EUROPEAN COMMISSION
5th Euratom Framework Programme

OECD NUCLEAR ENERGY AGENCY

International Standard Problem 46

THENPHEBISP

IRSN

THEMATIC NETWORK FOR A PHEBUS FPT-1 INTERNATIONAL STANDARD PROBLEM

CONTRACT N° FIKS-CT-2001-20151

COMPARISON REPORT ON INTERNATIONAL STANDARD PROBLEM ISP-46 (PHEBUS FPT1)

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Dissemination level : RE
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NOTE TECHNIQUE SEMAR 03/021

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SERVICE D'ETUDES ET DE MODELISATION D'ACCIDENTS DE REACTEURS

Cadarache, le 28/07/03

Nb de Pages: 188
+ appendices

NOTE TECHNIQUE SEMAR 03/021

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CE/CADARACHE - 13115 SAINT PAUL LEZ DURANCE - BAT 702/SEMAR - Téléphone : 33 4 42.25.76 46- Fax : 33 4 42.25.29 29

OECD/CSNI/GAMA Approval

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SERVICE D'ETUDES ET DE MODELISATION D'ACCIDENTS DE REACTEURS		
Nat. Document	NOTE TECHNIQUE SEMAR 03/0021	
TITRE	COMPARISON REPORT ON INTERNATIONAL STANDARD PROBLEM ISP-46 (PHEBUS FPT1)	
Auteur(s)	*B. CLÉMENT and T. HASTE*	
Type de Diffusion:	"Mots clés": PHEBUS, ISP-46, FPT1 N° Fiche Action: 244/2-046H/04-2	Nbre de pages: 188 + apps Nbre annexes: 10

Résumé:

L'objectif du Problème Standard International no 46 de l'OCDE/CSIN (ISP-46), basé sur l'expérience Phébus FPT1, est de tester la capacité des codes de calcul à modéliser, de manière intégrale, les phénomènes physiques intervenant lors d'un accident grave sur un réacteur à eau pressurisée. Il traite les aspects liés à la dégradation du cœur, au relâchement des produits de fission, actinides et matériaux de structure, à leur transport dans le circuit primaire et leur comportement dans l'enceinte de confinement. La participation à cet exercice a été importante: 32 organisations, incluant des organisations internationales, des exploitants, des autorités de sûreté et leurs supports techniques, des organismes de recherché et des developers de code provenant de 23 pays différents.

Les points principaux de l'essai FPT1 sont rappelés, avec une description du dispositif expérimental et de la conduite de l'essai. Les spécifications de l'exercice sont rappelées pour chacune de ses quatre phases: grappe, circuit, enceinte et chimie de l'iode.

Les résultats soumis par les participants ont été analysés en détail par les coordinateurs, pour chacune des phases individuelles, pour les calculs de base, et ceux dits "best estimate". Les accords et désaccords avec les résultats expérimentaux sont mis en lumière, avec des explications sur les causes lorsque c'est possible. L'analyse n'a pas seulement porté sur l'adéquation des modèles physiques individuels, mais aussi sur les aspects intégraux: en quoi des écarts sur la valeur d'un paramètre calculé va influer sur les modèles l'utilisant comme donnée d'entrée. Les aspects liés à la performance du code ont été aussi examinés. Pour chacun de ces points, des conclusions sont données et des recommandations faites en tant que de besoin.

Le comportement thermique de la grappe est généralement bien reproduit, ainsi que la production d'hydrogène. L'état final de dégradation du combustible peut être reproduit correctement en ajustant la température de relocalisation du combustible, mais il est peu probable que cet ajustement soit valable pour tous les essais similaires et les applications réacteur nécessitent donc des études de sensibilité dans l'état actuel de la modélisation.

Il est recommandé d'améliorer les modèles pour le relâchement des produits de fission semi-volatils, pour les matériaux de structure (Ag-In-Cd, Sn), ainsi que pour la cinétique du relâchement des produits de fission volatils.

La rétention globale dans le circuit est assez bien prédite, mais les dépôts dans la zone située au-dessus de la grappe sont sous-estimés, alors qu'ils sont surestimés dans le générateur de vapeur. La prédiction de la volatilité de certains éléments est aussi à améliorer.

La thermohydraulique de l'enceinte est en général calculée avec une précision suffisante. La vitesse de rabattement des aérosols est en général bien prédite, avec quelques difficultés pour reproduire la partition entre les différents mécanismes de dépôt.

Les calculs de chimie de l'iode dans l'enceinte posent plus de difficultés. Leur qualité dépend

fortement de celle des calculs de relâchement et de transport, dans les codes intégrés. Les principales difficultés concernent la présence d'iode gazeux dans le circuit primaire et la quantité d'iode organique dans l'atmosphère de l'enceinte.

Les développeurs de code ont analysé les résultats des calculs réalisés avec leur outil, en ont tiré leurs propres conclusions et défini les améliorations nécessaires. Cette analyse vient en complément de celle faite par les coordinateurs.

On a essayé de déterminer quelles étaient les implications pour les études réacteur. En ce qui concerne l'adéquation des modèles et des codes, l'ISP a permis d'identifier des améliorations nécessaires, les plus importantes étant:

- une meilleure estimation du relâchement des matériaux de structure, en particulier l'argent, et des produits de fission semi- et non-volatils,
- la possibilité de prendre en compte la présence d'iode gazeux dans le circuit primaire,
- la définition d'un jeu de paramètres optimisé pour les calculs de chimie de l'iode.

Le nombre important de calculs avec certains codes a permis de mettre en lumière les effets utilisateur, qui sont parfois assez importants.

Abstract:

The objective of OECD/CSNI International Standard Problem (ISP-46), based on experiment Phebus FPT1, is to assess the capability of computer codes to model in an integrated way the physical processes taking place during a severe accident in a pressurised water reactor, from the initial stages of core degradation, the fission product transport through the primary circuit and the behaviour of the released fission products in the containment. ISP-46 enjoyed very broad participation: 23 countries, 33 participating organisations, including international organisations, utilities, regulators, technical support organisations, researchers and developers. A wide range of calculations had been performed (47 base-case calculations, 21 best-estimate calculations), using fifteen different codes.

The main features of the FPT1 experiment are recalled including the experimental facility and the test conduct. The specifications are summarised, for each of the four phases of the exercise: bundle, circuit, containment and chemistry.

The results submitted by the participants were analysed in detail for each phase, for base case and best-estimate calculations. Agreements and disagreements with experimental data were pointed out, with explanations where possible. In addition to the adequacy of individual physical models, great attention was paid to integral aspects, i.e. to the consequences of discrepancies on output variables of one model on the calculations by other models using the values of these variables as input. Computing and code assessment aspects were also analysed. For each of these points, conclusions are given, and recommendations made when necessary.

The thermal behaviour of the fuel bundle is generally well captured, together with the hydrogen production. Good agreement for the final state of degradation could be obtained with suitable adjustment of bulk fuel relocation temperature, but this is unlikely to be representative for all similar tests. Therefore, plant studies need sensitivity calculations with the modelling in its current state.

It is recommended to improve models for semi-volatile fission product and structural material release (Ag-In-Cd, Sn), taking into account their radiological significance in determining the accuracy required, as well as time dependence of volatile release.

The overall retention in the circuit is quite well predicted, but the calculations underestimate deposits in the upper plenum above the fuel bundle, whereas they overestimate them in the steam generator. The volatility of certain elements should also be better predicted.

The thermal hydraulics in the containment is well enough calculated. The overall aerosol depletion rate is generally well predicted, but there are some difficulties with the partition of deposits amongst the different deposition mechanisms.

Calculation of iodine chemistry in the containment turned out to be more difficult. Their quality strongly depends of the calculation of release and transport in the integral codes. The major difficulties are related to the existence of gaseous iodine in the primary circuit and to the prediction of the amount of organic iodine in the gas phase.

In addition to this analysis, made by the co-ordinators of the exercise, there was feedback from the code developers who analysed the set of calculations made with the codes they are developing, and

drew their own conclusions on code capability and necessary improvements.

Finally, implications of the ISP-46 outcomes for plant studies are discussed.

Regarding adequacy of models and codes, the ISP has identified a number of necessary improvements in codes and models, of which the most important are:

- better estimation of structural material release, especially for control rod elements, and of semi- and low-volatile release;
- possibility to take into account the presence of gaseous iodine in the reactor coolant system;
- definition of optimum parameters for iodine chemistry codes.

The large number of submissions made using some of the codes allowed insights into the so-called "user-effect" that is significant for some parts of the calculations.

Repère bureautique: finrpt_v3.doc

Revision	Date	
3	July 2003	Draft 3 for review by CSNI GAMA
2	May 2003	Draft 2 for review by participants (without executive summary)
1	March 2003	Draft 1 for review by ISP-46 Final Workshop
0	February 2003	Draft 0 for preliminary circulation

Preface

Over the last thirty years, the Committee on the Safety of Nuclear Installations (CSNI) of the OECD Nuclear Energy Agency (NEA) has sponsored a considerable number of international activities - in particular, International Standard Problem exercises - to promote the exchange of experience between its Member countries in the use of nuclear safety codes. ISPs 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 experiment. A primary goal of these activities is to increase confidence in the validity and accuracy of analytical tools which are needed to assess the safety of nuclear installations, and to demonstrate the competence of the organisations involved.

