each specific plant design, including PWRs, depending on the specific application and purpose of the analysis, some 'tricks' may be required to properly model the system and to answer the particular purpose of the analysis.

It is not the purpose of the present report to address these problems because up to now, only a limited number of applications have been performed (with well known codes) to WWER, PHWR or RBMK designs and, therefore, no general conclusions can be drawn.

Some examples are listed in Table 3, to illustrate some of the difficulties that may be encountered, and some possible ways to handle them (with reference to in-vessel severe accident analysis) [28].

TABLE 3. SOME FEATURES OF REACTOR DESIGNS NOT ORIGINATING FROM THE USA OR WESTERN EUROPE WHICH ARE IMPORTANT FOR IN-VESSEL SEVERE ACCIDENT ANALYSIS AND MODELLING

PHWR

Fuel elements are horizontal, which leads to complex three dimensional configurations as soon as a large degradation is achieved. At least, specific thermohydraulics and melt relocation models must be developed for such reactors.

WWER-1000

This design is rather similar to western PWRs, and it is recognized that the main differences come from the materials used, especially in the core: Zr-1%Nb for claddings, and B₄C for control rods. Most codes can be used to calculate such designs, provided that some material properties of Zr are changed, as well as the Zr oxidation correlation. However, proper models for B₄C oxidation and subsequent interactions with other core materials are necessary to predict core heat-up (B₄C oxidation is very exothermic, whereas SIC is not oxidized), melt progression (the presence of carbon in the melt may lead to the existence of phases with high melting temperature) and fission product transport (CH₄ and boric oxide are produced in the same proportion as iodine). Another important difference is the horizontal steam generator tubes.

WWER-440

The same materials as for WWER-1000 and additional specific features:

- Large tubes of control material containing fuel rod bundles.
- After power shutdown, some fuel elements are moved below the initial core level.

These features usually require some ‘tricks’ to be modelled with widely used codes, and may lead to non-reliable results if the modelling is not assessed.

TABLE 3. SOME FEATURES OF REACTOR DESIGNS NOT ORIGINATING FROM THE USA OR WESTERN EUROPE WHICH ARE IMPORTANT FOR IN-VESSEL SEVERE ACCIDENT ANALYSIS AND MODELLING (cont.)

RBMK

This design is very different from western PWRs and is very difficult to model with standard codes. However, it should be noted that in each graphite channel, the fuel rods are similar to western ones: UO_2 pellet and Zr cladding. Therefore, the degradation process in each channel may be well predicted by standard codes (up to the graphite failure), provided that the thermohydraulic behaviour is modelled properly.

Among the specific features of RBMKs mentioned, the following are included:

- Weak self-shutdown of the chain reaction (coupling with neutronics at the beginning of the accident);
- Heat conductible, hot graphite with high heat capacity; strong heat exchange between channels and graphite; consequently, the low probability of fuel melt due to decay heat;
- Long fuel assemblies in the channels that are located in graphite and biological shielding, with the long piping of the cooling circuit located in the compartments below and above the reactor core;
- Relatively large (related to 1 MW power) amounts of water and steam as well as accumulated energy there; rather slow change of the steam pressure;
- Steaming and flow stagnation problems are possible in a peculiar geometry of reactor coolant system piping of the RBMK reactor — the complex steam separation, stratification and other similar phenomena can take place at low velocities of coolant flow;
- Axial heat and mass exchange in the steam without a closed circuit for its natural circulation, influencing also the steam starving of the steam-zirconium reaction;
- Rather limited strength of the reactor cavity (danger of upper metal plate lift-up by overpressure higher than 2 bar) in the case of multiple fuel channels rupture.

The accident localization system does not enclose the steam water piping, steam lines and drum separators, the untight reactor hall above the reactor and the drum separator compartments connected to this hall.

8.5. MAIN REQUIREMENTS FOR BEST ESTIMATE SEVERE ACCIDENT ANALYSIS

The aim of a best estimate analysis is to represent the plant behaviour as realistically as possible according to state of the art knowledge. A more

extensive explanation of the best estimate approach and the difference to the conservative approach is given in Ref. [6].

A completely conservative approach cannot be applied in the analysis of a severe accident because a conservative assumption for one parameter may lead to a non-conservative response for another parameter. For example, a low failure temperature (i.e. temperature for the onset of relocation of molten material) is conservative with respect to the time of vessel failure but not with respect to hydrogen production.

Use of a best estimate code is a basic requirement for a best estimate analysis. A best estimate code combines the best estimate models necessary to give a realistic estimation of the overall response of a plant during an accident. Thus, a best estimate code must, firstly, not contain models which are intentionally designed to be conservative (such models can be included as an option); and secondly, contain sufficiently detailed models to describe all the relevant processes during the transient of a severe accident.

The detailed codes are generally designed to be best estimate codes. For the early phase of a severe accident up to the formation of large amounts of molten fuel in the core, the experimental database is sufficiently large, an understanding of the phenomena is good and the models are adequately detailed and validated. However, for the late in-vessel phase of a severe accident, the experimental database is still poor (particularly with respect to the scale), the models have more modelling parameters, are less general and not well validated. Thus, there may be significant differences in the predicted trends of this phase of the accident, even using comparable detailed codes. As a result, it will be particularly important to assess the impact of modelling uncertainties on the predicted plant behaviour. The fast running codes may contain best estimate models for some phenomena, but not necessarily for all of the relevant phenomena. It is, therefore, difficult to use them for a best estimate analysis because of large uncertainties in some of the models. Their main fields of application are parametric studies and PSAs. However, even for PSAs, many organizations or institutes now use a combination of fast running code, best estimate codes (to justify some assumptions or provide relevant input to the fast running codes) and specialized codes (for lower head mechanical behaviour, for example).

Use of a combination of codes is recommended whenever a single code (even a best estimate code) cannot provide a relevant answer due to insufficient modelling or too large an uncertainty. In order to perform a best estimate severe accident analysis, the following requirements should be met:

- (a) Preferably use a detailed code for the analysis;
- (b) Choose the models and parameters regarded as best estimate;

- (c) Once chosen, these should normally be the default models and parameters;
- (d) In the case of a choice between several models, the sophisticated model is preferred over the parametric model, as it contains generally lower uncertainties;
- (e) The user guidelines of the code should be checked for recommendations;
- (f) Check the validation reports of the code if the validation work was performed with a common set of models and parameters or if the fitting of models and parameters was necessary in certain cases.

8.6. RECOMMENDATIONS FOR A BOUNDING ANALYSIS OF A SEVERE ACCIDENT

The choice of a bounding scenario of a severe accident is plant specific and, therefore, a unique bounding scenario for a particular plant design does not exist. It depends on the purpose of the analysis. The idea is to obtain the most severe response of the system related to a specific criterion. For example, if the analysis is done for the sizing of a recombination system, the bounding case would be a scenario that leads to highest and fastest concentrations of combustible gases. Another example is an analysis for determining a maximal source term. In this case, another scenario will represent a bounding case for the same plant design.

For the first example, most severe conditions appear in the case of a large break LOCA with a total loss of emergency core cooling system, because in this case, the time of corium ejection to the cavity is shortest, the decay heat associated with the corium is highest and the MCCI is most severe.

For the second example, the bounding case would be a case of early containment failure, followed by a major release of fission products to the environment. To define such a bounding case, it is necessary to determine the possible mechanism of early containment failure (DCH, steam explosion, hydrogen detonation, etc.), to determine the probability of the occurrence of each of these phenomena, as well as timing and size of impact on the containment integrity. As a result, it may be determined to be a bounding case, leading to the most severe source term as a result of an early containment failure.

8.7. ASSESSMENT OF UNCERTAINTIES

As set out above, a conservative approach is not appropriate for severe accident analyses. On the other hand, a best estimate approach requires dealing

with the related uncertainties. Three major sources of uncertainty in accident analyses have been identified and are discussed for design basis accident analysis in detail in Ref. [6], as follows:

- (1) Code uncertainty, which is associated with models and correlations, the solution scheme, model options, not modelled processes, data libraries and deficiencies in the codes;
- (2) Simulation uncertainty, associated with the inability to model the real plant exactly due to idealization of the complex geometry, three dimensional effects, scaling effects, simplification of systems, etc.;
- (3) Plant uncertainty, associated with errors in measuring and monitoring the real plant behaviour, such as reference plant parameters, instrument errors, system component set points, etc.

An additional source of uncertainty is user effects, which can be lumped with the three uncertainties presented previously. However, user effects can be reduced by training, availability of extensive user guidelines for the codes, input model verification and validation [6].

In the field of in-vessel severe accident analysis, code uncertainties exist with respect to the following issues:

- (a) Modelling of late phase phenomena, that is, molten pool formation and growth, corium slump, vessel failure mechanisms, etc., is not very sophisticated;
- (b) Measured material properties at high temperatures have large uncertainties; the fuel properties are changing with the burnup;
- (c) Many material interactions are not modelled directly in the codes but are taken into account by modifying melt temperatures in the input data; the mechanisms leading to early fuel slumping, as observed in the PHÉBUS-FP experiments, are not well understood.

In the field of the ex-vessel phase of severe accident analysis, code uncertainties exist with respect to the following issues:

- (a) Modelling of late phase in-vessel phenomena, in particular, reactor pressure vessel failure mechanisms leading to uncertain boundary conditions for the ex-vessel phase;
- (b) Modelling of the in-vessel melt oxidation and H₂ production;
- (c) Modelling of melt dispersal (if it takes place);
- (d) Material properties at high temperatures have large uncertainties;
- (e) Many material interactions are not modelled directly in the codes;

- (f) MCCI models do not always represent the physics and chemistry of the associated processes with sufficient detail;
- (g) Deficiencies of the lumped parameter codes in modelling the thermohydraulic response of the containment, with a tendency to give uniform distribution of steam and hydrogen concentration, underpredicting of thermal stratification, etc.;
- (h) Deficiencies of the lumped parameter codes in modelling the natural convection inside the containment with a tendency to give reduced flows, reduced flow velocities and, associated with that, reduced heat transfer coefficients between the containment atmosphere and the containment walls and structures;
- (i) Deficiencies in the prediction of possible gaseous iodine existing in the primary circuit;
- (j) Possible uncertainties of the influence of the in-vessel phenomena during the ex-vessel phase.

For more detailed information on uncertainties in the modelling of the relevant phenomena, see also Section 4.3 and Appendix II. Additional uncertainties may come from the extrapolation of small scale experiments to full scale plant calculations. The scaling uncertainties strongly depend on the particular phenomena.

A method often used to assess uncertainties is the performance of a parametric study. A few parameters or model options are varied independently to see their particular impact on key results. The selection of key results is dependent on the objectives of the analysis. If the analysis deals with hydrogen mitigation measures, hydrogen and steam production rates as well as the total amounts are of primary interest.

A general problem of the parametric method lies in the fact that, while varying one sensitive parameter for the others, best estimate values must be kept. Thus a huge number of calculations are required. To overcome this problem, different methods have been developed or are still being developed, including:

- (1) The uncertainty method based on accuracy extrapolation, developed by the University of Pisa, Italy [96]. This method uses a set of integral experiments to extrapolate the accuracy for experiment calculations to plant calculations.
- (2) The AEA-T method [97]. The uncertainties are characterized by reasonable uncertainty ranges and, by combining these ranges, a bounding analysis is performed.

- (3) The IPSN method using SUNSET [98], the GRS method using SUSANA [98] and the ENUSA [100] method assign probability distributions of selected sensitive parameters to uncertainty ranges for key results.
- (4) The code scaling, applicability and uncertainty methodology developed by the United States Nuclear Regulatory Commission (NRC) [101, 102].

The different methods were compared by an OECD/NEA/CSNI study using a small break LOCA experiment in the Large Scale Test Facility at JAERI, Japan [104, 105]. It came out that the major differences between the predictions of the methods came from the choice of uncertainty parameters and the quantification of the input uncertainties (uncertainty range, probability distribution).

The uncertainty methods listed above have not yet been applied extensively to real plant severe accident analysis although a form of the code scaling, applicability and uncertainty methodology developed for severe accidents [103] was utilized by the NRC in the resolution of DCH issues in the USA. Smaller applications, such as an IPSN uncertainty analysis with SUNSET and ICARE2 for the experiment PHÉBUS-FPT1 [88], have proved that these methods are suitable also for severe accident analysis. The methods provide a good picture of the uncertainty range of the examined parameters. A drawback of those methods is that they require the performance of many calculations, that is, they are more suited for the fast running codes, and that a lot of preparatory work is required to select uncertain parameters, to determine their range and probability distribution form.

For the design of accident mitigation measures, such a method which uses a mathematical tool to limit the number of required calculations is very helpful. The advantage of such methods is that the number of selected uncertain parameters does not influence the number of necessary calculations. Since it could be demonstrated that with complex system codes, such as MELCOR, uncertainty studies can be performed. These methods can be recommended, however, it is very important to start with a careful selection of uncertain parameters and their uncertainty range. Although an independent selection by different experts and use of a structured expert judgement procedure would certainly improve confidence in the uncertainty bands for the key results, it seems not yet adequate for usual plant analysis.

Other and simpler methods exist to quantify the uncertainty of a limited number of parameters. A limited number of calculations are performed, with variation of one or a few input parameters, regarded as sensitive by experience and expert judgement, to obtain an uncertainty range for one or a few output

parameters. Those methods can be used to quantify the uncertainties for special tasks, for example, corium coolability.

General uncertainties can be also defined by code to data comparisons for each code through development assessment and through independent validation activities. For example, see the discussion of uncertainties contained in Refs [104, 105] or the results from ISP 41.

Additionally to the uncertainty analysis, and sometimes together with it, it is useful to determine the sensitivity of the results to the input parameters. Several methods exist, which may help in the analysis of a result, and which would avoid the need for doing a large number of calculations to obtain a reliable result.

8.8. PRESENTATION OF RESULTS

8.8.1. Form of presentation

The recommendations for the presentation and evaluation of results given in Ref. [6] also apply to severe accident analysis. The results of the analysis should be structured and presented in an appropriate way to provide a good understanding and interpretation of the course of the severe accident. The primary targets of the analysis should be clearly addressed. The initial and boundary conditions and the representative parameters of the severe accident scenario chosen for the analysis should be clearly characterized.

The structure and format of the presentation should permit the entire process of the accident to be followed, in order to check easily the chosen acceptance criteria, and to compare the results of this analysis with the results of other analyses.

The results should include a set of key parameters, displayed as a function of time. The presentation of the results should contain at least key parameters reflecting the course of the severe accident and its main phenomena. These additional key parameters are for the in-vessel phase of a severe accident as a function of time and may include:

- (a) Temperatures of fuel, cladding and absorber materials;
- (b) Fill gas pressure and the maximum cladding diameter of the fuel rods (ballooning);
- (c) Hydrogen generation rate;
- (d) Fission product and aerosol release rates;
- (e) State of the core with loss of integrity of original core structures, relocation of liquefied material, molten pool formation and growth,

relocation of upper plenum structures, molten pool slumping, debris formation due to quenching or collapse of structures, etc.;

- (f) Masses, the state (solid or liquid) and the distribution of the different core materials, such as cladding, oxidized cladding, fuel and absorber — and overall values;
- (g) Mass and energy balance;
- (h) Time of cladding rupture (beginning of fission product release);
- (i) Time of molten pool formation in the core;
- (j) Time of corium relocation to the lower plenum;
- (k) Time of vessel failure;
- (l) Final state of the core with fractions of oxidized zircaloy, molten fuel and fuel relocated to the lower plenum;
- (m) Integral hydrogen generation;
- (n) Integral fission product release and aerosol generation;
- (o) The fraction of fission products retained in the fuel and in the primary circuits;
- (p) Maximum fuel temperature.

Examples of key parameters for the ex-vessel phase include:

- (a) Time of vessel failure and the mass of corium ejected to the containment;
- (b) Evolution of temperatures and pressure in the reactor cavity and in the containment;
- (c) Integral hydrogen generation inside the reactor pressure vessel;
- (d) Generation rate of combustible gases due to MCCI;
- (e) Fission product and aerosol release rates due to MCCI;
- (f) Energy rates due to decay heat, chemical reactions and heat transfer to the concrete and to the control volume (MCCI);
- (g) Energy balance for the MCCI — integral energies due to decay heat, chemical reactions and heat transfer to the concrete and to the control volume;
- (h) Masses, the state (solid or liquid) and the distribution of the different corium materials, stratified or mixed state, temperature, volume, height, density and mass of the layers at the bottom of the reactor cavity;
- (i) Aerosol distribution inside the containment and iodine volatile concentration evolution;
- (j) Distribution of combustibles inside the containment compartments, existing conditions for deflagration or for a deflagration to detonation transient;

- (k) Parameters related to a filtered venting system — filter loading with aerosols, decay heat inside the filter due to the accumulation of radioactive aerosols.

Use of a nuclear plant analyser (e.g. ATLAS [106] for ATHLET-CD, NPA and RELSIM for SCDAP/RELAP5, MELSIM for MELCOR) or other graphical displays (e.g. VISU for ICARE2, ATLAS for COCOSYS), capable of showing the state of core and vessel, the primary circuits and the containment as a function of time, is very important for the interpretation of results.

The report should also indicate results of sensitivity analyses and some indications of the code performance. The overall report of the analysis should allow the independent reviewer to be able to repeat the analyses solely using the information available in the report.

8.8.2. Evaluation and interpretation of physical phenomena in the results

After a set of calculations has been performed, the main physical processes and events should be identified and evaluated from the results, and interpreted in an evaluation report. Interrelation of different physical processes (e.g. thermohydraulics and fission product transport, or thermohydraulics and hydrogen distribution) should be evaluated if applicable.

Depending on the purpose of the analysis, a proper acceptance criterion should be selected and the results should be compared with the selected value.

Selecting a bounding case, which leads to more serious conditions for the evaluated accident, may ease the categorization of the accidents and of the obtained results (see Section 8.5).

The recommendations for the presentation and evaluation of results given in Ref. [6] apply also to severe accident analysis. The results of the analysis should be structured and presented in an appropriate way to provide a good understanding and interpretation of the course of the severe accident. The primary targets of the analysis should be clearly addressed. The initial and boundary conditions and the representative parameters of the severe accident scenario chosen for the analysis should be clearly characterized.

The results must be documented according to the quality assurance requirements. Finally, the presentation of the results should contain conclusions clearly addressing the achievement of the primary objectives.

9. SUMMARY AND CONCLUSIONS

The continued reduction in the potential for, and consequences of, severe accidents will play an important role in the operation and development of NPPs and the associated improvements in standards of living worldwide. Improved training, effective accident management strategies and, ultimately, the development of more advanced reactor designs will continue to be the cornerstone of such a reduction. Fortunately, these activities can benefit from more than two decades of severe accident research and, in particular, the extensive suite of severe accident codes that embody the lessons learned from that research. However, the successful application of these codes requires that the end-user have a firm understanding of the important trends and phenomena associated with severe accidents.

As discussed in Sections 2 and 3, the behaviour of a plant during a severe accident is affected by a complex range of thermal, mechanical and physical processes. For example, the consequences of reflooding the reactor core will depend on the state of the core at the time of reflood. Reflooding during the initial stages of an accident, before melting of any rods or structures has occurred, should result in the rapid quench of the core. Reflooding during the early phases of core degradation can result either in the shattering of fuel rods, formation of debris and release of fission products into the containment, or even, if the peak temperature is higher, in an increase of zircaloy oxidation and rapid heat-up of some parts of the core, leading to the formation of large blockages or even molten pools, and the release of significant quantities of hydrogen and fission products. Reflooding during the later stages of the accident, once molten pools have been formed, may be largely ineffective in cooling much of the core. The exact response associated with reflood will also depend strongly on the reactor design. The injection point and mode of flooding, that is, top (from hot leg) or bottom (from cold leg) flooding, the use of control rod drives, or ex-vessel flooding may also determine the effectiveness of the flooding process. The design of the reactor core is also important in determining the impact of different severe accident phenomena. For example, the type of grid spacers used, such as Inconel or zircaloy, may determine the temperature at which fuel cladding liquefies and initial fission product release from the fuel rod occurs. The design of the reactor cooling system can also be critical in the overall performance of the plant during a severe accident. The location of loop seals and the orientation of the piping may determine when and where the initial failure of the system occurs. Hot leg natural circulation, for example, can be a significant factor in determining the

likelihood of high pressure failure of the vessel, melt ejection and spreading (DCH risk), and the likelihood of early containment failure.

The ability to accurately predict the response of the NPP during a severe accident using a severe accident code will also depend on the type of computer code used, the accuracy of the modelling options used in the code, and the experience of the code user. As discussed in Sections 4 and 5, there is a wide variation in the type of modelling approaches and the accuracy of the individual models used. In general, integrated codes allow the user to model both the reactor coolant system and the containment but have more parametric models that must be tuned by the user. Because these codes were intended to be fast running, modelling accuracy was of less concern than speed. In addition, the users of integrated codes can have much more impact on the overall predicted response of the plant, because of the large number of modelling parameters that must be set. The mechanistic or detailed system thermohydraulic codes are typically limited to the analyses of the reactor coolant system. In these codes, modelling accuracy is more important than speed, so the level of modelling detail and the number of phenomena considered is higher than in the integral codes. In their case, the user also has a much more limited set of modelling parameters to set and so has less impact on the overall results. The dedicated codes typically are the most detailed but are limited in the scope of the phenomena that can be considered. In cases where the data are limited, these dedicated codes are often used to help define the accuracy of the detailed codes or to reduce the overall uncertainties when analysing a particular process. For example, a detailed three dimensional stress code may be used to reduce the uncertainties in vessel failure times and locations, as predicted by the other codes using zero dimensional or one dimensional models.

The overall accuracy of the codes and, in some cases, the expected uncertainties in important processes, are determined through extensive verification and validation activities. As discussed in Section 6, the results of these activities are normally described in the documentation included with the codes. In addition, independent validation activities, performed by organizations outside the group developing the code, are carried out for many of the codes discussed in this chapter. As a result of these activities, it has been generally concluded that the uncertainties in predicting the early phases of a severe accident are relatively small, in particular for the detailed codes, while the uncertainties for the later stages are still relatively large. In addition, the uncertainties associated with the reflooding of damaged cores or debris beds are also still relatively large.

Unfortunately for the end-user of the codes, particularly those users who have not previously been involved in severe accident research programmes, quantitative conclusions regarding the overall accuracy of the severe accident

codes and models for a full range of accident conditions are still incomplete. There are a number of reasons why such definitive conclusions are lacking. However, most importantly: (a) the difficulty of running severe accident experiments, particularly for the late stages of the accident; and (b) the large number of important phenomena – the number of experiments that have been performed is still limited, relative to the large number of experiments performed to validate system thermohydraulic codes for design basis accident conditions. As a result, the scalability of such experiments to the size of the NPP and to plant designs other than TMI-2 is still uncertain. In addition, multi-dimensional effects, particularly as far as the coupling between vessel thermohydraulics and core degradation is concerned, are not well characterized. For this reason, dedicated codes, such as CFD codes, have been employed to help define the uncertainties in many of the codes, and in some cases, are still being used along with the detailed codes to help reduce uncertainties for specific applications.

The qualifications of the end-user also have a significant impact on the overall uncertainties in the prediction of plant behaviour. As noted in Section 4.3, the effect of the user may be increased due to the necessary estimate of modelling parameters that may have a significant impact on the results. This is particularly true for the integral codes, where parametric models with extensive user parameters are used. The user effects are also increased because the application of these codes requires some understanding of severe accident phenomena that may be rarely discussed at the university level. Thus, additional, specific training for individual users is often required when using these codes to cover the lessons learned from the past and ongoing severe accident research programmes.

As discussed in Section 7, applications of severe accident analysis and codes have increasingly moved to support training, the development and validation of accident management programmes and severe accident mitigation, and plant simulators. Application of severe accident analysis and codes has also increasingly been used to support the design and operation of new plants. Other more historical applications still continue. For example, integral codes are still widely used to support PSA activities, while the detailed codes are being used to help resolve important severe accident issues. Yet, in recent years, detailed codes have also been used at some stages of PSAs, to justify some assumptions. The newer applications, training, accident management and mitigation, and plant simulators have, to a large extent, been supported by the enormous increase in computing power as well as work to improve the speed and reliability of the different severe accident codes. In some cases, even the detailed codes can run real time applications on relatively inexpensive personal computers or workstations. Applications to training and

plant simulators have also been increased by the development of improved graphics displays that help users to interpret the results faster with a comprehensive view of the situation.