Following an offer made by the French Institute for Radiological Protection and Nuclear Safety (IRSN) in 1998, the CSNI has devoted its 46th International Standard Problem to a code comparison exercise based on the Phebus FPT1 experiment. The ISP-46 exercise is part of the programme of work of the CSNI Working Group on the Analysis and Management of Accidents (GAMA) both in the field of in-vessel behaviour of degraded cores and in the field of fission product release, transport, deposition and retention. Its objective is to assess the capability of computer codes to reproduce an integral simulation of the physical processes taking place during a severe accident in a pressurised water reactor, i.e. including fuel degradation and associated hydrogen production and fission product release, fission product and structure material transport in the primary circuit, aerosol behaviour in the containment and iodine radiochemistry. Beyond the ISP-46 exercise, computational benchmark exercises on reactor accident sequences (TMI-2 accident) will be organised, in order to investigate further the ability of current advanced codes to predict core degradation and to evaluate the confidence we can have in code extrapolation to reactor scale.

The European Commission, a major sponsor of the Phebus FP programme, helped the organisation of the ISP under the EC Nuclear Fission Safety 5th Framework Thematic Network "THENPHEBISP", contract number FIKS-CT-2001-20151, including financial support of the coordinators and many European partners.

1. Introduction

From the beginning of nuclear power plant developments, it has been realised that a severe accident in which the normal core cooling is lost could lead to fuel elements melting and fission product release beyond the plant limits. Nuclear power plants are designed with engineering systems and associated operational procedures which provide an in-depth defence against such accidents.

It is now common practice to assess the risks to the population associated with severe accident conditions in commercial plant, using computer codes to model the accident progression, core degradation, and potential source term to the environment. The source term analysis involves calculation of quantity, timing and forms of the fission products (FP) and structure aerosols released as well as the activity released into the atmosphere. Indeed, the knowledge of FP release, which is closely coupled to the degraded core state and the associated circuit and containment conditions, is essential to efficient accident management.

Development and assessment of the computer codes used for such analysis has taken place on an international basis using a wide range of integral and separate-effects experiments. The Phebus FP programme [1] [2], in which four of a planned five experiments have so far been carried out, is investigating key phenomena involved in LWR severe accident sequences, through a series of in-pile integral experiments. The facility provides prototypic reactor conditions which allow the study of basic phenomena governing the releases, transport, deposition and retention of the fission products. The phenomena studied take place in the core region, in the primary system components and in the containment building; the processes involved in these studies are thermal-hydraulics, physics, chemistry and radioactivity which are closely coupled.

The second experiment in the series, namely Phebus FPT1 [3], Figure 1, was chosen as the basis for ISP-46. This provides for the first time the opportunity to assess the capability of systems-level severe accident modelling codes in an integral manner, covering core degradation through to the late phase (melt pool formation), hydrogen production, FP release and transport, circuit and containment phenomena, and iodine chemistry, in one experiment. The possibility also existed to compare the performance of detailed-level codes covering one aspect of the accident progression, for example core degradation, with the systems-level codes, thus providing benchmarking of the different levels of modelling.

The ISP was conducted as an open exercise, with all the relevant experimental results being available to the participants. The specification report was provided in three versions: an initial draft[4] provided for comment at the Preliminary Workshop in November 2001, a definitive version[5] which was the basis for the participants' submissions, and finally a revised version[6] which included additional material provided during the calculational phase of the exercise.

The present document reports the conclusions of ISP-46. It covers the objectives of the exercise, indicates the timescale, summarises the Phebus facility and the test itself, indicates the material supplied to and requested from the participants, discusses the analysis by the coordinators of the different phases separately and in an integral manner, and finally lists the overall conclusions. Appendices give additional information relevant to the ISP, and list information on code models and their use provided directly by the participants and code developers.

2. Objectives and Organisation

The general objective of ISP-46 was to assess the capability of computer codes to model in an integrated way the physical processes taking place during a severe accident in a pressurised water reactor, from the initial stages of core degradation through to the behaviour of released fission products in the containment. This helps in the evaluation of the uncertainties associated with calculation of the source term and of the core final state, and aids identification of remaining modelling needs. The objectives were realised through analysis of Phebus FPT1, whose test facility incorporates scaled-down representations of a reactor core, primary circuit including a steam generator, and containment. The test section included a silver-indium-cadmium control rod, as used in most Western PWR designs.

The areas covered by the experiment, and therefore by the Standard Problem, are fourfold:

1. Fuel degradation, hydrogen production, release of fission products, fuel, and structural materials ('bundle' part of the ISP);
2. Fission product and aerosol transport in the circuit ('circuit' part of the ISP);
3. Thermal hydraulics and aerosol physics in the containment ('containment' part of the ISP);
4. Iodine chemistry in the containment ('chemistry' part of the ISP).

Participants were encouraged to perform integral calculations covering all four aspects of the exercise. However, the ISP was so organised that it was also possible for participants to calculate any of the above phases in a stand-alone manner, using detailed-level mechanistic codes that treat for example core degradation or containment thermal hydraulics and aerosol physics on their own. In this way, advantage could be taken of experience with relevant ISP's such as ISP-28 (Phebus B9+, early phase core degradation) [7], ISP-34 (FALCON, fission product and aerosol transport in circuit and containment) [8], ISP-37 (VANAM, containment thermal hydraulics and aerosol physics) [9], ISP-40 (STORM, aerosol physics and resuspension) [10], ISP-41 (RTF, iodine behaviour in the containment) with its follow-up exercises [11], ISP-44 (KAEVER, containment aerosol physics) [12] and ISP-45 (QUENCH, bundle heatup, hydrogen production, quenching) [13]. The exercise did go further down to the level of detailed phenomena, for example three-dimensional natural circulation in the containment.

The Phebus FP experiments are being analysed in detail through Interpretation Circles organised under the auspices of the European Commission and the Phebus project itself. As their names imply, the activities of these groups are primarily oriented towards detailed interpretation of the experimental results and investigation of the physical phenomena involved. This often involves the generation of special code versions and very complex noding schemes in an attempt to capture fine details of the data. It was not the intention of the present ISP to duplicate these activities, but rather to concentrate on the overall performance of the codes used in a similar manner as they would be used for plant studies, employing standard models and options as far as possible, with representations of the facility in similar detail as used for plant studies. This was intended to facilitate evaluation of lessons learned regarding analysis of real plant and of uncertainties in risk analysis.

To the latter end, recommendations were made regarding the noding to be used in the analysis, for two cases; a base case with discretisations similar to those that could be used in a reactor study, and for an optional, more detailed, 'best estimate' case more typical of those used in experimental interpretation. It was hoped that participants would be able to perform two sets of calculations for

each code they had chosen to employ, so the effect of fineness of noding could have been examined. The submission for each code (not limited to one per organisation) could consist of a base case and a best-estimate case for each of which numerical data would be provided, accompanied by such sensitivity studies to illuminate the results as the participant thought fit. However the first set of calculations was deemed to be more important.

3. Timescale

The ISP was organised following normal practice on an approximately two-year timescale, as shown in Table 1. A key event was the general release of the Phebus FPT1 Final Report worldwide in September 2001, thus making the results available outside the Phebus project partnership. The issue of a preliminary version of the Specification Report in advance of the Preliminary Workshop allowed time for comment, particularly relevant to those participants outside the Phebus project who might not have analysed Phebus experiments before. The most intensive phases were preparation of the specification (4 months), participants' calculations and submission of their results (7 months), and the co-ordinators' analysis of the results and draft of the Comparison Report (7 months).

4. Participation

The ISP was well supported, with participation from 33 institutes, companies etc. in 23 countries and international organisations. The latter comprised EC-JRC, Austria, Belgium, Bulgaria, Canada, Croatia, Czech Republic. France, Germany, Greece, Hungary, Italy, Japan, Korea, Mexico, Russia, Slovenia, Spain, Sweden, Switzerland, Turkey, UK and USA. As can be seen from the list in Table 2, the participating organisations included utilities, regulators and their technical support organisations, research institutes and private engineering consultancy companies, thus providing a good range of backgrounds to the technical work. Fifteen different codes were used: ASTEC, ATHLET-CD, COCOSYS, CONTAIN, ECART, FEAST, IMPACT/SAMPSON, ICARE/CATHARE, IMPAIR, INSPECT, MAAP4, MELCOR, SCDAP/RELAP5, SCDAPSIM and SOPHAEROS, of these 4 are integral codes (ASTEC, IMPACT/SAMPSON, MAAP4 and MELCOR). For the base case, 47 calculations were received, with 21 for the optional best-estimate version. Of the base case calculations, 14 were integral (defined as including calculations for 3 or 4 phases). A notable feature was the relatively small number of participants attempting the containment chemistry phase.

Further details regarding the participation are provided in Appendix 1. This contains contact information, data concerning the material supplied by the participants, and a bibiliography of the technical reports that formed part of each submission.

5. Summary of the experiment

5.1. The Phebus FP project

The Phebus FP programme comprises five integral experiments on reactor severe accidents dealing with fuel degradation, hydrogen production, fission product release, transport and behaviour in the containment. It is undertaken by the French Institute for Radiological Protection and Nuclear Safety (IRSN) in close collaboration with the European Commission, using the experimental facilities of the "Commissariat à l'Energie Atomique" at the Research Centre of Cadarache (France) and promoting extensive collaboration amongst international partners from Europe, North America and the Far East.