Selection of the most appropriate severe accident code or codes should consider: (a) the potential use of the code; (b) the definition of the pertinent acceptance criteria for each application; and (c) the relative ranking (and availability) of the code. Applications requiring the highest level of accuracy, such as training, plant simulators, or development of accident management or severe accident mitigation strategies, may require a combination of detailed codes and dedicated codes, depending on the level of accuracy required. Applications requiring lower levels of accuracy, such as the support of a severe accident or, more specifically, integrated source term calculations, may require a combination of the integral codes and detailed codes, again depending on the level of accuracy required. The definition of pertinent acceptance criteria, in particular, those applications requiring the highest level of accuracy, will define the need for and specific type of dedicated code that may be required. Use of steam explosion codes, for example, may be necessary to look at the relative risks associated with flooding of the outside of the vessel to prevent vessel failure, that is, the potential reduction in risk associated with the successful termination of the accident without vessel failure versus the additional risk of containment failure in the event that the flooding was not successful. The final ranking and selection of the code, once the uses and acceptance criteria have been defined, will depend on such factors as the availability of technical support and training, the range of physical phenomena covered by the code, the quality of the models, and the overall reliability, accuracy and speed of the code or codes.

As discussed in Section 6, once the code or codes are selected, there are several components involved in the completion of an analysis of severe accidents, including: (a) development and validation of the input models for the facility to be analysed; (b) checking the results; (c) assessment of the uncertainties in the results; and (d) presentation and publication of the results. The effort involved in the development and validation of the input models is strongly dependent on the type of code that is selected and the availability of existing plant models for design basis accident calculations. In particular, the use of existing design basis accident input models as a starting point for severe accident analysis can significantly reduce the effort involved in the development and validation of severe accident input. In this instance, existing design basis accident plant models can be used directly in the detailed severe accident codes, that is, RELAP5 (or ATHLET, CATHARE) input models can be used in SCDAP/RELAP5 (or ATHLET-CD, ICARE/CATHARE, respectively). The effort involved in the checking of the results and assessment of the

uncertainties in the results is also significant. However, selection of a code or codes that includes extensive publication on the validity of the code can significantly reduce the effort involved, particularly if the code has been validated for similar transients and plant designs. The use of systematic methodologies discussed in Section 8 can also help reduce the effort, if a code is being applied for conditions where limited code specific validation documentation is available. The final step, presentation and documentation of the results, can also be simplified through the use of a nuclear plant analyser or other graphical displays showing a comprehensive view of the circuits and the state of core degradation. Specific features, such as on-line visualization or the possibility to replay the calculation, may be very useful for a quick verification of the relevance of the calculation, and for an easier interpretation of the results.

Conclusions

The ability to include severe accident conditions in the design and operation of plants, in the development of accident management and severe accident mitigation strategies, and in training activities, has been dramatically enhanced over the past few years as many severe accident research programmes have been completed and mature codes have become available for general use. The rapid growth in the speed of computers and the enhanced performance and reliability of these codes have also been a significant factor, making such activities much more affordable. However, systematic training of analysts in severe accident phenomena and in the severe accident codes being used, use of systematic methodologies to ensure the validity of any calculations or plant simulations, and the participation in technical exchanges on severe accident research and code applications, as well as participation in international research projects and ISPs, are crucial to any successful application of severe accident technology.

In addition, the continued application of these tools and the lessons learned from the past two decades of severe accident research to the development of advanced plants, operating procedures and training will help ensure that future work is devoted strictly to hypothetical severe accidents.

Appendix I

RECOMMENDATIONS FOR CONTAINMENT NODALIZATION

This section presents some recommendations on modelling of short and long term containment behaviour using lumped parameter computer codes.

I.1. GENERAL REQUIREMENTS FOR CONTAINMENT NODALIZATION

The input deck should provide reasonable estimates for severe accident behaviour under diverse accident conditions. The nodalization should provide a feasible model of the thermohydraulic response of the system for each phase of the severe accident progression. Due to the prolonged duration of severe accidents, the input deck must be reasonably simplified — a trade-off between accuracy and performance.

The input model should reflect plant specific features which may influence the overall course of the accident progression. While developing the nodalization of the system, the following must be pursued:

- (a) Realistic prediction of the timing for key events during the accident progression;
- (b) Realistic timing and rate of fission product release and retention in the containment system;
- (c) Realistic evaluation of the integral quantity and generation rate of combustible and non-condensable gases;
- (d) Proper modelling of the decay heat distribution;
- (e) Ability to model the application of severe accident management guidelines;
- (f) Proper models and logic of the engineered safety features;
- (g) Special attention to the heat structure models;
- (h) Retention of radionuclides and the expected source term depends strongly on the amount of surfaces introduced in the model (in particular, horizontal facing upward heat structures);
- (i) The thermohydraulics response of the containment — decay heat distribution, heat transfer between adjacent compartments.

In theoretical terms, the best way would be to start with a fine nodalization or with a corresponding CFD calculation and then simplify the nodalization where possible. In day to day work, the user should try to make use of already existing nodalizations and the experience gained with them.

I.2. SPECIFIC REQUIREMENTS AND GENERAL REMARKS

The node size is governed by several factors:

- (1) Numerical stability;
- (2) Run time and time step management;
- (3) Spatial convergence.

Therefore, it is advisable to avoid nodalization, where a sharp density gradient coincides with a junction (a liquid interface, for example) during most of the transient. It is good practice to eliminate minor flow paths that do not play a role in system behaviour or are insignificant compared to the accuracy of the system representation. Numerical stability requires that the ratio of the node length to diameter be greater than 1. This is a lower limit for node sizing. The modeller should try to obtain the length of volumes in such a way that they have similar material Courant limits. Portions of the model containing a 'free surface' are nodalized in such a way that the free surface lies approximately midway between the node boundaries. Multiple, parallel flow paths generally must be combined. In many cases, the nodes correspond to compartments in the building or several lumped together rooms to a single volume. Often it is necessary to subdivide one compartment (e.g. containment dome).

The model of the environment zone as a sink for potential leaks should be modelled, considering that it is the sink for the source term (leak of fission products) and that it provides the thermal boundary conditions for the outer walls of the containment.

I.3. NODE SIZE

Typical node sizes for containment models are in the order of 10–1000 m³. In many cases, the nodes correspond to subcompartments in the building, but the user has the freedom to lump together several rooms to form a single computational zone. Lumping together rooms, or artificial subdivision of large volumes (e.g. the dome), is guided by an engineering idea about the anticipated thermohydraulic behaviour, with assumptions about zones of thermal stratification or homogeneous conditions. The user must provide sufficient degrees of freedom for the model in order that the relevant conditions can be mathematically simulated, subject to a number of consistency conditions.

I.4. NUMERICAL DISPERSION

In lumped parameter models, the advective transport of heat, humidity or gas concentrations is calculated by a numerical scheme with first order accuracy only. This numerical method results from the basic assumption of homogeneous conditions within the control volumes and the lack of long-distance, relative spatial ordering information. It is equivalent to the well known upstream differencing scheme in the theory of CFD. While this scheme avoids unphysical overshoot or undershoot and is numerically stable for Courant numbers $Co < 1$, it leads to a considerable numerical dispersion. The advection velocity, u , and the time step, t , are such that the Courant number is 0.5, which means that concentrations are transported by half the control volume during one time step. The dispersion effects are caused by iterative homogenization of the concentration distributions within each control volume.

The dispersion coefficient is often much greater than the molecular or turbulent effective diffusion coefficient. For example, the thermal diffusivity of ambient air is about $2 \times 10^{-5} \text{ m}^2/\text{s}$. For typical containment conditions, $u = 0.5 \text{ m/s}$, $x = 5 \text{ m}$ and $t = 2 \text{ s}$ give an artificial diffusion coefficient of $D = 1 \text{ m}^2/\text{s}$, which is five orders of magnitude greater than the thermal diffusivity. The artificial diffusion may vary locally according to the local Courant number. It can be reduced by mesh refinement, introducing smaller values for x , but only at the expense of enhanced numerical effort. There is no simple way to estimate the errors introduced by this numerical dispersion, but experience from simulating large scale experiments can help to assess the errors that would be expected for real plant predictions.

I.5. ARTIFICIAL NATURAL CONVECTION

In a lumped parameter containment model, flow velocities in junctions connecting different control volumes are calculated from the pressure differences across these junctions. Under hydrostatic equilibrium conditions, flow velocities should be zero. However, even under hydrostatic equilibrium, artificial convective flow velocities will be generated in the model by an improper nodalization scheme, as described in the following.

In the nodalization on the left hand side in the figure mentioned, the vertical hydrostatic pressure distribution differs between the left hand single node and the right hand stack of two nodes. Even if the temperature is equal for all nodes, the gas compressibility leads to a density difference between the upper and the lower node. This difference leads to corresponding hydrostatic pressure differences between the left and right flow channels, which cause an

artificial convection flow in the model. An improved nodalization is shown on the right hand side of the figure, where all vertical node elevations are aligned on horizontal planes. This alignment is necessary to avoid nodalization induced convective flows.

It is recommended that complex nodalizations be qualified with respect to the absence of artificial convective flow by running an undisturbed transient simulation with isothermal and homogeneous initial conditions. Model simulations with artificial flows would indicate a well mixed state of the atmosphere, while in reality, stratification could be present with enhanced hydrogen concentrations, etc. Thus, the errors introduced by artificial convection could lead to non-conservative conclusions.

The introduction of unspecified buoyancy sources (instrument cooling at elevated positions, hot walls or hot pools at lower positions) may lead to false predictions of convective flows. At present, there is insufficient knowledge about the interrelation of hot condensate water distribution and natural convection flow in the containment atmosphere.

I.6. CONVECTIVE MIXING

In a lumped parameter model, flow junctions generally allow only unidirectional flow, not countercurrent flow. As a consequence, if a single junction is connected to a dead end control volume, this volume will not exchange a significant amount of atmospheric mass over this junction, even if thermo-hydraulic conditions physically lead to an intense convective mixing.

The nodalizations in the upper part of the figure below do not allow the simulation of convective mixing of the cold and hot atmospheres because of the dead end configurations of the cold zones. In the lower part of the figure, additional junctions have been added to enable convective mixing flows. On the lower left hand nodalization, an additional subdivision of the top cold zone has been introduced. Without such a subdivision, both junctions to the top node would experience identical boundary conditions, which also would inhibit any countercurrent flow. The lower right hand nodalization does enable countercurrent flow if the two junctions to the cold zone are specified to have different elevations; it is recommended that each of these junctions represent half of the actual vent flow area.

Some caution is necessary if vertical double junctions are applied. Artificial convective flow may be generated over such double junctions if the junction elevations are not identical, because this will lead to differences in the junctions' hydrostatic pressure gradients.

I.7. MODELLING OF INJECTION SOURCES

In the vicinity of injection sources, such as primary system leaks or pressure relief valves, large spatial gradients exist in the temperature, concentration and velocity fields. Injection of hot primary system fluid into a large zone of the containment model leads to an immediate dispersion because the material is assumed to be homogeneously distributed over the injection zone. Thus, the large gradients are neglected almost completely. In reality, a jet or a buoyant plume may develop at the injection location, which carries most of the injected fluid to a different location.

The steam injection into zone 2 led to a calculated convective flow loop in a counterclockwise direction: zones 2, 3, 5, 4 and 2, in contrast to the experimental observation. A closer inspection showed that a buoyant steam plume carried most of the injected fluid from the injection position into zone 1, which then gave rise to a convective flow loop in a clockwise direction. A simple correction to the model was achieved by relocating the steam release position to zone 1, which resulted in the proper calculated flow direction. Another approach would be to introduce a more refined subdivision of the computational mesh in the region covered by zones 1 and 2. This approach should work even without utilizing the engineering knowledge which indicates that a steam plume is likely to exist. Evaluation of the plume behaviour at the injection point may indicate that mixing will only take place in a higher compartment.

I.8. HEAT SLABS

Heat conducting structural walls are generally modelled by one dimensional heat slabs. For practical containment analyses, it is recommended that, at most, three types of heat slabs be modelled in each zone: one for concrete, one for thin steel (up to 1 cm) and one for thick steel. An effective thickness should be defined such that total heat capacity and surface area are represented correctly. A variable discretization should be applied for the one dimensional heat conduction solution, beginning with a node spacing around 0.2 mm at the slab surface and increasing the spacing by a factor of 2 (or less) for each following interior node. A total of 10–15 nodes should be sufficient for each heat slab. The coating should be taken into account if present. When two slabs representing different materials are in contact, the mesh size near the interface should be approximately the same on both sides.

For long transients, heat transport from one zone to another by heat conduction through a common wall can be of importance, especially if the temperature levels of both zones are different over long times. In this case, the

wall should be modelled with heat exchange to both zones. In most other cases, heat slab modelling of internal walls can be simplified by assuming adiabatic boundaries at the wall midplanes, and attributing every half-wall to the adjacent fluid zone.

Appendix II

AN EXAMPLE OF DEMONSTRATING THE STEPS FOR THE ANALYSIS OF SEVERE ACCIDENTS: ANALYSIS OF SEVERE ACCIDENT TRANSIENTS IN THE SURRY NUCLEAR POWER PLANT USING SCDAP/RELAP5/MOD3.2

II.1. EXAMPLE SHOWING THE STEPS FOR ANALYSIS

SCDAP/RELAP5 and other codes, mentioned in the main body of this report and other appendices, have widely been used over the past 10–15 years to perform several accident analyses. Although the specific steps and the effort involved in these calculations have varied because of the varying objectives of the analysis activities, nearly all have included many, if not all, of the steps discussed in Section 8. Although it was necessary to select one code for the purposes of this example, it is recommended that the readers review the detailed document available for each of these codes. The reference manuals for these codes provide examples of the applications of such codes, along with detailed user guidelines which help with the specific tasks of input model development and application of these codes to a variety of problems.

The analysis of severe accident transients in the Surry nuclear power plant using SCDAP/RELAP5 has been documented in a series of publicly available reports starting in the late 1980s, published by the NRC, with the analysis of natural circulation and now including the assessment of SCDAP/RELAP5/MOD3.2, direct containment heating and steam generator tube rupture. Although several of the references are included at the end of this appendix, much of the material presented in this example was taken directly from the Development Assessment Volume of the SCDAP/RELAP5/MOD3.2 code manuals [65], which was available over the Internet from the NRC. It is suggested that this publication be reviewed for more detailed information about the input model and results obtained.

Although the development and refinement of the Surry input model, the preparation of scenarios to be analysed and other steps of the analysis activities were performed by a series of analysts over a period of years as the needs of the NRC evolved, this example summarizes the primary activities that were involved and provides very general estimates of the level of effort that might be involved at each of the representative steps of the analysis activities. The level of effort presented reflects a relatively advanced level of experience by the analysts, as well as the fact that the code has been widely used for such applications for over 15 years.

Step 1: Specification of the facility and the objectives of the accident analysis

The Surry NPP was selected as a representative 3-loop Westinghouse plant. In this case, detailed information was available for the plant that allowed the analysts to develop accurate representations of the facility. This plant had also been used by the NRC in a variety of analysis activities using other codes, thus, the selection also allowed the NRC and analysts to make comparisons with other calculations.

The objectives of the accident analysis effort included the following:

- (1) Developmental assessment of various versions of SCDAP/RELAP5;
- (2) Determination of the likelihood of steam generator tube rupture under a range of accident conditions;
- (3) Determination of the likelihood of high melt ejection under a range of accident conditions (to support the resolution of direct containment heating issues).

The level of effort for this step was minimal in this example, since the plant was selected on the basis of the availability of plant data and the intended objectives were not critically dependent on the plant type selected. In most cases, the choice of the facility will be equally obvious, thus, the level of effort for other applications should be comparable. In the event that the objective is defined as a validation activity, selection of the appropriate experimental facility may be more complicated because more effort may be involved in assessing the capabilities of the facility and experiments in terms of the type of validation activities needed.

Step 2: Selection of the approach to be used

Because of the variety of objectives, relative high uncertainty in the later stages of the accidents, and the importance of the results to regulatory decisions, a combined approach using a detailed (mechanistic) code with best estimate models and (in the case of steam generator tube rupture and high pressure melt ejection) conservative model input assumptions was selected. The limited number of conservative model input assumptions were established jointly by the NRC staff, analysts and code developers.

The level of effort for this step was also limited in this example. In most cases, the effort expended in this and the following step, selection of the appropriate code, will be determined primarily by the availability of alternative codes and the level of expertise of staff in the use of these codes. In the event that a code and approach are selected that have not been previously used by

staff, a significant effort might be required to review the different code options, obtain access to the code or codes, and obtain training in the use of this software. In this case, selection of the approach and the code (including time for training and technical support from the development staff of the code) may involve several weeks to a few months of effort, depending on the expertise of staff and the training available for each code.

Step 3: Selection of the code to be used

In the case of the first objective — the validation of RELAP/SCDAP/MOD3.2 — the selection of the code was obvious. For the second two objectives, the NRC had the option of using MELCOR or SCDAP/RELAP5. SCDAP/RELAP5 was selected because it was felt that a detailed analysis would be required, given the importance of the results. In this case, modelling accuracy was of prime concern. In addition, it was not necessary to model the containment performance, except for the thermohydraulic feedback to the reactor coolant system. The NRC also had an independent group of analysts run a limited series of MELCOR calculations and VICTORIA calculations to provide additional confidence in the results. The VICTORIA code is a very detailed fission product transport code and was used to check for the potential of accelerated reactor coolant system failure due to the deposition of fission products. The SCDAP/RELAP5 results were used to provide the thermohydraulic boundary conditions for VICTORIA.

The level of effort involved in this stage was minimal for this example. It is useful to refer to the comment in the previous step for the level of effort that might be required in the event that alternative codes must be reviewed and acquired, and training would be obtained.

Step 4: Determination of the methodology

The methodology to be used depended to some degree on the objective of each analysis activity. However, all methodologies had common features. Firstly, prior to the start of plant calculations, the best estimate modelling parameters were defined through a combination of direct code to data comparisons (typically, for the early phase of the accident), comparisons with other more detailed codes or models (typically, for the late phase of the accident where experimental results are limited), and engineering judgement. In this case, best estimate modelling defaults were established for the code and published in the developmental assessment reference manual for each version. In the case of SCDAP/RELAP5, once the modelling defaults are set and published by the code developers, the code will automatically use those

defaults. It is recommended in the user guidelines for the users not to override the defaults unless bounding calculations are specifically required. Secondly, representative plant nodalization studies are performed using the default modelling options. Thirdly, comparison studies are performed between the current version of the code and the previous version of the code. All these results are published in the developmental assessment reference manual. Fourthly, when bounding calculations are to be performed, the appropriate model parameters are established jointly by the analysts and the code developer (in most cases, the NRC staff).

For the first objective, the developmental assessment of SCDAP/RELAP5/MOD3.2, the approach consisted of the first three stages noted in the previous paragraph. In this case, bounding calculations are not normally performed as part of the developmental assessment. For the calculations involving steam generator tube rupture, in very simple terms, the base calculations are performed using the model defaults and level of nodalization established through the developmental assessment process, and then bounding calculations would be performed to determine the range of conditions necessary for steam generator tube rupture. In this case, bounding input model assumptions would be used that would give the earliest time of steam generator tube rupture. Similar methodologies would be used in the case of high pressure melt ejection. However, in this case, bounding input model parameters would be used that would result in the latest time for reactor coolant system failure and depressurization, and the earliest time for molten pool slumping and vessel failure.

In this case, the effort to perform the initial assessment of the code would require several months of work by the developer, since a wide range of experiments would have to be analysed and evaluated. If such results are available for the code selected in Step 4, then it would only be necessary for the analysts to review the results from the code developer's assessment activities. In some cases, it may be desirable for the analysts to repeat a representative set of the assessment calculations in the event that their experience with the code is limited. Representative assessment input models are normally included with the code, so it would not normally be required that new input models be prepared. The level of effort required by typical analysts will depend on their experience but an effort in the order of a few weeks would probably be appropriate. The effort involved in establishing the methodologies for a calculation of the steam generator tube rupture and high pressure melt ejection was in the order of a few weeks because of the importance of the anticipated results. In this case, the code developers, analysts and the NRC were involved in the decision making. The level of effort involved by the typical analyst under

similar circumstances would probably be the same with any variation, depending primarily on the level of external review and discussions required.

Steps 5–9: Input data preparation — collection of plant data and establishment of a plant database, development of an engineering handbook, verification of input data and validation of input data

In this example, a pre-existing SCDAP/RELAP5/MOD3.1 input model for Surry was used. Since there were some input changes required because of modelling improvements added to SCDAP/RELAP5/MOD3.2, it was necessary to make those changes to the plant model. Since the changes did not require any changes in the plant data, it was only necessary to review the input manuals for the new version of the code.

In this case, the experienced analysts required a few days to review the manuals, make the changes, and test and publish the changes. Less experienced users would require additional time to review the manuals, but the time involved should not increase significantly.

Although they were not necessary in this example, four other basic options were available for the development of the input models for SCDAP/RELAP5/MOD3.2, including the conversion of an existing RELAP5 input model to include the SCDAP input options, conversion of an existing input model for another detailed system thermohydraulic code, such as TRAC, conversion of an input model from a comparable plant, and the development of a new input model. The order of these options also reflects an increasing level of effort, with a few days required to convert an existing RELAP5 model, a few weeks to convert a model from another detailed system thermohydraulic code, a few weeks to several months to convert from an input model for a comparable plant (the time depends on differences between plants), and between one year to one and a half years to develop a new model. The primary factor that determines the level of effort for the conversion of a model from a comparable plant or the development of a new plant model is the availability of detailed plant design information. In general terms, the most common approach used for SCDAP/RELAP5, because of the wide use of RELAP5 and large variety of plant input models available for the code, is the conversion of an existing RELAP5 plant model by adding the SCDAP modelling options to the input.

Step 10: Preparation of scenarios

In this case, the preparation of accident scenarios included a discussion with the NRC staff to determine the scope of the effort, and the review of representative PSAs for the Surry or comparable plants to determine the

scenarios of interest. In the case of the development assessment objective, scenarios were chosen that were of interest or of possible future interest to NRC staff, so the nodalization and other assessment calculations would be the most useful. For the other two objectives, risk dominant high pressure scenarios were selected because they would be the most likely to result in steam generator tube rupture and high pressure melt ejection.

In this example, the level of effort was minimal since PSA results were readily available that allowed the selection of risk dominant scenarios that would be of general interest. In the event that such information was not available or the calculation results revealed insights into the accident scenario that had not been considered in the original PSA, the selection process could be much more time consuming and might involve an iterative process with the selection of scenarios, performance of calculations, review of the results, and an adjustment of the scenarios.

Steps 11–13: Execution of the calculation, checking of results, and presentation and publication of results

In this example, a large series of calculations were performed using different variations of the same input model (for nodalization and time step studies) and with different accident scenarios, so the execution of calculations, checking of results, and presentation and documentation of results were performed in parallel and somewhat iteratively. In most cases, checking of results was by far the most time consuming task due to the large amount of information that is computed by the code. In addition, in many cases, a review of results led to an increase in the number of new calculations. The total effort involved was several weeks, with each plant calculation normally taking between 20 and 70 hours to complete. This time was provided for a DEC 3000 workstation in 1997, run times for the Surry model from accident initiation to lower head failure at between 5 and 6 h are now typically between 5 and 20 h of CPU time on a typical personal computer.

II.2. APPLICATION OF THIS EXAMPLE TO OTHER SEVERE ACCIDENT ANALYSIS ACTIVITIES

In the example, a series of calculations was performed and documented in a matter of a few months from the initial definition of objectives to the completion of a detailed report. Two activities dominated the effort involved: review and discussion of the activities with the NRC (refining the objectives and methodologies), and review and documentation of the final results. At the

time that this work was performed, the time required to perform the calculations was a significant factor, however, this is becoming much less important as the speed of the code (through improvements in the numeric and other user features) and the speed of commonly available computers continues to improve. The preparation of input models, including the definition of accident scenarios, was a relatively small contributor because of the level of experience of the analysts, the technical support provided by the code development staff, and the ability to use an existing input model as a starting point. All three factors are important considerations when applying the lessons of this example to other accident analysis activities. Through proper training of the analysts, the selection of codes that include a strong level of technical support by the developers, and the adaptation of existing input models, the level of effort required for severe accident analysis activities can be reduced significantly. In addition, careful attention to these three factors can play an important role in ensuring the accuracy of analysis activities.

Appendix III

AN EXAMPLE OF A CALCULATION: DETERMINATION OF THE LEVEL OF NON-UNIFORMITY OF THE HYDROGEN DISTRIBUTION INSIDE A WWER-1000 CONTAINMENT IN THE CASE OF A SEVERE ACCIDENT

In general, a prerequisite to obtain qualitatively and quantitatively good predictions of the phenomena associated with the ex-vessel response of a plant under severe accident conditions is a proper modelling of the thermohydraulic response of the containment. This appendix presents an example of the methodology applied to the modelling of the containment of a WWER-1000 with the MELCOR code, including validation and application of the model. The purpose of the analysis was to determine the hydrogen distribution during a severe accident inside the containment compartments for designing and sizing a hydrogen recombination system.