The overall aim of the Phebus FP programme is to investigate key phenomena involved in LWR severe accident sequences, through a series of in-pile integral experiments. In detail, there are three main objectives:

1. to use global experiments to check the assumptions made in code models, namely:
    - combination of separate effects phenomena,
    - ensuring that no major phenomenon has been omitted in the code modelling.
2. to obtain experimental data to check/validate the code systems used in the safety analysis for the source term evaluation.
3. to improve the understanding of severe accidents, and to make available a technical and scientific data base:
    - for a better evaluation of the radioactive release hazard,
    - for assisting the specification of operational accident management procedures,
    - for improving the evaluation of the moment at which they should be implemented,
    - for defining further studies related to post-accident management.

The facility provides prototypic reactor conditions which allow the study of basic phenomena governing the releases, transport, deposition and retention of the fission products. The current test programme involves five tests, of which four have so far been conducted, see Table 3 for a summary of the main conditions concerning the test bundles. It should be noted that the experiments do not simulate the period from the initiating event to the heatup phase, involving two-phase flow in the bundle and primary circuit; only heatup, degradation and release in single-phase steam is considered.

5.2. The experimental facility

5.2.1. General

The test train is located in a loop crossing the central part of the Phebus driver core which supplies the nuclear power. In tests FPT0, FPT1, FPT2 and FPT3 the fuel rods are 1.13 m long with a 1 m long

fissile zone (total mass of UO_2 about 11kg), are held in place by two Zircaloy spacer grids and are arranged in a 5x5 square lattice on a pitch of 12.6mm, without the four corner rods, as shown schematically in Figure 2 for the radial configuration and in Figure 3 for the vertical configuration. In FPT1 the spacer grids are of depth ~0.043m and are positioned at elevations 0.24 and 0.76m from the bottom of the fuel column. The two grids are linked to four Zircaloy stiffeners. The absorber rod in the centre of the bundle contains Ag-In-Cd in the first three of these tests and B_4C in FPT3. Only the first test FPT0 was performed using trace-irradiated fuel. For the rest of the matrix, irradiated fuel rods (~ 23 GWd/tU for FPT1 and ~ 32 GWd/tU for FPT2) are used.

The subsection below provide summaries of various parts of the facility. Further details including exact dimensions may be found in the FPT1 Final Report and in the FPT1 Data Book[14]. Location of instrumentation is given in Appendix 2, along with details of the mass inventories of the bundle.

5.2.2. The bundle

The test bundle is surrounded by an insulating zirconia shroud with an inner circular ZrO_2 or ThO_2 layer (ThO_2 in FPT1), an external ZrO_2 layer and a pressure tube of Inconel coated on the internal face by flame-sprayed dense ZrO_2. These three annular structures are separated by two gaps under cold conditions. The outer pressure tube is cooled by an independent pressurised cooling circuit, with a high mass flow of water at a temperature of 438K. The rods are cooled by a measured gaseous flow of steam imposed at the entrance.

Measurements in the bundle involve mainly temperatures: fuel centreline and cladding (for fresh fuel rods), control rod, stiffeners, shroud and coolant. After failure of the rod thermocouples (TCs), the bundle temperature is controlled by shroud TCs located inside and on the outer surface of the external ZrO_2 insulating layer. Two ultrasonic thermometers enable improved control of bundle temperatures at different levels. The tests involving irradiated fuel rods (FPT1, FPT2, FPT3) include 18 rods with intermediate burn-up (no TCs) and 2 fresh fuel rods to enable the implementing of some rod TCs allowing a direct measurement of fuel temperature. Coolant flow rates, hydrogen production and FP are measured in the circuit. In particular, an On Line Aerosol Monitor (OLAM) device enables the detection of major events of the core degradation. The measurement system for the power of the driver core and fission chambers located around the bundle can also detect significant core material relocation events.

Gamma-scanning examinations of some FPs and activation products of bundle structures enable the mean axial profiles of fuel and control rod mixtures to be measured. In addition, a large set of tomographies is performed enabling a rapid and precise overview of the bundle degradation and of the final axial distribution of bundle materials on the basis of their densities. Final destructive examinations include cross and axial cuts for more detailed quantification of the bundle degradation.

5.2.3. The circuit

The pipework between the upper end of the fuel bundle and the entrance into the containment tank consists, for the Phebus FP tests except FPT4, of the following components , see Figure 4 for a schematic view:

- the upper part of the test section (vertical line, ~3m high, internal diameter 0.073m reducing in stages to 0.048m then 0.03m, see Table 4), where the gas temperature drops to 970 K,
- an isothermal (970 K) horizontal line (~9m long with an internal diameter of 0.03m), with sampling devices inside a furnace (point C),

- the vertical steam generator U-tube (~4m high with an internal diameter of 0.02m), with pipe walls maintained at 420 K,
- another isothermal (420 K) horizontal line (~4m long with an internal diameter of 0.03m), with sampling devices inside a furnace (point G), and the connection to the containment vessel.

The vertical and first horizontal line together simulate the hot leg of a PWR primary circuit, while the second horizontal line simulates the cold leg.

5.2.4. The containment vessel

The volumetric scaling factor of this 10m³ vessel (5m in height with an inner diameter of 1.8m) corresponds to the core mass ratio between a 900 MW(e) pressurised water reactor (PWR) core and the Phebus FP test fuel bundle, viz. 5000 : 1.

As for the circuit, representative fission products concentrations are therefore preserved.

Heat transfer and steam condensation phenomena in a reactor containment are simulated by three vertical condensers. Their cooled surfaces are covered with epoxy paint as a possible source for molecular iodine trapping and organic iodine formation. Non-condensing painted structures are attached to the three condensers.

The outer walls of the vessel are slightly superheated in order to prevent any steam condensation and to minimise aerosol deposition.

The lower vessel part is closed by a curved bottom structure including a $0.1m^3$ sump. The sump has a diameter of only 0.584m in order to reproduce a representative atmosphere-water exchange surface. It contains a painted structure. The sump water is recirculated by an auxiliary loop. In the washing phase another circuit injects water onto the vessel bottom structure, thus washing settled aerosols into the sump.

5.3. Phebus FPT1 test conduct

The following summary of the experiment is mainly quoted from the FPT1 Final Report. Illustrations are provided from the same source to show examples of the boundary conditions and experimental results to be simulated in the Standard Problem calculations (section 6). Many illustrations refer to specific instruments in the bundle, circuit and containment; these are illustrated in Appendix 2 with further details in the Final Report.

5.3.1. Pre-conditioning phase

The FPT1 test bundle which included 18 PWR fuel rods (~6.85% initial enrichment in U^{235}) previously irradiated to a mean burn-up of 23.4 GWd/tU, two instrumented fresh fuel rods (~3.5% enrichment in U^{235}) and one silver-indium-cadmium (AIC) control rod, was pre-irradiated for ~7 days with a mean bundle power of ~205 kW in the Phebus reactor before the experimental phase of the test itself in order to generate short-lived fission products in the fuel.

After the pre-conditioning phase, a period of 36 hours was necessary to bring down reactor xenon poisoning and to establish the boundary conditions of the experimental circuits. In particular, this so

called transition phase was also used for drying the bundle using neutral gas. The experiment itself then began by injecting steam into the bundle and gradually increasing the core nuclear power.

5.3.2. Degradation phase

The fuel degradation phase of the test lasted about 5 hours, during which the inlet steam flow rate injected at the bottom of the test train varied from 0.5 to 2.2 g/s providing oxidising or "steam-rich" conditions for fission product chemistry, while the bundle power was progressively increased up to 36.5 kW. The injected fluid was pure steam, with no additional substances such as boric acid or hydrogen. The pressure in the experimental circuit during the test was maintained roughly constant at ~2 bar.

The bundle degradation phase consisted of two main periods. The first one, devoted to the thermal calibration of the bundle and with measurement of the coupling factor between the experimental bundle and the driver core, lasted ~7900 seconds. During this period, the bundle power and the steam flow rate were increased step by step in order to check the thermal response of the bundle. The steam flow rate was first reduced from 1.8 to 0.5 g/s, meanwhile, the bundle power† was increased in steps from 0 to 3.90 kW, Figure 5. The second period was the real temperature transient and degradation phase of the test, lasting from ~7900 to ~17000 seconds. The degradation phase was specifically devoted to the release of fission products, and bundle, structure and control rod material in order to study their transport and retention in the experimental circuit. The thermal hydraulic conditions for the degradation phase were: (1) an initially constant steam flow rate which then decreased from 2.2 to 1.5 g/s and, (2) a bundle power progressively increasing from 3.90 kW to 36.5 kW. Typical temperature histories in the bundle and shroud are shown in Figure 6. During the degradation phase substantial hydrogen production was observed, particularly around 11000s at the zirconium oxidation peak, Figure 7, as well as fission product release, particularly for volatile species, Figure 8.

Following the detection of a second temperature peak in the lower part of the shroud, the degradation phase was terminated by shutdown of the nuclear power at 17039s, and the bundle was cooled in a steam flow of 1.5 g/s. At the end of this cooling phase the containment was isolated at 18660s. The interrelation amongst the different events is shown in Figure 9.

The sequence of events in the bundle during the degradation phase is reflected in the thermal hydraulic conditions in the circuit and containment. Moving along the circuit, the conditions in the vertical line, hot leg, steam generator tube and cold leg are shown successively in Figure 10, Figure 11, Figure 12 and Figure 13 respectively, while conditions in the containment are shown in Figure 14, Figure 15 and Figure 16 for the gas temperature, pressure and humidity respectively.

The bundle degradation phase was followed by three other phases restricted to the containment. These successive phases are briefly described below, with temperature and pressure histories shown in Figure 17 and Figure 18.