Based on the plant specific geometry of the containment compartments, it was supposed that there would be a rather uniform hydrogen distribution under post-severe accident conditions. The purpose of the exercise was to:

- (1) Prove that the hydrogen distribution was rather uniform and that local accumulations which may threaten the containment integrity could not be expected;
- (2) Determine the extent of applicability of a relatively simplified containment model as part of an integral plant model (primary/secondary system and containment) for a lumped parameter code for analyses of the containment response under severe accident conditions.

In Section III.1, the methodology used for the analyses is presented: description of the models and input decks; and determination of the level of modelling detail, verification and qualification of the input deck used for determination of the hydrogen distribution and recombination. In Section III.2, the level of non-uniformity of the hydrogen distribution inside WWER-1000/V-320 containments has been determined. This appendix serves as proof that a correct methodology has been applied and contributes to the credibility of the correctness of computational results.

III.1. METHODOLOGY USED FOR THE ANALYSES: A DESCRIPTION OF THE WWER-1000/V-320 CONTAINMENT MODEL

For the purposes of analysing the hydrogen distribution inside the containment compartments, three MELCOR models with different levels of detail were developed and used:

- (1) Containment model with 11 control volumes (extracted from the full plant MELCOR model);
- (2) Ad hoc developed detailed MELCOR containment model with 29 control volumes.

Figures 2 and 3 present the nodalization schemes used for modelling of the containment of WWER-1000/V320. The WWER-1000 containment is characterized by relatively open compartments. The flow paths between the rooms have significantly large flow areas. As a result of this feature of the containment, the computational results show that thermal, steam and hydrogen stratification are not expected for all possible break locations inside this type of containment.

The containment of WWER1000/V-320 is designed in a cylindrical shape with an internal diameter of 45 m, covered with a hemispheric dome, with a total free volume of approximately 60 000 m³. The lower elevation of the containment is 13.40 m and the upper elevation is 65.25 m (the highest point of the containment dome). The borated water tank, which is designed as a main recirculation sump, is located under the containment foundation slab and is a part of the containment hermetic zone. The internal volume of the containment consists of approximately 60 compartments.

The MELCOR – 11 control volumes model of the containment is based on the information about the geometry, free volumes, surfaces, etc., as determined in the containment database. The nodalization used in the model is shown in Fig. 3 and is summarized in Table 4.

In order to achieve a better predictability of long term convection processes inside the containment, which consequently determine the resulting hydrogen distribution, a model with refined nodalization was developed. The nodalization scheme of the containment is developed in such a way as to allow tracking of the global convection flows between compartments. The model was developed with consideration to the recommendations in Appendix I, that is, mainly an attempt to eliminate artificial natural convection.

For both models, there were realistic plant specific values for the free volumes of individual compartments, as well as for the heat structures (floors,

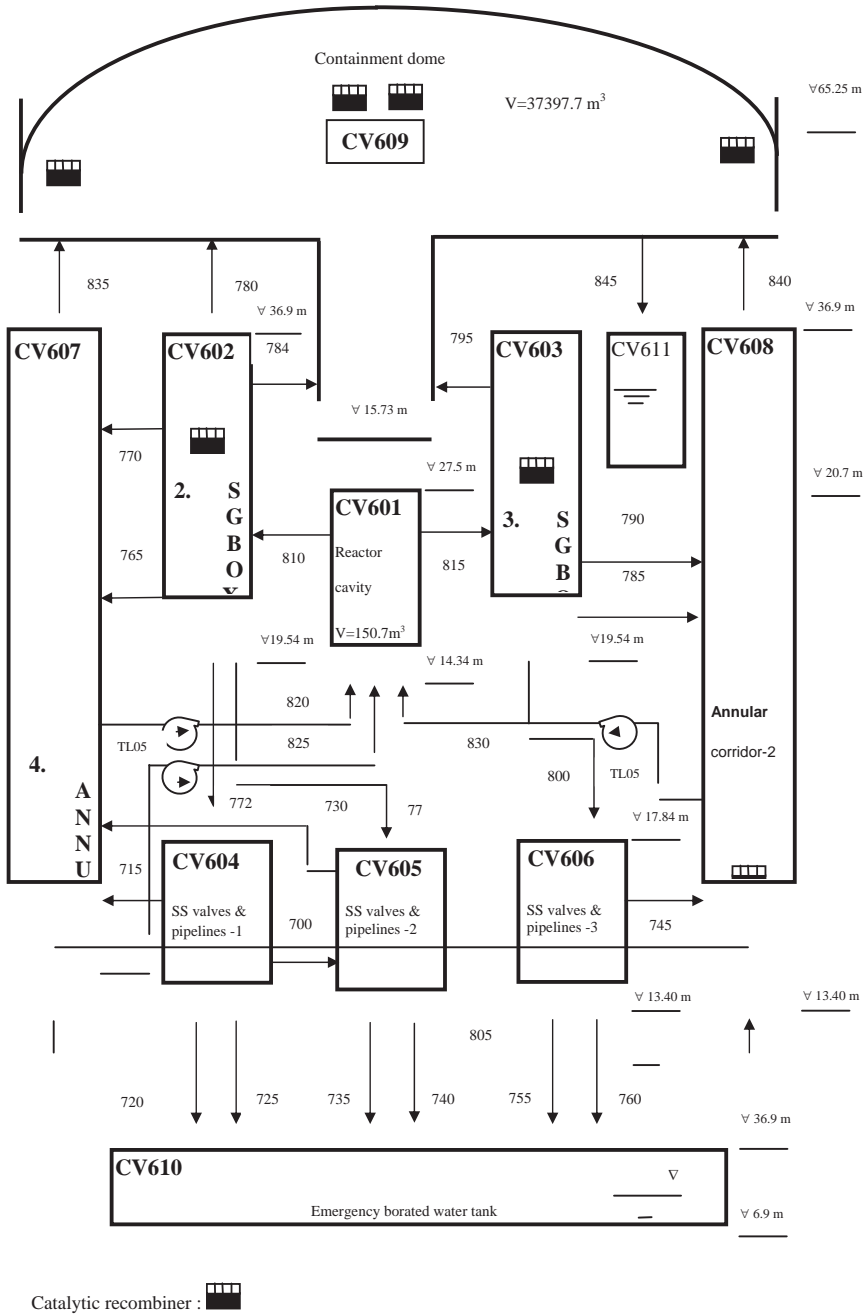


FIG. 2. Containment nodalization of WWER-1000/V-320.

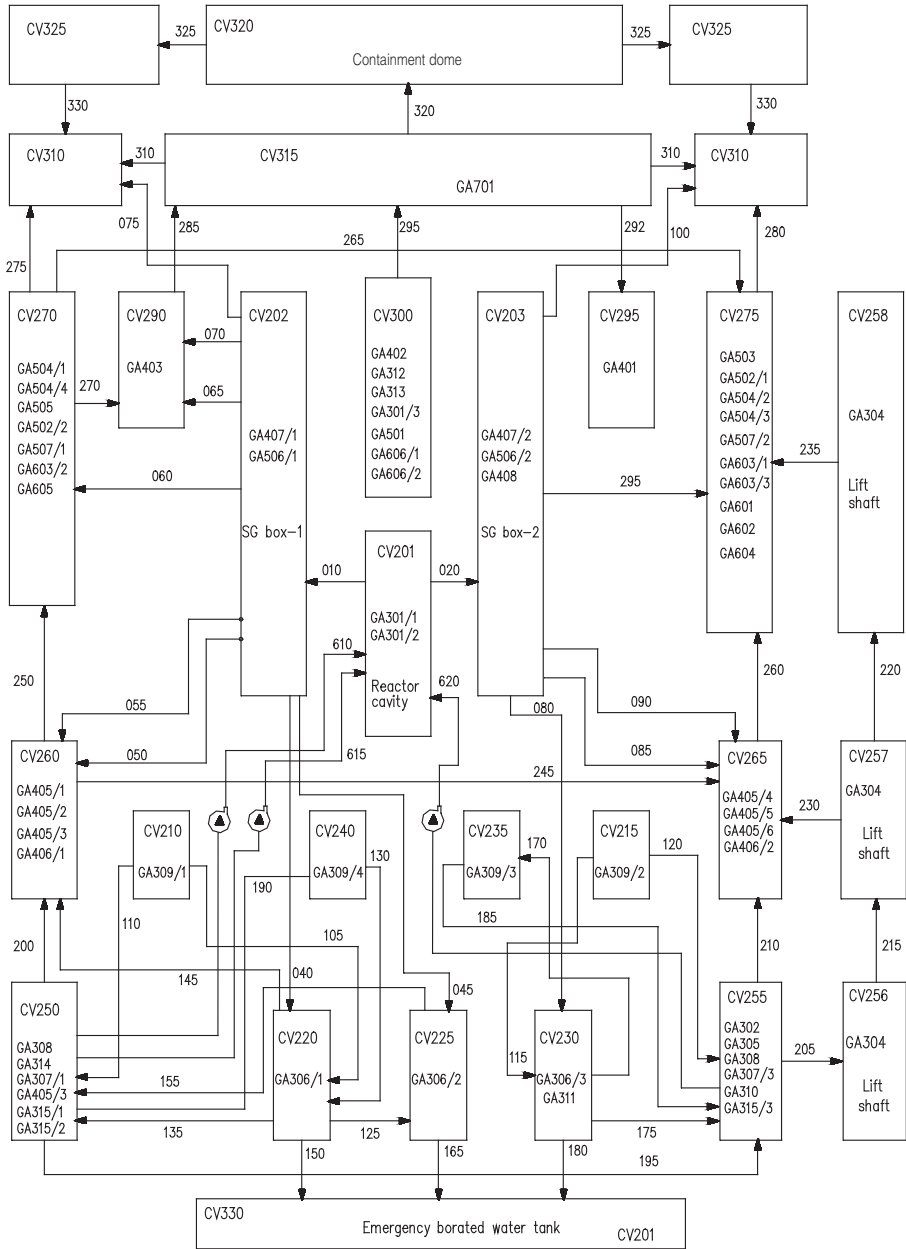


FIG. 3. Detailed nodalization of the WWER-1000 containment model for MELCOR.

TABLE 4: CONTAINMENT NODALIZATION — 11 VOLUME MODEL FOR ANALYSING THE HYDROGEN DISTRIBUTION IN A BEYOND DESIGN BASIS ACCIDENT

Node no.	Compartment name	Node identifier	Free volume (m ³)
1	Reactor cavity (GA301)	CV601	150.51
2	Steam generator box (GA407/1; GA403/1,2; GA506/1)	CV602 (<i>break</i>)	2 892.63
3	Steam generator box (GA407/2; GA408; GA506/2)	CV603	3 449.66
4	SS valves and pipes GA306/1	CV604	362.21
5	SS valves and pipes GA306/2	CV605	437.74
6	SS valves and pipes GA306/3; GA311	CV606	460.09
7	Annular corridor GA307/1,2; GA309/1,4; GA315/1–3; GA405/1–3; GA406/1; GA502/2; GA504/1,4; GA507/1; GA601; GA603; GA605	CV607	6 377.95
8	Annular corridor GA302; GA303; GA304; GA305; GA307/3; GA308; GA309/2,3; GA310/1,2; GA314; GA315/1,3; GA405/4–6; GA406/2; GA502/1; GA504/2,3; GA507/2; GA603/1–3; GA604	CV608	6 480.52
9	Containment dome (reactor hall) GA312; GA313; GA401; GA402; GA501; GA505; GA602; GA701; GA702/1–4	CV609	37 980.81
10	EBWT (sump) GA201	CV610	706.91
11	Spent fuel pool GA401	CV611	1 130.97
		Total	60 430.00

walls, ceilings, equipment) of the compartments made of concrete, steel and other materials which were introduced into the containment model.

The nodalization scheme of the detailed model (see Fig. 3) presents the control volumes and the lumping together of the compartments for each of the control volumes. Rooms with relatively big openings are lumped into single control volumes. All compartments of the hermetic zone are represented by 29 control volumes. The steam generator box compartments (GA407/1, GA506/1 and GA407/2, GA560/2) are modelled with two control volumes of

approximately equal free volume. There is no separate compartment for each primary loop. Two primary loops are located in CV202, and another two loops are located in CV203.

The pressurizer compartment (GA403) adjacent to the steam generator box is modelled as a separate cell (CV290), and the spent fuel pool (GA401) is represented as a single control volume (CV295). The four MCP motor compartments are lumped together with the corresponding parts of the upper corridor: control volumes CV270 and CV275, respectively. The reactor shaft is artificially divided into three separate rooms: lower part GA301/1, middle part GA301/2 and upper part GA301/3, to avoid artificial convection (see Section 6). The control volume CV201 corresponds to the lower and middle part of the reactor cavity, up to the bellows sealing (at elevation 26.87 m). The upper part of the reactor shaft is lumped together with the shaft for wet refuelling and cable rooms (GA606/1,2) into control volume CV300. The corridor (GA308) and the compartments of the ventilation system TL05 (307/1,2,3) at elevation 13.4 m are represented by control volumes CV250 and CV255, respectively. The three compartments of the safety systems valves and pipes (GA306/1–3) are represented as single control volumes: CV220, CV225 and CV230. The control volumes CV260 and CV265 include the middle corridor at elevation 19.54 m (GA406) and the compartments of the cooling system TL01 (GA405/1–6). The compartments, which are not in the line of the flow paths and constitute dead ends, are lumped together with their neighbouring compartments. The upper part of the containment consists of a large volume: the dome (GA701). The dome volume is modelled in such a way as to allow simulation of the convective mixing of the atmosphere in the upper part of the containment, therefore, an additional subdivision of the top zone of the containment into four volumes is introduced.

In the lumped parameter computer code MELCOR, the flow rates in the flow paths connecting different control volumes are calculated based on the pressure difference in the ‘from’ and ‘to’ volumes. When there are equilibrium conditions, the flow velocities should be zero. Even under hydrostatic equilibrium conditions, however, artificial convective flows between the control volumes may be established. The control volume pressure in MELCOR is estimated at the phase interface. If there is water in the volume, the pressure is estimated at the interface surface between the water and the atmosphere above. If the volume is filled only with steam/gas, the volume pressure is estimated at the bottom of the control volume. Therefore, two volumes with different bottom elevations create a driving pressure difference and an artificial non-physical convection.

To avoid such non-physical convection in the containment model, the elevator shaft (GA304) was divided into three control volumes. The circular corridors (lower, middle and upper corridor) were also divided into three

separate volumes: CV250, CV260 and CV270; and CV255, CV265 and CV275 for the first and second corridor, respectively (see the nodalization). The elevator shaft is modelled with CV256, CV257 and CV258.

Modelling of the heat structures was done as precisely as possible according to the plant database. The containment walls, floors, ceilings and metal internals (pipelines, vessels, equipment, etc.) are modelled by 50 heat structures. In the detailed containment model, all heat structures are represented with only one side facing a control volume. The other side is modelled as adiabatic. Therefore, there is no heat exchange between the control volumes. For the simplified containment model, the heat structures are modelled with the respective adjacent control volumes as boundary conditions.

The heat structures are split to about 10–15 temperature nodes (depending on the total thickness of the structure), representing stainless or carbon steel liner on the internal surface, thermal insulation (for the equipment, pipelines, etc.) and the concrete structures. All in all, four materials are used for modelling the heat structures.

The main differences between the detailed and the simplified models are:

- (a) Dome subdivided into four control volumes (CV325, 320, 310 and 315) in an attempt to model the influence of the parts of the dome that are near condensation surfaces and the resulting convection. This was intended to better represent the connections of the volumes that are below the dome with the dome itself.
- (b) Each of the annular corridors and the lift shaft are subdivided into three vertical control volumes for the elimination of artificial driving forces that appear in the case of the connection of volumes with different heights.
- (c) Compartments of the CVCS filters (CV210, 215, 235 and 240) have been modelled as separate CVs because they have relatively small openings compared with the rest of the containment compartments. In the simplified model, they are lumped together into CV607 and CV608.

III.2. DETERMINATION OF THE LEVEL OF NON-UNIFORMITY OF THE HYDROGEN DISTRIBUTION IN THE CONTAINMENT

For verification and qualification of the integral plant model, a stand-alone, detailed 29 volume model of the containment was developed. Comparative analyses were performed for an LB CL LOCA (DN200), with a total loss of the emergency core cooling system. The analyses were performed using the integral MELCOR model that includes the primary/secondary systems and the containment (full plant model). A comparison of the results

with the stand-alone detailed containment model was performed only for the in-vessel part of the severe accident progression.

The purpose of the comparative analysis was to:

- (1) Prove the correctness of the coupling of the stand-alone model to the boundary conditions;
- (2) Determine the behaviour of the hydrogen distribution using the detailed model.

The boundary conditions were modelled using time dependent volumes and time dependent flow paths. The boundary control volume (break volume) was modelled as three control volumes at equilibrium saturation conditions, each containing: (1) only water; (2) only steam; and (3) only hydrogen. The time dependent flow path velocities were determined based on the density of the respective medium that is discharged to the containment (the density inside the time dependent control volume) and the mass flow rates, as determined by the full plant model. For checking the boundary conditions, the integral mass flows were compared, determined by the full plant model analyses and as introduced to the stand-alone 29 volume containment model. The comparison of the integral mass flows shows a satisfactory agreement of the boundary conditions introduced to the stand-alone containment model – within 1% deviation between the integral and stand-alone models.

Results from the comparative analyses of the simplified and the detailed models are presented in Figs 4–9. The containment pressure and the hydrogen

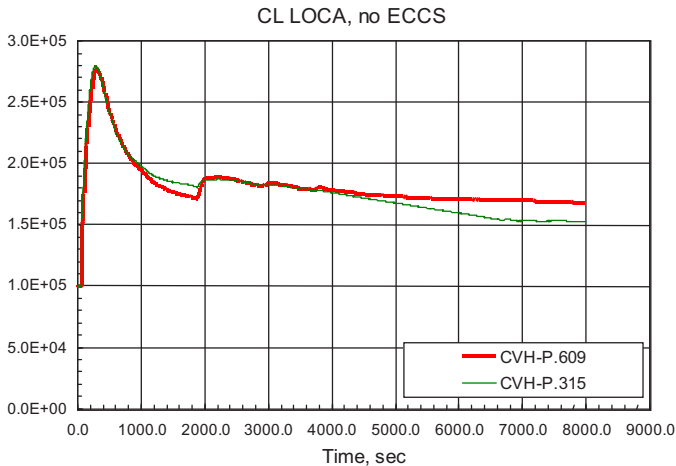


FIG. 4. Containment pressure (Pa).

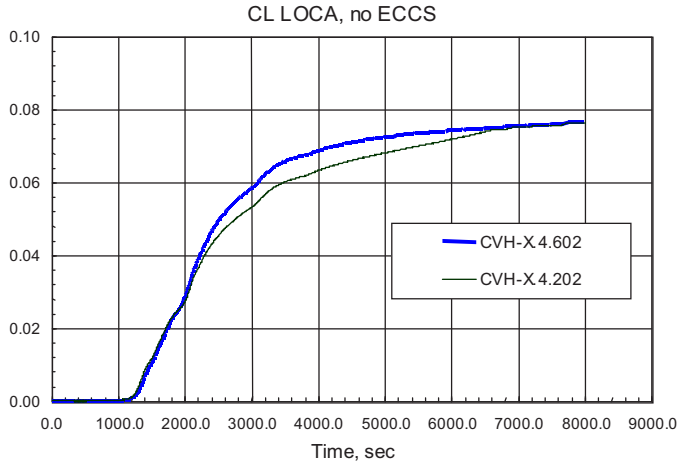


FIG. 5. Hydrogen volumetric concentration in the intact steam generator box.

volumetric concentrations in various compartments of the containment were compared.

From this comparison of the predicted hydrogen concentrations, it is seen that for the two models — simplified and detailed — the results are rather similar. The main conclusion from this verification analysis is that the two models and input decks reflect the containment behaviour in a very similar

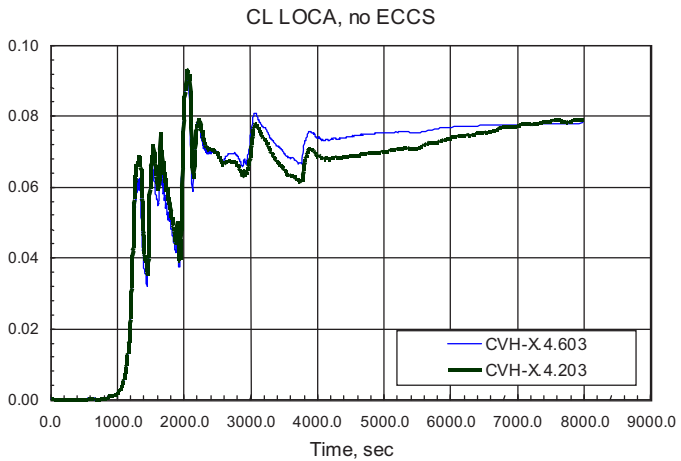


FIG. 6. Hydrogen volumetric concentration in the steam generator box with break.

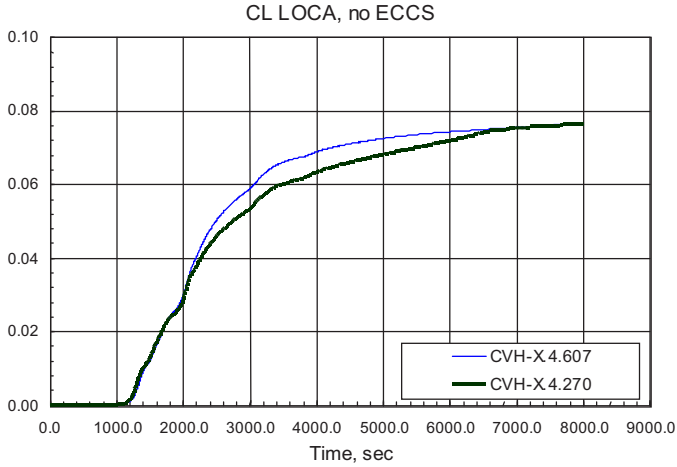


FIG. 7. Hydrogen volumetric concentration in the annular corridor.

way, that is, there are no major errors in the system representation as a computer model.

In Figs 10 and 11, the hydrogen concentrations are presented in various compartments, as predicted by the full models. The major conclusion from these results is that the compartments of the WWER-1000/V-320 containment are rather open and the hydrogen distribution may be considered uniformly

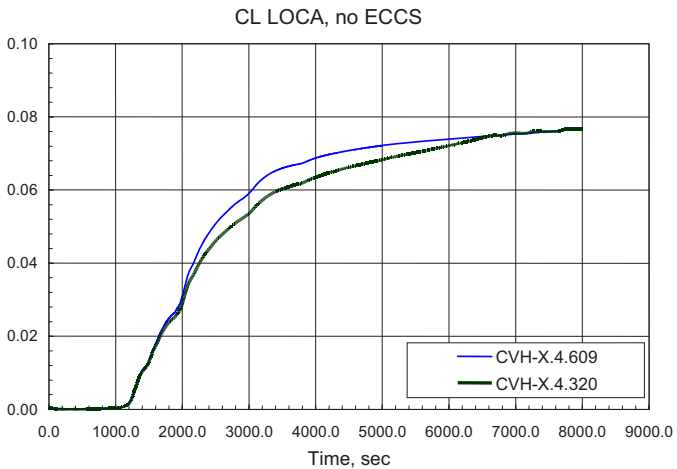


FIG. 8. Hydrogen volumetric concentration in the containment dome.

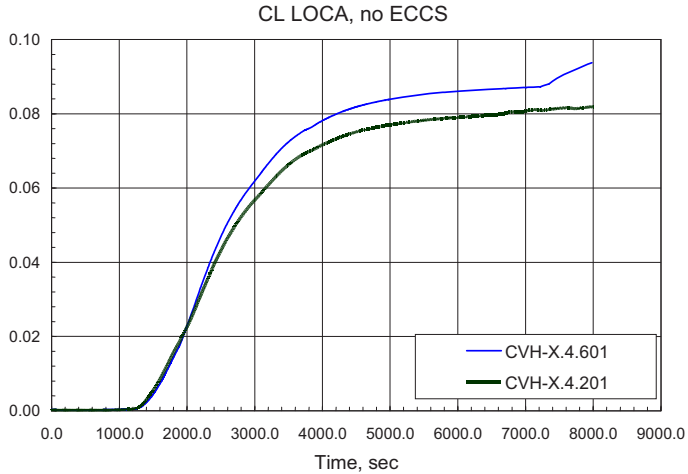


FIG. 9. Hydrogen volumetric concentration in the reactor cavity.

distributed. This result was obtained for a rather fast process of hydrogen generation, as a result of severe core degradation. Therefore, for the purpose of determination of the hydrogen distribution after a beyond design basis accident, use of a simple containment model as part of the integral MELCOR model of WWER-1000 is fully justified. This conclusion, however, is true only

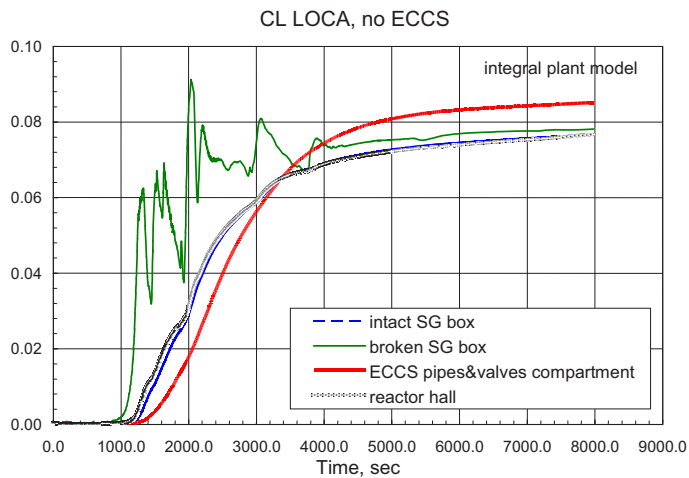


FIG. 10. Hydrogen volumetric concentration in various compartments — simplified model.