† *Note:* The powers quoted here in the text are revised upwards by about 7% from those given in the FPT1 Final Report, which are shown in Figure 5. The revised figures used are illustrated in Figure 30. Further details were provided in the Specification Report.

5.3.3. Aerosol phase

The aerosol phase was devoted to studying fission product and bundle, structure and control rod material settling in the containment. It lasted approximately 64 hours, starting with the containment isolation from the experimental line. During this phase, the sump temperature was maintained at 90°C. After about 23000 seconds (6.4 h), steam condensation stopped and the condensers and gas temperature reached, respectively, stable values of 92 and 108°C. Once the thermal boundary conditions became stable, an average relative humidity ratio of about 60 % was maintained throughout the aerosol phase. No further steam condensation occurred on the condensers. The duration of this phase was much longer than needed for aerosol depletion. This was intentionally achieved in order to reach stationary conditions for iodine chemistry.

5.3.4. Washing phase

This phase lasted 21 minutes during which the containment elliptic bottom was washed by a sump water spray. The spray, collecting the deposited aerosol, drained into the sump water in order to initiate the radiolysis process. Before washing the elliptic bottom, it was necessary to change the thermal hydraulic conditions of the containment in order to minimise, as far as possible, vaporisation of the water from the sump during the washing phase. The thermal hydraulic conditions were therefore changed during the so-called washing preparatory phase (of duration 4.5 hours) by decreasing the condenser wet part temperatures from 92 to 49°C to reduce the humidity in the tank and reducing the sump water temperature from 90 to 47°C.

5.3.5. Chemistry phase

This final phase, lasting 17 h 35 min, was devoted to studying containment chemistry. Investigation of the iodine chemical behaviour in the sump under radiation and the release of gaseous iodine from the sump into the containment atmosphere due to radiolysis were priorities. For this phase, the thermal hydraulic conditions of the containment were once again changed. The containment wall, condenser wet zones and sump temperatures were increased to reach respectively 128, 113 and 90°C in order to reach a humidity ratio of about 31%. The aim was to reach a stationary state for iodine chemistry, differing from the one obtained during the aerosol phase, mainly for iodine concentration and dose rate in the sump water.

5.3.6. Summary of fission product results

The experiment produced a very large quantity of data related to the time dependence of the fission product release, speciation, deposition, and iodine chemistry in the containment. As detailed in the Final Report, the devices and methods used include on-line instrumentation such as gamma spectrometers, sampling instruments requiring post-test analysis of their contents, and detailed post-test examination of the damaged bundle which reveals amongst other data the amount of fission products retained in the fuelled section. Typical results are indicated in the figures below, while a summary of the release and transport data is provided in Table 5.

Firstly, Figure 19 shows the release rate of a typical (and important) species I^{131} during the degradation phase showing the relationship to other experimental parameters. In Figure 20 the mass flow of Xe^{135} in the circuit is shown, compared with containment data. An example of the data obtained by post-test examination of the bundle is shown in Figure 21, similar axial distributions were obtained for many species. Turning to the circuit, deposition in the steam generator was

measured as a function of time, Figure 22, and the spatial distribution was measured at the end of the experiment, Figure 23. In the containment, measurements were made of the aerosol mass injected, suspended and deposited for individual species such as iodine, Figure 24, and in total, Figure 25. From these results, the amounts entrained and deposited by different mechanisms were evaluated, Figure 26. The activity in the containment sump was monitored in the long term to determine the amounts of various species there present, Figure 27 and Figure 28. Finally, specific measurements of iodine were performed, for example the gaseous iodine fraction in the atmosphere, Figure 29.

5.3.7. Revisions to Final Report experimental data

In the production of the Specification Report, it was found that various clarifications, revisions and additions needed to be made to the experimental data from the Final Report, to provide consistent information sufficient for all participants. The major items are given below:

- Revision to the bundle power, Figure 30 (note that this figure has since been revised again), axial power profile, self-shielding factors;
- Thermophysical properties of the shroud, and of other structural materials such as Inconel;
- Bundle inventory of Pu;
- Pre-irradiation history in the BR3 reactor, for the irradiated rods;
- Fission product inventory for FPT0 (useful for deriving the inventory of the unirradiated rods separately);
- History of iodine injection into the sump, Figure 31;
- Reconciliation of event timings given in different parts of the Report;
- Provision of derived fission product sources at bundle exit, point C and point G, with additional derived information on cadmium and tin release;
- Correction of some of the stated thermocouple positions in the bundle upper plenum.

Also. for the circuit phase, an input dataset was provided for the SOPHAEROS code, to give a reference picture of the dimensions in the circuit.

These additional items are conveniently gathered together in the final version of the Specification Report.

6. ISP Specification

6.1. General

The sources of information for the ISP were, in descending order of priority:

- the Specification Report;
- the FPT1 Final Report;

- the FPT1 Data Book.

In addition, detailed data were provided in numerical form in supplementary files in electronic form, for example source term data and experimental measurements such as temperatures in the circuit which are not all provided in the Final Report.

6.2.Computational domain

The temporal and spatial domains for the four parts of the analysis are defined as follows, where zero time refers to the start of the bundle degradation phase, 10h15min00s on 26 July 1996.

6.2.1. Phase 1: Bundle

- Spatial domain - fuel rods, control rod, shroud, coolant channel, axial length 0-1.0825m (top of fuel & control rods), radial dimension to 0.056m (outside surface of the Inconel pressure tube). The zero level in the bundle is -7987mm (Bottom of Fissile Column, Final Report figure 2.4-2, reproduced here in Appendix 2) with respect to the circuit.
- Temporal domain - 0 to 18660s (containment isolation).

6.2.2. Phase 2: Circuit

- Spatial domain - in length from top of fuel bundle (-6904.5m) to entrance to containment, radially to inner heated surface maintained at constant minimum temperature for the hot leg, steam generator and cold leg, same radial position for the unheated part of the upper plenum 1, coolant channel.
- Temporal domain - 0 to 18660s (containment isolation).

6.2.3. Phase 3: Containment

- Spatial domain - inner containment walls including those of sump and condensers, atmosphere, sump liquid.
- Temporal domain - 0 to 30000s (end of aerosol settling, note detailed experimental containment data end at 28540s).

6.2.4. Phase 4: Chemistry

- Spatial domain - as for the containment.

Temporal domain - 0 to 341400s (end of chemistry phase).

6.3. Initial and boundary conditions

The subsections below list the minimum conditions that were specified. The following two conditions were common to all:

- Geometry;

- Material properties.

The lists below assume stand-alone calculations; for coupled calculations the input conditions for a following stage may be available from the stage before.

6.3.1. Phase 1: Bundle

- Nuclear power history;
- Power distribution (axial, radial);
- Inlet steam flow history and pressure;
- Fission product inventory;
- Thermal boundary conditions at the outer radial surface of the computational domain.

6.3.2. Phase 2: Circuit

- Inlet steam and hydrogen flow rate histories;
- Inlet fluid pressure history;
- Inlet temperature history;
- Wall temperature evolution in the upper plenum;
- 'Constant' wall temperature evolution along the length of the circuit;
- Fluid temperature evolution in the circuit;
- Fission product and structural material release rates.

Note: these conditions imply that the wall and fluid conditions are to be derived from the experimental data rather from a separate thermal hydraulic calculation for the circuit, which would take into account all heat sources and losses, thermophysical properties of insulating materials etc. Such a calculation (i.e. circuit thermal hydraulics) is out of the scope of this ISP. An example how the wall and fluid conditions could be derived from the experimental data was provided in the Specification Report.

6.3.3. Phase 3: Containment

- Inlet steam and hydrogen flow rate histories;
- Draw-off (sampling) flows;
- Inlet pressure history;
- Inlet temperature history;
- Temperature evolution of the outer walls, condensers and sump;
- Aerosol granulometry (AMMD and geometrical standard deviation);
- Fluid temperature evolution in the sump;
- Fission product and structural material release rates.

- Initial composition of the atmosphere (i.e. at room pressure and temperature before heatup of the vessel).

6.3.4. Phase 4: Chemistry

As for the containment, with in addition:

- Gaseous iodine fraction entering the containment;
- History of iodine injection into the sump during release and aerosol depletion phases;
- Iodine inventory in the sump water before and after washing;
- Additional iodine transfer to sump water during the washing phase;
- Condensing flow rate on the condensers;
- Radiation dose rate;
- Volumes of each water phase;
- Interface area between sump and atmosphere;
- Mass transfer coefficients;
- Oxidised silver fraction in the sump;
- pH evolution in the sump water.

6.4. Recommendations on noding for reference case and sensitivity studies

The noding schemes recommended below were intended in the first case to approximate to a noding density appropriate to that for a reactor calculation, taking into account the need for some extra detail owing to the boundary conditions, while the second case is generally more detailed, similar to some of those used in interpretation of the experimental results. Comparison of these gives some insight into what level of detail is required to give spatial convergence.

6.4.1. Reference calculation

6.4.1.1. General principles

- noding density defensible in reactor calculation context (if these are different, a justification should be provided);
- node centres correspond as far as possible to instrumentation positions to avoid interpolation problems;
- user parameters broadly consistent with those used in plant calculations (again, if these are different, a justification should be provided).

6.4.1.2. Bundle

- 11 axial nodes in heated length, top and bottom 50mm length, rest at 100mm intervals so centres correspond with the thermocouples;

- 5 components representing control rod, inner ring of irradiated rods, outer ring of irradiated rods, outer fresh rods, shroud; radial noding in components left free;
- number of thermal hydraulic channels left free.