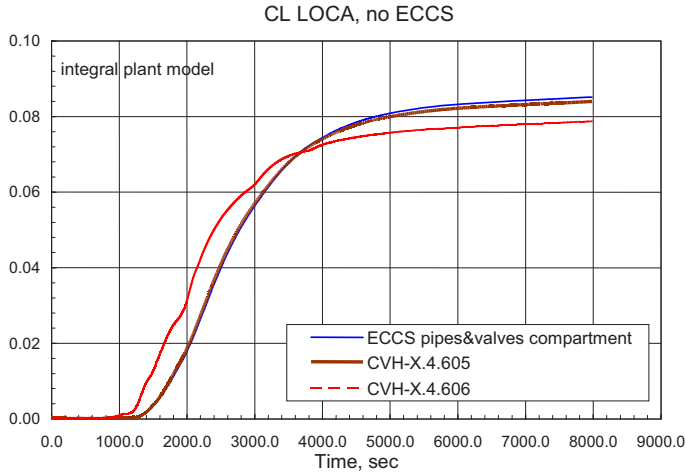


FIG. 11. Hydrogen concentration in various compartments — simplified model.

for this particular type of containment and should not be generalized for any containment design. In addition, the results from the detailed model have shown that there is no stratification inside the long vertical volumes (the circular corridors).

From the comparative analyses described previously, it is possible to conclude the following:

- (1) Hydrogen distribution inside the WWER-1000/V-320 containment is rather uniform and does not require multiple volume models or an application of CFD codes.
- (2) For the severe accident case with core degradation, special attention has to be paid to volumes with possible breaks due to greater H_2 concentration gradients expected there.
- (3) The detailed model gives similar predictions to the model with simplified containment nodalization. The full model may be used with sufficient confidence for beyond design basis accident analyses and a prediction of the distribution of non-condensable gases inside the containment.
- (4) The simplified model is sufficient for the purpose of these analyses: determination of the hydrogen distribution at design basis accident conditions and determination of the number and location of passive autocatalytic recombiners.

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Annex I

MAIN FEATURES OF SELECTED SEVERE ACCIDENT CODES

In the following, the integral codes ASTEC, MAAP and MELCOR, and the detailed mechanistic codes ATHLET-CD, ICARE/CATHARE and SCDAP/RELAP5, are briefly described. More detailed information can be obtained from Table I-1, in which the covered physical phenomena are listed for each of these codes.

Table I-2 presents an overview regarding the main validation work for the different codes. Since for this overview only so-called key experiments have been taken into account, it may cause a wrong impression about the real status of validation work. In particular, for the detailed codes ATHLET/CD, ICARE/CATHARE and SCDAP/RELAP5, many additional experiments have been used for the validation and the definition of uncertainties.

I-1. ASTEC

The accident source term evaluation code, known as the integral code ASTEC [I-1], is being developed by the IRSN (Institut de radioprotection et de sûreté nucléaire), France, and the GRS (Gesellschaft für Anlagen- und Reaktorsicherheit mbH), Germany, since 1994. The aim of this close cooperation of both companies is the creation of a fast running integral code which allows the calculation of the entire sequence of a severe accident in a light water reactor from the initiating event up to the release of fission products into the environment, covering all important in-vessel and ex-vessel phenomena. The main fields of application of this code are PSA Level 2 studies, accident sequence studies, uncertainty and sensitivity studies, and support to experiments.

Since the 1980s, a two-tier approach has been applied by the IRSN and the GRS, based on the simultaneous but independent development of both integral and detailed mechanistic codes. During this time, the IRSN has developed the integral code ESCADRE, and the GRS has modelled the containment behaviour using two codes: RALOC for thermohydraulics and hydrogen distribution, and FIPLOC for aerosol behaviour. For the first ASTEC version (called V0), it has been decided to gather in the same system the best candidates which can be provided by the two companies. Thus, ASTEC V0 consists of a combination of some modules of ESCADRE (for the reactor cooling system, core degradation, fission product release and transport, corium ejection from the vessel, direct containment heating and iodine chemistry in

the containment) and of the containment part of ASTEC (module CPA), which combines the RALOC and FIPLOC codes. The V0.3 version of the code was released in October 2000 to 16 European partners within the EVITA project of the fifth framework programme. A new version V1 is under development, which will include the front end phase.

I-2. ATHLET-CD

ATHLET-CD [I-2] is being developed by the GRS in cooperation with the Institut für Kernenergetik (IKE) of the University of Stuttgart, Germany, and the IRSN at Cadarache, France.

The mechanistically based code consists of the ATHLET part, which describes the circuit thermohydraulics, non-condensable gases, the thermal behaviour of the structures, neutron kinetics, reactor typical control systems, and the CD part, which allows the behaviour of the core to be simulated (PWR and BWR) in the case of a severe accident. The CD part, which is based on selected models of the KESS-III code (developed by IKE), simulates the following phenomena: structure heat-up, cladding and crust oxidation, hydrogen production, ballooning, mechanical rod failure, UO_2 dissolution, melting and relocation of metallic and ceramic materials, fission product release and transport.

I-3. ICARE/CATHARE V1

ICARE/CATHARE [I-3] is being developed by the IRSN at Cadarache for the simulation of severe accident sequences in PWRs.

The behaviour of the core in the case of a severe accident (ICARE part) is described by mechanistically based models and comprises the heat-up of core structures with consideration to convection and radiation, oxidation, hydrogen production, ballooning, mechanical rod failure, UO_2 dissolution, melting and relocation of metallic and ceramic materials, formation and behaviour of debris beds, behaviour of the molten pool, lower head mechanical behaviour and fission product release. The recent incorporation of ICARE into the thermohydraulics code CATHARE now enables full plant analyses for severe accident scenarios in typical PWRs.

I-4. MAAP 4.03

MAAP Version 4 is a computer code [I-4] that can simulate the response of light water reactor power plants, both current designs and advanced light water reactors, during severe accident sequences, including actions taken as part of accident management. There are two parallel versions of MAAP 4, one for BWRs and one for PWRs. The code can be used for Level 1 analyses to determine whether a given specification of initiating events and recovery times leads to core damage and/or recovery. It can be used in Level 2 analyses to determine the containment response and fission product release histories to the environment.

MAAP 4 is categorized as an 'integral severe accident analysis tool', which means that it integrates a large number of phenomena into a single plant simulation (nuclear steam supply system + containment + eventually auxiliary building) such as: thermohydraulics; core heat-up and melt progression; lower plenum debris behaviour; thermal and mechanical responses of the reactor pressure vessel lower head; hydrogen production, transport and possible combustion; DCH; MCCI; fission product release, transport and deposition. Models are included for engineered safeguard system logic and performance. Also, operator actions are simulated by the specification of intervention conditions and responses.

I-5. MELCOR 1.8.4

The integral code MELCOR [I-5] is being developed by Sandia National Laboratories, USA. For in-vessel analysis, the existing version of the code (the validation review is performed for Version 1.8.4 only) contains highly parametric models allowing the simulation of entire severe accident sequences leading to the release of fission products and their behaviour within the reactor coolant system and the containment.

The flexible nodalization of the reactor coolant system allows the simulation of different kinds of LWRs: PWR, BWR and WWER. The code consists of different packages describing the relevant phenomena in the case of a severe accident. Control functions increase the flexibility with respect to the simulation of auxiliary systems as well as the output information.

I-6. SCDAP/RELAP5/MOD3.2

The SCDAP/RELAP5 code [I-6], which is designed to describe mechanistically the thermohydraulics of the overall reactor coolant system and connecting systems, as well as core damage progression, has been developed by the Idaho National Engineering and Environment Laboratory. The code consists of the SCDAP part, which deals with the description of core heat-up and degradation in the case of a severe accident, COUPLE, a module which allows the simulation of a debris bed or molten pool in the lower head, and the RELAP5 thermohydraulic code for a description of the behaviour of the reactor coolant system and other required systems. SCDAP includes core models for both, representative PWRs and BWRs. One can postulate that, at present, SCDAP/RELAP5 is the most detailed and complete severe accident analysis code; it has been used worldwide for detailed full plant analysis.

The publication of MOD3.3 has been released recently [I-7]. MOD3.2, however, is still being used widely, thus a review of the code features and the validation is performed for the latter one.

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TABLE I-1. MAIN FEATURES OF SEVERE ACCIDENT CODES

Phenomenon	ASTEC V0.3	MAAP 4.0.3	MELCOR 1.8.4	ATHLET-CD	ICARE/ CATHARE V1	SCDAP/ RELAP5 3.2
Fission and decay:						
Recriticality	—	—	—	✓	—	—
Boron dilution effects	—	—	—	✓	—	—
Absorber/fuel separation	✓	✓	✓	✓	✓	✓
Thermohydraulics:						
2-phase	— ^a	✓	✓	✓	✓	✓
Thermal non-equilibrium	—	—	—	✓	✓	✓
Momentum equation	—	—	✓	✓	✓	✓
Flexible nodalization reactor coolant system	✓	—	✓	✓	✓	✓
Core reflood	—	—	—	✓	✓	✓
Non-condensables	✓	✓	✓	✓	✓	✓
Impact of core degradation on flow paths	✓	✓	—	✓	✓	✓
Impact of blockage formation	✓	✓	—	✓	✓	✓
Core bypass	✓	User input	—	✓	✓	✓
Reflux condenser mode	—	✓	✓	✓	✓	✓
Natural gas convection within reactor pressure vessel	✓	✓	—	✓	✓	✓
Natural gas convection within reactor coolant system	—	✓	—	✓	✓	✓ ^b

For footnotes see end of table.

TABLE I-1. MAIN FEATURES OF SEVERE ACCIDENT CODES (cont.)

Phenomenon	ASTE V0.3	MAAP 4.0.3	MELCOR 1.8.4	ATHLET-CD	ICARE/ CATHARE V1	SCDAP/ RELAP5 3.2
Core heat transfer						
Radiation radial	✓	✓	✓	✓	✓	✓
Radiation axial	✓	?	✓	✓	✓	—
Radiation from molten pool	✓	✓	✓	—	✓	—
Initial core damage						
Fuel/cladding contact	✓	?	—	✓	✓	✓
Ballooning	✓	✓	—	✓	✓	✓
Oxide flowering	—	—	—	—	✓	—
Oxide shattering	—	User input	—	—	—	✓
Irradiated fuel effects	—	—	—	—	—	✓
Non-fuel dissolution	—	✓	✓	—	✓	✓
Fuel dissolution	✓	✓	✓	✓	✓	✓
Oxide shell failure	—	P ^c	P ^a	P ^a	✓	✓
Absorber models	AIC and B ₄ C	AIC or B ₄ C	AIC and B ₄ C	AIC or B ₄ C	AIC and B ₄ C	AIC or B ₄ C
Spacer grid	—	—	—	—	✓	✓
Canister wall	—	✓	—	✓	—	✓
Lower core support plate model	✓	✓	—	—	✓	—
Upper plenum structure model						✓
Oxidation and hydrogen						

TABLE I-1. MAIN FEATURES OF SEVERE ACCIDENT CODES (cont.)