6.4.1.3. Circuit

- 3 nodes in upper plenum and rising line;
- 2 nodes in hot leg with zone C;
- 4 nodes in SG up;
- 1 node for SG top;
- 1 node for SG down;
- 1 node for cold leg with zone G.

Stand-alone calculations may require an additional node at the start to represent the bundle.

6.4.1.4. Containment

- 2 nodes suggested; main vessel and sump, others may be used to define boundary conditions.

It should be recalled that the ISP-46 objective is not to validate detailed thermal hydraulic calculations.

6.4.2. Optional best-estimate calculation

6.4.2.1. General principles

- noding scheme takes into account Phebus-specific features without excessive detail;
- node centres correspond as far as possible to instrumentation positions to avoid interpolation problems;
- user parameters may be chosen to account for Phebus-specific features, but justification for the choices should be supplied.

6.4.2.2. Bundle

- 20-25 axial nodes in heated length, chosen so for each t/c there is a node corresponding with the centre;
- 5 components representing control rod, inner irradiated rods, outer irradiated rods, outer fresh rods, shroud; radial noding in components left free;
- number of thermal hydraulic channels left free.

6.4.2.3. Circuit

The following were minimum numbers:

- 4 nodes in upper plenum and rising line;
- 3 nodes in hot leg with zone C;
- 7 nodes in SG up;
- 1 node for SG top;

- 2 nodes for SG down;
- 2 nodes for cold leg.

Stand-alone calculations may require an additional node at the start to represent the bundle.

6.4.2.4. Containment

- 9 nodes suggested; basically top, double annulus over lower wet and total dry condenser, and over injection point, bottom, sump (data for 5 levels quoted in final report, average temp is over these levels), others may be used to define boundary conditions (note, increased noding is not so important in the containment, 2 nodes could be used if 9 are impracticable).

It should be noted that such a refined noding is useful only if it impacts on the aerosol depletion pattern; containment thermal hydraulics per se can be better studied by analysing other experiments where the study of these is the main objective.

7. Deliverables from participants

7.1. General

Participants were asked to provide a summary description of their codes, a description of how they modelled the Phebus facility, a summary table of key events (Table 6) similar to that often requested in plant sequence calculations, information on computing performance, an assessment of their own results, lessons learnt regarding plant studies. In addition to this written information, detailed numerical results were requested as given in the next section. During the course of the initial analysis of the results, the coordinators also requested the completion of questionnaires to provide information on code models and user parameters chosen, in a common format. The response of the participants is summarised in Appendix 4.

7.2. Detailed numerical results

This section summarises the results that were requested for each phase in turn. A separate file was requested for each phase of the calculation (e.g. for integral codes) so that the results of integral and separate-effects codes can be more easily compared

7.2.1. Bundle phase

- Bundle temperature, thermal hydraulic, fission product release and other time-dependent quantities as listed in Table 7;
- Snapshots of the bundle state at a range of times in the degradation phase as listed in Table 8;
- Schematic pictures of the bundle state at the times indicated in Table 8 showing the final state of the bundle in the radial noding scheme chosen, with information at least on the UO_2, ZrO_2, Zr disposition in intact state and if possible in the relocated state. An example was provided in the Specification Report.

7.2.2. Circuit phase

- Thermal hydraulic conditions and in the circuit and fission product release data through the C and G points as a function of time, as listed in Table 9;
- Fission product deposition data through the circuit as listed in Table 10.

7.2.3. Containment phase

- Thermal hydraulic conditions in the containment and aerosol physics data in the containment (including atmosphere, sump and deposition) as a function of time, as listed in Table 11.

7.2.4. Chemistry phase

- Time dependent iodine chemistry data, as listed in Table 12.

8. Analysis of results

This section gives an account of the detailed analysis of each phase, followed by more generalised analysis covering all phases. As this integral ISP has generated a vast amount of numerical data, more than in previous ISPs which have a more 'separate-effects' character, it has been judged appropriate at this stage not to concentrate on very detailed aspects of individual submissions (such as the effect of varying each user parameter), but to take more of an overall view, indicating which areas might benefit from further analysis later, possibly in follow-up studies that take account of the results of other relevant work.

The general methodology was firstly to check the incoming numerical data for completeness and for formatting and units errors, for example, correcting as necessary, then to generate global plots of key variables that compared all submitted results against the corresponding numerical data. From these plots, representative cases were chosen to make a comparison amongst the results from different codes, effectively eliminating the 'user effect'. For now, the analysis has focused more on the results of the base cases, rather than on the best-estimate cases, though results from the latter are taken into account where possible. A full comparison of best versus base cases has not been possible at the present stage, but may be possible later.

To give a fuller picture of the participation, and to form a basis for further study, appendices have been provided giving information on the submissions. Appendix 3 lists the summary tables supplied by the participants, which give the key results in a compact format. Appendix 4 gives the replies to questionnaires which give details of the models used and some of the more important user input parameters. Appendix 5 gives details of the results of the computing benchmark, while Appendix 6 gives short summaries of each code used in the exercise, kindly supplied by the code authors or by experienced users. Appendix 7 gives the conclusions of each submission as extracted from the technical reports of the contributors, while Appendix 8 gives the views of the major code developers on the outcome of the analysis. Appendix 9 is a compendium of comparison plots produced during the exercise, while finally Appendix 10 gives additional information provided by participants after the final deadline for submitting results (December 2002).

8.1. Bundle

8.1.1. Introduction

The bundle phase of the ISP, Phase 1, enjoyed a strong participation, with 34 base case and 13 best-estimate cases being received. For integral calculations, results were provided by (developers indicated in *italics*):

- ASTEC V0.3, V0.4 by EC, *GRS*;
- ASTEC V1 (2 submissions) by *IRSN*;
- ATHLET-CD/COCOSYS by *GRS*;
- IMPACT/SAMPSON by *NUPEC*;
- MAAP-EDF 4.04.c by *EDF*;
- MELCOR 1.8.4 by Enproco, Gidropress;
- MELCOR 1.8.5 by CSN, JSI(2) ,KAERI, KINS, NRI, NUPEC, PSI, *SNL*, Studsvik, UP Madrid;

while for the stand-alone option:

- ATHLET by *GRS*, U Bochum;
- ICARE2 by ENEA, KFKI, FZK, *IRSN*;
- SCDAP/RELAP5/MOD3.2 by FZK;
- SCDAPSIM by CNSNS, U Zagreb, RDIPE, U Hacettepe, SCK, Gidropress.

In addition, *ISS* provided an overview of the SCDAPSIM contributions.

The analysis was mainly on the basis of the base cases, as being more representative of plant studies, with best-estimate results being used as necessary.

8.1.2. Overview of results

Given the large number of submissions with some codes, it was necessary to select representative cases that represent best each code's capability; this reduces the user effect. The selection was made on the following basis:

- quality of selected key output variables: history of hydrogen production, 2nd ring fuel temperature at 400mm, guide tube temperature at 800mm, inner shroud temperature at 200mm and 600mm (former indicates melt relocation), fluid outlet temperature, history of iodine release;
- completeness and accuracy of energy balance information;
- integral preferred over separate-effects (given the object of the exercise);
- inclusion of code developers;
- availability of detailed information in the documentation.

The basic selected cases were as follows:

- ASTECV0.4 - GR3;
- ASTECV1 - IP3;
- ATHLET/COCOSYS - GR4;
- ICARE2 - EN2, IP2;
- IMPACT/SAMPSON - NP1;
- MAAP4 - EF1;
- MELCOR - PS1, NR1, SI3, US1, NP2, KA1;
- SCDAP/RELAP5/MOD3.2 – FZK;
- SCDAPSIM - MX1, CR1, TU1.

Minor adjustments to the list were made in individual cases to illustrate specific points

As an indication of the noding schemes adopted, examples are given for an integral/base case NR1 (MELCOR), Figure 32 (note that the cold leg of the steam generator is here divided into 3 nodes, rather that 1 as recommended, and that there are 3 radial rings in the bundle whereas some calculations used up to 5), a detailed/base case MX1 (SCDAPSIM), Figure 33, and a comparison of base and best cases for FZ3 (ICARE2), Figure 34. As seen, the bundle was normally discretised into separate radial rings representing the irradiated rods (usually subdivided into 2 or 3 components), unirradiated rods, control rod (where possible) and shroud. One or (preferably) two thermal hydraulic channels were used. Participants adopted various devices to include the Zircaloy of the stiffeners (not a standard component) and of the grids and thus to give a good overall mass balance and hence improve the hydrogen production calculation. A common approach was to smear the mass of the stiffeners over the inner surface of the shroud.

The main parameter choices of the participants are listed in Appendix 4. For the treatment of experiment-specific features, information is provided on modifications to the nuclear power and to the shroud thermal properties, and on the treatment of gap closure in the shroud as the bundle heats up (neglect of this can result on the bundle radial heat loss being calculated too low at high temperatures). The usual approach for the last point was to modify the thermal conductivity of the gap so it rose to a very high value after the gap had been calculated to close. Regarding chemical processes modelled, information is provided on the treatment of Zircaloy oxidation by steam, modelling of diffusive limitation on this oxidation in the gas phase (important for the high rates seen in the excursion phase), oxidation of Zr-bearing mixtures, and the dissolution of UO_2 by Zircaloy. In the first of these, the Urbanic/Heidrick parabolic approach sometimes combined with that of Cathcart/Pawel at lower temperatures was a popular choice, while for the second a heat/mass transfer analogy was normal. The Prater/Courtright correlation was little used. Most participants calculated oxidation of mixtures (otherwise hydrogen production is too low particularly in the late phase), usually taking the rate for metal weighted by molar fraction. A variety of options was used for fuel dissolution by Zircaloy, including the treatments of Kim/Olander and Hofmann.

Turning to melt relocation parameters, information is given on the breach criterion for oxidised clad, the criterion for bulk fuel movement, the physical properties of U/Zr/O mixtures, and any modifications made to the material properties. For the first, the most common approach is still the empirical treatment based on temperature, taking account of the oxide thickness; no mechanistic model yet seems available. One temperature is used if the oxide thickness (or oxidised fraction) is

less than a preset value, and a higher one if it is greater. For example, for SCDAPSIM calculation CR1, the criterion is (1) T>2500K and oxfraction <0.6, then (2) T>2950K; the latter corresponds to the ceramic melt temperature. MAAP4, submission EF1, uses a different approach, based on the Larson-Miller criterion which involves calculation of a damage fraction. For bulk fuel movement, it is normal just to use a temperature; this is sometimes termed a 'melting' temperature whereas 'relocation temperature', 'collapse temperature' or something like this would be better, as it is by no means clear that the relocating fuel is completely molten (a slurry composed of solid pellet fragments and liquid U/Zr/O mixture containing also structural and materials such as Fe seems more likely). A collapse temperature of 2500-2600K was a common choice, sometimes achieved by artificially lowering the fuel melting point from the normal ceramic value (care needs to be taken here to avoid inconsistencies with the U/Zr/O phase diagram). For material data, MATPRO was the most common choice. It is noteworthy that in MELCOR1.8.5 the default bulk relocation temperature was lowered to give answers consistent with FPT1; this is not necessarily appropriate as other irradiated fuel experiments such as Phebus FPT2 and PBF SFD 1.4 show relocation at higher temperatures, what is needed here (and for other empirical model parameters) is a demonstration of global agreement across a range of similar experiments, with best-estimate (to be the default) and limiting values being recommended by the code developers following a programme of assessment.

A full set of comparison plots is provided in Appendix 9.1. A subset which forms the basis for the discussion which follows is indicated in the text as each figure arises.

8.1.3. Nuclear power

The nuclear power is one of the most important inputs to the calculation, governing the bundle heatup and subsequent degradation. The nuclear power histories submitted by the participants are illustrated in Figure 35 and Figure 36 for the base and best-estimate cases respectively. In order to give a better match to the measured bundle temperature histories, many participants adjusted the power input (normally a reduction) and/or the shroud thermal conductivity; these changes were within the uncertainty ranges quoted.

For the power, the reduction tended to be in the range 5-10%, as seen in the figures, this helped to prevent early calculation of the oxidation excursion. However other differences in the curves are apparent, particularly towards the end of the bundle phase. In many cases these are due to the fact that in some cases the power plotted was the input power, in others it was the power deposited in the bundle, including the effects of relocation and self-shielding. It needs to be made clear in the code output which is meant. Ideally, both should be available, to see if these latter effects are important (not so much in Phebus, but may be in plant calculations). The power deposited in the bundle is the one needed for energy balance assessment.

Modelling closure of the shroud gaps on heat-up is also considered important. If neglected, the shroud acts as too good an insulator later on in the transient, as mentioned in the previous sub-section.

8.1.4. Energy balance

Checking the energy and mass balance should be an essential part of any experimental analysis and plant calculation, but only a few cases were reported by the participants. Thus some analysis was performed by the coordinators as part of the ISP. The assessment of the energy balance in the bundle involves consideration of the nuclear power, the power released by oxidation of the metals

by steam (mainly of Zircaloy), the heat loss by convection to the coolant, and heat lost radially through the shroud. Many participants were able to provide at least the oxidation power by reference to standard code outputs.

The oxidation power is illustrated for base cases in Figure 37. It shows primary peaks at the time of the main oxidation excursion, with generally secondary peaks later (consistent with the observed hydrogen production). Apart from isolated spikes, the oxidation power is lower than the nuclear power. Some of the peaking is due to noding effects, as the continuous progression of the flame front which would give a smoother behaviour cannot be exactly captured by the axial discretisation. However some MELCOR cases especially gave unphysically large spikes, inconsistent with the hydrogen production. A problem with the code output seems likely, which should be checked. As an illustration, participant PS1 provided a power obtained by scaling the hydrogen production rate by the heat of reaction (assumed constant), as well as the code's advertised oxidation power, these are compared in Figure 38. The good agreement away from the big spikes provides support for the view that it is the code output rather than the calculation itself that is the problem.

The convected power lost to the fluid and the power lost through the shroud are shown for the base cases in Figure 39 and Figure 40 respectively. The convected power may be correlated with the fluid temperature change up the bundle (strictly speaking the difference between the input and output fluid enthalpy). There is a wide scatter in the results, broadly consistent with this fluid temperature change (see below). There may be a problems with output parameter definitions in some cases, e.g. not including all surfaces.

The power lost through the shroud is typically 2-3 times that lost to convection, given the low sink temperature on the outer shroud, and is sensitive to the thermal properties assumed. The power losses here mainly bunched together - low values may indicate problems with the definition of the output quantity (e.g. neglect of radiation); this is often not a standard output parameter and in many cases needed to be defined by the user, which leads to extra work and the potential for error (similar remarks apply to the convected power too). Again, occurrence of spikes needs to be checked by the user, as these are unphysical.

The overall energy balance was analysed in selected cases, and the results are illustrated in Figure 41 to Figure 46. The best cases show heat loss through the shroud of typically 66% at the end of the P2 plateau, with convective loss about 33%; the shroud loss then increases as temperatures rise. The derived quantity 'stdht' which is the difference between heat generated and heat loss (nuclear heat + oxidation heat – convected heat – heat loss through the shroud), in principle should be the rate of change of gain in stored heat, and resemble in shape the bundle heatup history. Since the bundle temperatures are reasonably well calculated (see next section), stdht is expected to vary little amongst the best calculations, however variations of up to a factor of 2-3 are seen (but note these are differences of similar large numbers). This could be due to differences in material properties, or, more likely, differences in the definition of the energy output of the code (in ISP-45, QUENCH-06) problems of energy balance were also noted). This is another area where the codes need to be checked for consistency. It is interesting to note how little of the power actually goes into heating the bundle, and how much is lost to the shroud.

8.1.5. Fluid temperatures

The bundle inlet and outlet temperatures are illustrated in Figure 47 and Figure 48 respectively. It should be noted that these are respectively below and above the heated length 0-1000mm; the inlet measurement is at -107mm while the outlet is at 1077mm (not 1025mm as erroneously stated in the

FPT1 Final Report Figure 4.1-10 and thus in the ISP specification). For the inlet this does not matter as the temperature gradient approaching the bundle inlet are small, but at the outlet there is a steep gradient going into the upper plenum. This requires therefore accurate interpretation of the results of the codes, making sure that the output is quoted at the right axial position.

The inlet temperature was provided as input data, and this is reflected in the figure at least in the early stages. Rises in the temperature in the later stages indicate more clearly plotting of the calculated nodal temperature rather than of the imposed boundary condition, and also the calculated presence of hot relocated material (which cools afterwards) which causes some local blockages to the coolant flow. Concerning the outlet temperatures, there is a general tendency of the supplied results to overcalculate this quantity, by up to many hundreds of degrees, although some codes managed to give good agreement with the data. There are potentially both experimental and calculational reasons to explain partially this overcalculation:

- the outlet fluid thermocouple TCW46 is near to outer rod 16 facing the shroud above the heated section, and so it may measure lower than the average fluid temperature; the shroud temperature would be a conservative lower bound;
- the calculated temperatures would not be referred to 1077mm, but to 1025mm (being higher), it is also possible that some participants would have used the temperature at the middle of the topmost fuel node, 975mm (giving higher temperatures still).

The magnitude of these effects was investigated by ICARE2 calculations based on the submission IP2, and results are illustrated in Figure 49 at levels from 975mm to 1077mm, for the inner fluid channel 1, the outer fluid channel 2, and the surface of the shroud facing the coolant. At the plateau around 15000s, the difference between channel 1 and channel 2 at the same elevation is about 60K, and between channel 2 and the shroud wall larger at about 220K, whereas the axial difference between 975mm and 1077mm is about 200K (70K between 1025mm and 1077mm). These differences, while significant, are not sufficient to explain the wide spread in the results, this conclusion is supported by the spread in the convective heat loss, which cannot be explained by errors in the elevation quoted for the temperature data. One can therefore conclude that there is a genuine tendency to overpredict the outlet fluid temperature, even taking these uncertainties into account. If a code is forced to match the measured history, the convective heat loss can become unphysically small, even negative, Figure 50.

While there is little impact on the predictions for the bundle, these overpredictions feed through into the circuit calculations, especially in the rising line, affecting the calculated deposition of the fission products.

8.1.6. Shroud temperatures

The shroud temperatures have no direct physical significance regarding plant safety assessment, but nevertheless provide complementary information regarding radial heat losses, which form the largest component of the overall heat loss. Too little radial heat loss can lead to too a high convective loss, and therefore to excessive outlet temperatures, for a given input power and fit to the rod temperatures. Given the dominance of the radial heat losses, the choice of shroud properties affects these outlet temperatures, and therefore circuit conditions; this is also not prototypic, but must be considered in the interpretation of the results. As the radial heat loss is large compared with the convective loss, relatively small changes in the shroud properties can have a disproportionate effect on the outlet gas temperatures (taking differences of large numbers magnifies the potential uncertainty).