Phenomenon	ASTEC V0.3	MAAP 4.0.3	MELCOR 1.8.4	ATHLET-CD	ICARE/ CATHARE V1	SCDAP/ RELAP5 3.2
Zirconium	✓	✓	✓	✓	✓	✓
During quenching	No dedicated model	No dedicated model	No dedicated model	✓	No dedicated model	✓
Double-sided oxidation	✓	User input	—	✓	✓	✓
U-Zr-O	✓	✓	—	—	✓	✓
During fuel/coolant interaction	No dedicated model	No dedicated model	No dedicated model	No dedicated model	—	No dedicated model
Particulate debris	—	✓	✓	—	✓	✓
Stainless steel	—	✓	✓	—	✓	✓
B ₄ C	—	—	✓	—	✓	✓
Impact of air	—	—	✓	—	✓	—
Relocation and pool formation	—	—	—	—	—	—
Relocation velocity	—	User input	User input	User input	✓	✓
Heat transfer to cladding	✓	User input	User input	✓	✓	✓
Formation of particulate debris	✓	—	—	—	✓	✓
Coolability model for particulate debris	—	✓	✓	—	✓	No dedicated model
Formation of metallic blockages	✓	—	✓	✓	✓	✓
Radial spreading	—	User input	?	—	✓	✓

For footnotes see end of table.

TABLE I-1. MAIN FEATURES OF SEVERE ACCIDENT CODES (cont.)

Phenomenon	ASTECC V0.3	MAAP 4.0.3	MELCOR 1.8.4	ATHLET-CD	ICARE/ CATHARE V1	SCDAP/ RELAP5 3.2
Molten pool behaviour in the core						
Stratification (metallic/oxidic)	—	—	—	—	—	✓
Heat transfer (transient/steady state)	—/✓	—	—	—	✓	—
Interaction with supporting structures	✓	—	✓	—	✓	✓
Melting of structures above the core	—	✓	✓	—	✓	✓
Failure criteria for crusts/structures	—	✓	—	—	—	✓
Relocation of non-molten structures	✓	—	—	—	—	✓
Fuel-coolant interaction:						
Melt fragmentation	✓	✓	User input	—	—	User input
Melt dispersal	—	—	—	—	—	—
Reactor coolant system pressurization	✓	✓	✓	✓	✓	✓
Steam explosion	—	—	—	—	—	—
Lower head behaviour:						
State of the metallic and oxidic melt	Mixed	User input	Mixed	—	Mixed	Mixed
Debris coolability model	—	✓	✓	—	✓	✓
Pool coolability model	—	Optional	—	—	✓	—
Detailed lower head failure model	—	✓	✓	—	✓	—

TABLE I-1. MAIN FEATURES OF SEVERE ACCIDENT CODES (cont.)

Phenomenon	ASTEC V0.3	MAAP 4.0.3	MELCOR 1.8.4	ATHLET-CD	ICARE/ CATHARE V1	SCDAP/ RELAP5 3.2
Fission product release from fuel:						
High volatile fission products	✓	✓	✓	✓	✓	✓
Medium and low volatile	✓	✓	?	✓	—	?
Release from molten pool	—	User input	—	—	—	—
Fission product transport in reactor coolant system and connecting lines:						
Deposition in main coolant lines	✓	✓	✓	✓	—	^d
Revolatilization in main coolant lines	✓	✓	✓	✓	—	—
Deposition in connecting lines	—	—	✓	✓	—	—
Revolatilization in connecting lines	—	—	✓	✓	—	—
Pool scrubbing	—	✓	✓	—	—	—
Deposition in dry steam generator	✓	✓	✓	✓	—	—
Chemistry:						
Iodine	—	—	—	—	—	—
B ₄ C	—	—	✓	—	✓	✓

^a The entire reactor coolant system is not yet modelled, i.e. the analysis can only start at core uncovering. Thermohydraulics in the loops is single phase, and a swollen water level is simulated in-vessel.

^b No specific model, but simulation is possible by an appropriate nodalization.

^c User parameter.

^d Model available but not validated.

TABLE I-2. VALIDATION OF IN-VESSEL SEVERE ACCIDENT CODES BY KEY-TEST

Code	PBF SFD	ACRR	NRU FLHT	LOFT LP	PHÉBUS CSD	PHÉBUS FPT	CORA	QUENCH	TMI-2 (phase)	Thermohydraulics	Core heat-up	Clad deformation	Core degradation	AIC CR	B ₄ C CR	UO ₂ /Zry interaction	Reloc. CR melt	Reloc. U-Zr-O	Hydrogen generation	Quenching efficiency	Natural circulation	FP release	FP transport			
ASTEC, ESCADRE	1-4 MP2									P	P	P	P	P	P	P	P	P	P			P				
						B9+					P	P		P		P		(✓) ^a	(✓) ^b	P						
								13			P	P		P		P		P		P						
											P	P		P		P		P		P						
								1			P	P		P		P		P		P				P	P	
											✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
											✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
											✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
											✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
											3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
ICARE/ CATHARE	1-4 MP1 MP2									✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓			
										✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓			
											✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		
											✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		

TABLE I-2. VALIDATION OF IN-VESSEL SEVERE ACCIDENT CODES BY KEY-TEST (cont.)

Code	PBF SFD	ACRR	NRU FLHT	LOFT LP	PHÉBUS CSD	PHÉBUS FPT	CORA	QUENCH	TMI-2 (phase)	Thermohydraulics	Core heat-up	Clad deformation	Core degradation	AIC CR	B ₄ C CR	UO ₂ /Zry interaction	Reloc. CR melt	Reloc. U-Zr-O	Hydrogen generation	Quenching efficiency	Natural circulation	FP release	FP transport
			5							✓	✓	✓	✓	✓	✓	✓	(✓) ^a	✓	✓	✓	✓	✓	✓
	FP2									✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
					B9+					✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
						1				✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
							13			✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
							W2			✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
									1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
									2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
MAAP										✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
MELCOR	1-4									✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
										✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
		ST1								✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
		DF4								✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
		MP2								✓	✓	✓	✓	✓	✓	✓	(✓) ^c	(✓) ^c	✓	✓	✓	✓	✓
										✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

For footnotes see end of table.

TABLE I-2. VALIDATION OF IN-VESSEL SEVERE ACCIDENT CODES BY KEY-TEST (cont.)

Code	PBF SFD	ACRR	NRU FLHT	LOFT LP	PHÉBUS CSD	PHÉBUS FPT	CORA	QUENCH	TMI-2 (phase)	Thermohydraulics	Core heat-up	Clad deformation	Core degradation	AIC CR	B ₄ C CR	UO ₂ /Zry interaction	Reloc. CR melt	Reloc. U-Zr-O	Hydrogen generation	Quenching efficiency	Natural circulation	FP release	FP transport										
SCDAP/ RELAP5	1-4	5		FP2	B9+	1	13	03	1-2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓										
										✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓			
										✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
										✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
										✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

^a Steel rod.

^b Starting from a debris bed.

^c Model available but not validated.

Annex II

COMBINATION OF LUMPED PARAMETER AND CFD MODELLING FOR HYDROGEN COMBUSTION ANALYSIS

As discussed in Section 5.1.6, if there is a need to consider the hydrogen combustion process in detail (e.g. because of concerns over the pressure or temperature loading), a promising approach is to couple a CFD combustion code with a lumped parameter model of the whole containment. This annex provides an example of such an approach.

The interface between the codes can be arranged in such a way that all slow and long term processes are included in the standard lumped parameter models, and all fast and flow dependent phenomena in CFD models. The two groups of models have to communicate on-line to provide the necessary data exchange.

Instead of using a built-in combustion model, for example, DECOR in COCOSYS [II-1], an interface can be developed to include an external CFD combustion code. Using this approach, it is expected that the increased capabilities of CFD combustion modelling can be made available to long term system codes. The interface is characterized by the following:

- (a) The codes to be involved were developed independently and should retain their individual structure. This eases later inclusion of modified code versions or other codes.
- (b) A message paradigm, parallel virtual machine (PVM), is used to provide on-line data transport between the codes. Additional modules in the codes are needed to send and receive data.
- (c) With respect to a nuclear safety application, the lumped parameter code is considered the basic code running all the time. If combustible conditions are detected anywhere in the spatial model, the CFD combustion code with actual initial conditions is activated and starts providing combustion data.
- (d) The computational grids of the areas in question have to be created prior to the coupled run and are not subject to data exchange. They must be consistent.
- (e) The combustion model in the lumped parameter code is only partially used. It obtains combustion rates from the CFD code and sends back actual boundary conditions. It is expected that the CFD combustion code models only a section of the total system, therefore, it needs the actual conditions at the boundaries.

This type of coupling has been implemented in the CFD combustion code BASSIM [II-2] and in COCOSYS. The principal data flow between these codes is outlined in Fig. II-1.

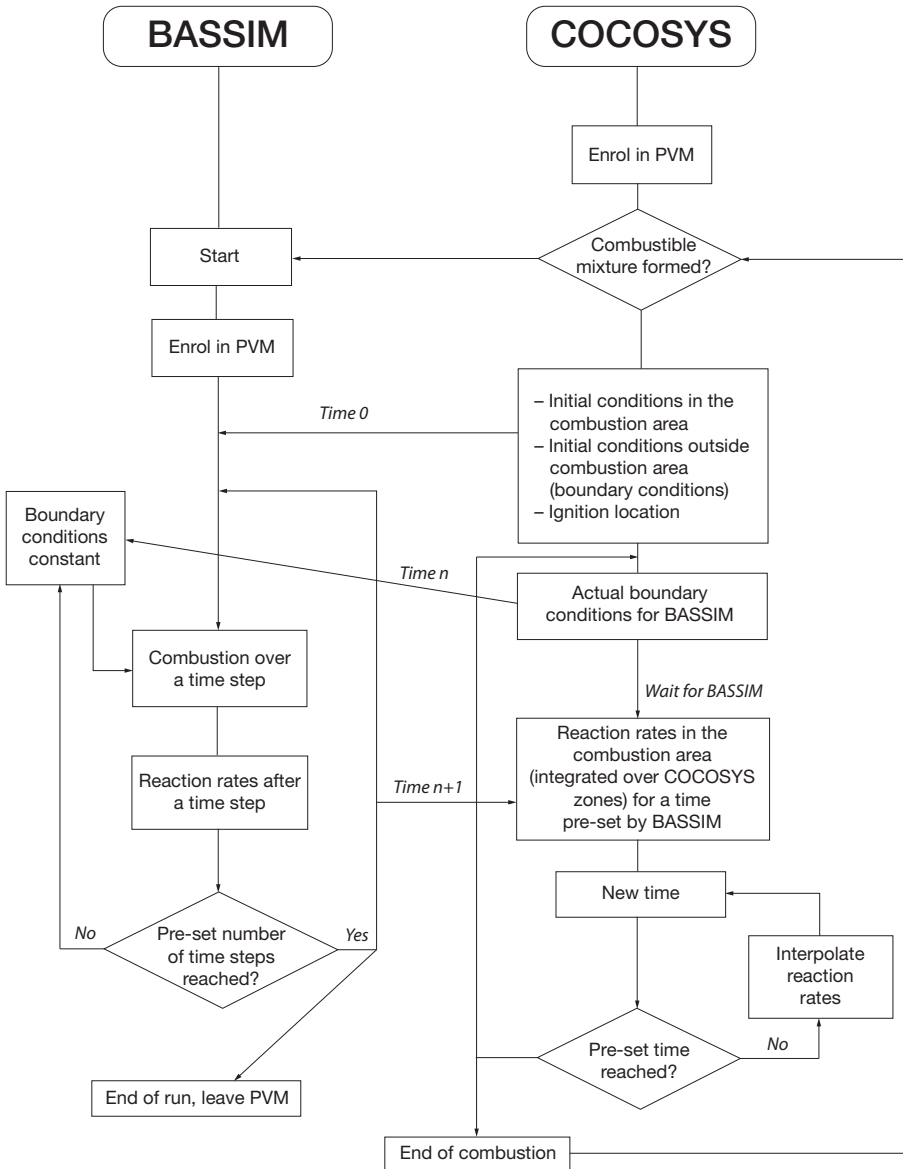


FIG. II-1. Outline of data exchange between BASSIM and COCOSYS.

COCOSYS has the general control and spawns also BASSIM as a child process when combustible mixtures have been detected. It is possible to have several child processes, which means combustion at different isolated locations. During combustion, the CFD code has time control because it is easier to synchronize both codes by steering the lumped parameter code accordingly. Pressure, temperature and concentrations in zones surrounding the combustion area (boundary conditions) are held constant during a CFD time step. Computing times of the CFD code are approximately ten times higher than those of the lumped parameter code. This code is, therefore, often in a wait cycle. A different data flow is also available for a coupling when solely gas mixing is of interest.

REFERENCES TO ANNEX II

- [II-1] KLEIN-HEISSING, W., et al., COCOSYS V1.2, Programme Reference Manual, GRS-P-3/2 (2000).
- [II-2] RASTOGI, A.K., MARINESCU-PASOI, L., “Numerical simulation of hydrogen dispersion in residential areas”, World Hydrogen Energy (Proc. 10th Conf. Cocoa Beach, FL) (1994) 245–254.

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