Graphs comparing the calculated and observed temperatures at the 200mm and 600mm levels in the inner shroud are shown in Figure 51 and Figure 52. Noteworthy features are the tendency to overpredict temperatures, and the sudden rise in temperature after 200mm for both codes and data, indicating relocation of hot material to this position. As with the outlet gas temperatures, the spread is surprisingly large, considering the generally good prediction of the bundle temperatures, see below. Some of this may be due to the use of too high an input power[1], or to a inappropriate radial location having been chosen for the code output (the radial temperature gradients in the shroud are very steep, see Figure 6 for example, so a small error in radial positioning could have a big impact on the temperature quoted). However in the time available it was not possible to take this analysis further, given the higher priority afforded to parameters of more significance to reactor safety.

Given the uncertainties in power and shroud properties, the need for tuning these quantities to give a fit to both the shroud and outlet temperatures seems essential to give good agreement with the overall temperature profiles and therefore to the bundle degradation and fission product release. The MELCOR contribution PS1 shows better agreement with a power reduction of 10% and an increase of shroud thermal conductivity of 20%, both of which are within their uncertainty bands.

8.1.7. Bundle temperatures

Good prediction of the fuel rod temperatures is clearly essential for accurate calculation of the bundle degradation and fission product release, similar remarks apply to the control rod degradation for structural material release that forms the larger part of the aerosols transported into the circuit. Graphs comparing the calculated fuel temperatures against experimental data are shown in Figure 53 to Figure 58 for a selection of axial elevations and base/best cases. Similar information for the control rod (guide tube and absorber material) is given in Figure 59 to Figure 62.

Concerning fuel temperatures, fuel temperatures in the centre of the bundle (peak region, 400-700mm) were generally well calculated. There was a slight tendency to overprediction at 300mm, where some participants calculated an excursion where none was observed. Some early excursions are predicted at all elevations, as indicated before (too high input power, low heat losses). Agreement tended to be better for the best-estimate cases than for the base cases, with a lower spread in the results (possible effect of more experienced user as well as of more refined noding). Some participants made no distinction between the outer irradiated rods and the fresh fuel rods. Some variations in clad burst temperature (from ballooning) were noted, but these are unlikely to influence substantially the subsequent damage progression. On fission product release, there would only be an effect here on the timing of relatively small release of volatile fission products from the gap.

Regarding control rod temperatures, there were stronger variations in the agreement of the calculated temperatures with the data, especially at higher elevations (overprediction at 1000mm), but the overall trend is again well calculated. Some participants could not model the individual parts of the control rod; this may be important for more detailed relocation and release models. In some cases a problem of residual mass after relocation was noted; a nominal mass is left behind which follows the gas temperature (this shell is often left to preserve the original view factor matrix, the mass is negligible so the heat conduction calculation is not affected). Care needs to be taken that this mass does not cause unexpected logical effects in tests for the status of control rod degradation

[1] The nuclear power input given in the specification report was the best estimate at the time of its publication, but this is now considered ~10% higher than the present best estimate. This is consistent with many participants' findings.

at these levels. Variations in control rod failure temperature affect the timing of the initial cadmium burst release, these are to be examined later if possible, using other relevant data, e.g. from the CORA series where greater volumes of data are available. However, it may be noted that the control rod failure temperature of ~1623K observed in FPT1 lies with the range seen in CORA (1493-1695K), note also that FPT0 gives an earlier failure at about 1473K.

Overall, it may be concluded that the calculation of bundle temperatures was satisfactory, and in the best cases, good.

8.1.8. Bundle degradation

A comparison was carried out between the measured axial mass profile for the final state and the calculated profiles, inspecting the distribution amongst the various species present for the calculations. The results are shown for selected cases in Figure 63 to Figure 70. It would be desirable to investigate the progression to the core final state, and to compare the results with the experimental results available as a function of material density, but this was not possible in the time available.

With a suitable choice of input parameters, the best calculations could give a good representation of the bundle final state, and overall there was not a large difference on the whole between the base and best-estimate cases (the latter showing at best only a mild improvement over the base cases). In the best cases, the agreement could be excellent. A major consideration is relocation of U/Zr/O (following breach of the clad oxide shell) and UO_2 (bulk fuel relocation). The bulk fuel relocation temperature needs to be reduced from ceramic values (over 2700K) to give good agreement with the blockage profile. In the SCDAP model (SCDAP/RELAP5 and SCDAPSIM) this temperature is fixed as the ceramic melting point; so, there is little relocation calculated. There is incomplete mass balance for some codes, e.g. ASTEC, as some material data cannot there be output (U/Zr/O …), so there is need for output enhancement here.

Other experiments, e.g. Phebus FPT2 and PBF SFD 1.4, show evidence for higher bulk relocation than in FPT1; so, any change of default values should not be made on the basis of FPT1 data alone. It therefore seems unlikely that a simple temperature criterion will suffice; more detailed model development, possibly needing new separate-effects data, is therefore indicated, as the mechanisms involved are not clear (effect of irradiated fuel, presence of iron in the melt, …). In the meantime, plant calculations should be performed with sensitivity studies on the bulk relocation temperature to bound the effect.

In principle it would be possible to gain additional information by analysing the progression to the final state, for example looking at the effect of changing the oxide shell breach criterion which affects the initial relocation of U/Zr/O, in comparison with early phase melt progression ISPs such as Phebus B9+ (ISP-28) and CORA-13 (ISP-31), but this was not possible in the time available. Similar remarks apply to the fuel dissolution by molten Zircaloy, where there are strong indications that irradiated fuel is dissolved more quickly than fresh fuel[15,16]. Such analysis could also take advantage of axial material profile data as a function of density, which discriminate between oxidised Zircaloy and UO_2. In the meantime, similar remarks are made as for the control rod failure temperature and the bulk fuel relocation temperature, viz. sensitivity studies need to be done in plant calculations based on the parameters obtained by fitting to a range of relevant experiments.

Blockage and material distribution data are not easily available from most code standard output, despite the fact that core final state is a key signature of an accident sequence. Sometimes it is only

available after manual post-processing of results, giving extra work and scope for error (omission or double counting of material, found in a few cases here). It follows that the blockage and material distribution data should be available both in printed output ('major edits') and in graphics dump files as a standard feature of the codes.

8.1.9. Hydrogen production

Hydrogen production is relevant to safety issues, for example to the risk of deflagration and/or detonation in the containment, and is therefore included as a separate item. It is obviously closely linked to the oxidation power, discussed above. Comparisons of calculated hydrogen mass flow rate against experimental data are shown in Figure 71 and Figure 72, while similar comparisons for the integrated amount are shown in Figure 73 and Figure 74.

Most codes predict a final value in the upper end of the uncertainty range (~ 10 %), but with pronounced differences in evolution correlated with the temperature history; so, the shape discriminates better than the total amount. There is little sensitivity to base versus best-estimate cases. Most codes calculate the second peak due to oxidation of U/Zr/O melt, a positive feature.

Overall, the agreement seems reasonable. In principle, it should be possible to compare the relative merits of the various Zircaloy oxidation correlations such as Urbanic/Heidrick, Prater/Courtright, etc. by inspection of the detailed shape of the hydrogen production curve, particularly in the region up to the top of the oxidation peak where rod-like geometry is still mainly preserved (avoiding uncertainties due to breach of the cladding oxide shell which can lead to removal of Zircaloy from the hot zone and thence delays or even stops its subsequent oxidation). However such an analysis would probably be confounded by the much larger uncertainties concerning the radial heat losses in these experiments. So, equally good agreement could be found after using a different oxidation correlation, then making a change to the shroud thermal conductivity within the rather large uncertainty band. It would be more productive to use experiments such as those in the CORA (ISP-31) or QUENCH series (ISP-45), which are more specifically targeted towards hydrogen production issues.

8.1.10. Fission product release

The calculated fission product release from the fuel has a strong impact on the transmission through the circuit and the source to the containment. The analysis here considers release from volatile, semi-volatile and low-volatile species. The results are shown in Figure 75 to Figure 92 for the species Xe, I, Cs, Te, Ba, Sb, Mo, Ru and U.

The total release for volatiles was generally well calculated, with little difference between base and best-estimate cases. There were substantial differences in the release kinetics, even for similar fuel temperature histories in good agreement with the data. The trend was towards too rapid a release in the early stages, typical of CORSOR-type approaches (in MELCOR for example) with only a temperature dependence. More recent models, such as ELSA2 (in ASTEC V1 and ICARE2) which consider the fuel state and the oxidation potential of the coolant, show promise but their development is not yet complete. A similar approach which considers stoichiometry has been introduced into IMPACT/SAMPSON, Appendix 10.1.

For semi/low-volatile release, much more scatter is exhibited. The tendency is to calculate low for Mo, high for Sb, and very high for Ba. Concerning molybdenum, the higher than calculated release has already been evidenced in annealing tests such as the VERCORS ones, especially in an

oxidising environment, that is the case during most of the FPT1 transient. Improvements could be made in integral codes by revising the correlation for vapour pressure, taking account of the oxygen potential. A more detailed approach is also possible with mechanistic codes such as MFPR or VICTORIA, which calculates the repartition of fission products in the different solid phases, and their vapour pressure over these phases. However, it is unlikely that such detailed models can be incorporated in an integral code in the near future. The quality of the prediction for antimony could also be improved by modifying the vapour pressure correlation. However, this is less important, given the rather low radio-toxicity of antimony. The case of barium is different. In annealing tests, the release might be very high, whereas in the Phebus bundle tests, it is very low. An interpretation has been proposed[17] based on on a reduction of barium total pressure in the solidus-liquidus transition zone in the U-Ba-O phase diagram, and due to interaction with iron and zirconium oxides. Improvements of models could be done following this approach; they would require a good coupling between degradation and fission product release models.

For the low-volatiles U and Ru, there is a reasonable order of magnitude agreement in most cases. The best-estimate cases appear to give better agreement and less scatter, but these are generally from more experienced users. There is probably room for improvement in predicting more accurately the release of the different actinides (uranium, plutonium, americium and curium), that actually differ, whereas they are generally assumed to be identical. However, this should be made on the basis of a more extensive data base than the FPT1 test. Ruthenium has a very specific behaviour. The rather good agreement observed must be tempered by the fact that what is calculated is the release from fuel and what is measured is the release from the bundle zone. Indeed, most of the ruthenium released remained trapped in the fuel bundle zone, and no code was able to capture this behaviour.

Some MELCOR participants volunteered additional output, giving the total release from the rods as well as release from the exit of the bundle (the latter was the requested parameter). Results are typically 5–10 % deposited in the bundle, Figure 101; there is more in proportion for the less-volatile species. This additional output could aid additional interpretation of the results, and this could be profitably employed in the analysis of other Phebus tests too. At present, MELCOR appears to be the only code that can calculate release and deposition in the same volume; this is a feature that could be considered for other integral codes too, as in the general reactor case it will not be clear in advance whether a particular node should be considered as an emitting or receiving volume. This seems to be a matter of code logic rather than new model development, as the relevant models already exist.

8.1.11. Structural material release

This subsection considers the release of tin from the Zircaloy cladding, and silver, indium and cadmium from the control rod absorber materials. The results are presented in Figure 95 to Figure 100 respectively.

Tin is important for tellurium transport, as the tellurium might be transported as SnTe (the elements are found together in transmission and deposition, although this precise species has not been observed directly). The structural tin is released from burning of the Zircaloy cladding; so, there is a close resemblance to the hydrogen production/Zircaloy consumption curve, Figure 102 (whose absolute values for Zircaloy consumption assume that all the hydrogen comes from the production of this metal).

Many codes start with a reasonable release rate, but continue onwards, to give too high a release eventually, and overall there is a wide scatter of results. No physically-based model is yet available, so development should be attempted. It is known that at least under steam-rich conditions, some tin migrates into the unoxidised metal to form a tin-rich layer, allowing the remainder to be released as aerosol; the FPT1 results suggest that 60-70% of the tin in the hot zone could be available in this way. Tin aerosol was also observed in the CODEX air ingress tests[18], suggesting that oxidation by oxygen could also be effective in promoting tin aerosol formation. What is not clear is whether oxidation is essential for the tin release process; would heating tin in an inert atmosphere to similar temperatures give any release? Upcoming results from Phebus FPT2, which had a oxidation in an extended steam starvation period, may shed some light on this question.

Concerning control rod materials, there is a general difficulty with the releases of silver, indium and cadmium (SIC). These are essential for accurate calculation of circuit chemistry for the iodine; the main need is to saturate the iodine reactions. There is no accepted model as yet; a variety of approaches was tried (as a scaled-up fission product release, a 'burst'-type release, ad-hoc empiricism etc.) leading to a wide range of answers, as the likely dominant mechanism in the earlier stages after the initial Cd burst release (evaporation from a molten SIC pool held in a 'crucible' formed by the oxidising metallic cladding/guide tube stub) is not captured. The ELSA2 model attempts to link with the control rod degradation state, but the model, while promising, needs additional development.

The silver release results range from zero (no model) to 66%, with only a very few calculations showing an acceptable time dependence and final amount. It is judged that in a blind calculation (as for a plant transient) such agreement would be unlikely. However it is better to have even a crude model than no model at all, as at least there is a chance that there would be enough Ag released to react with the iodine, as observed.

There is again no accepted model for indium release, and there is an even wider range of answers, from nothing to a 100% burst release on control rod failure (most unlikely). The time dependence, too, is not represented. The more physically-based model ELSA2 in ASTEC V1 gives a better time dependence but too high a release, probably because of incorrect speciation (oxide versus metal).

The cadmium results show a similar very wide scatter, from virtually zero (like a non-volatile fission product, unscaled), to 100% burst release on control rod failure, some participants also treated it as a scaled fission product, giving an inappropriate time dependence as the burst release is not represented. The likely mechanism is burst release followed by evaporation from the molten SIC pool. The burst release is not 100% as data from CORA and Phebus FPT0 shows Cd in the refrozen melt (50-70% from the SIC molten at control rod failure seems reasonable under these condictions). ELSA2 models this process but the burst release is too high and too early, seen also as excess early suspended mass in the containment. Sometimes unphysical step changes in the Cd release were calculated, followed by long periods of zero flow, these are associated with noding effects and are something that need to be eliminated in future model development (these changes can be averaged out by hand for input into a stand-alone circuit calculation, but this cannot be done for an integral calculation).

The overall conclusion is that modelling of structural material release is inadequate and substantial model development is necessary.

8.1.12. Conclusions for bundle phase

8.1.12.1. Modelling aspects

- In general, the temperature history of the bundle and the total hydrogen production are well enough predicted, though some tuning of the bundle power and shroud thermal conductivity seem always to be necessary;
- The best calculations can reproduce the bundle final state well, but it is not clear that the same choice of parameters would work as well for other bundle tests;
- The total volatile fission product releases agree well with the data, though there is a tendency to over-predict at low temperatures (but better with the newer models);
- The semi-volatile and low-volatile results are much more mixed, with some good results (maybe fortuitous) amongst wide disagreement; improvement is needed;
- Control rod material and tin (clad) release models also need improvement, taking into account the bundle state.

8.1.12.2. Further analysis

In the time available, only the main features of the results have been analysed. The following suggestions are made for further work:

- Oxidised clad breach criterion: correlation with U/Zr/O release and hydrogen production (removal of oxidising molten Zircaloy from the hot zone);
- Dissolution of fuel by molten Zircaloy, difference between fresh and irradiated fuel;
- Final state of bundle: check with the additional data on material density to give more information on relocation as a function of material composition;
- Hydrogen production: look for correlation with the model used (Urbanic-Heidrick was a popular choice), and check for consistency with other ISP results (but may be compromised by uncertainty in boundary conditions, so a lower priority).

8.1.12.3. Integral aspects

- The fission product releases are of obvious importance for the onward circuit transport and source term calculations, so improvements are needed as indicated above (the errors in the bundle source term propagate right through the rest of an integral calculation):
  - this is especially important for iodine and species it can react with (Ag, Cd, …);
  - it is better to have even a simple empirical model giving an order-of-magnitude answer, than no model at all;
  - consider concentrating first on improving models where there is the greatest radiological impact (the species themselves, and those that can react with them).
- Accurate calculation of the bundle outlet temperature is also needed for good calculation of retention in the circuit (especially in the upper plenum and rising line).

8.1.12.4. Recommendations

- Improve models for bulk fuel movement, taking into account differences between irradiated and unirradiated fuel, checking the results across a range of integral tests (as FPT1 indicates a lower relocation temperature than most);
- Improve models for semi-volatile, low-volatile and structural material release (SIC, Sn), taking into account their radiological significance in determining the accuracy required; also, time dependence of volatile release;
- Perform follow-on analysis if possible especially for, oxide shell breach criteria, material relocation and hydrogen production, in the light of the results of other relevant ISPs and separate-effect tests.

8.2. Circuit

8.2.1. Introduction

In the experiment, fission products are mainly retained in two different zones where the thermal gradient is important:

- Just above the fuel bundle, where the main mechanisms for deposition are vapour condensation on walls and thermophoresis of nucleated particles;
- In the rising line of the steam generator, where not already condensed elements (iodine and cadmium) nucleate, and others are deposited by thermophoresis.

Retention in other zones of the circuit, measured and calculated, are small and will not be analysed in detail.

The largest number of submissions for this phase comes from MELCOR integral calculations, with thirteen results for the base case. A second group can be made with integral or semi integral calculations using SOPHAEROS as a transport module, including ASTEC calculations, two ATHLET-CD/SOPHAEROS and one COCOSYS/SOPHAEROS calculation for the base case. Other integral calculations have been made using MAAP4 and IMPACT/SAMPSON. It should be noted that this last calculation should be more considered as a stand-alone one, as it uses measured release instead of calculated ones.

Stand-alone calculations have been made using ECART, FEAST and SOPHAEROS.

Some participants have provided best estimate calculations and sensitivity studies. The study performed by NRI, with MELCOR and SOPHAEROS calculations using the same source is of particular interest. Sensitivity studies performed by PSI also provide helpful information for the analysis.

A full set of comparison plots is provided in Appendix 9.2. Selected figures are reproduced here as Figure 103 to Figure 132.

8.2.2. Wall and fluid temperatures

As mentioned before, most of the deposition takes place in zones where the thermal gradient is important. From the analysis of phase 2 results, we know that calculations have a general tendency to overestimate the fluid temperature at the bundle outlet. It is thus expected to observe a similar behaviour in the lower part of the vertical line. This is the case at elevation -6192, where most of the calculations overestimate the fluid temperature (see Figure 103), by 500K for some of them. What is more surprising is the propagation of this overestimation At the -4330 elevation, if we except two extreme calculations, the calculation results are randomly distributed during the heat-up phase, ranging from underestimation by about 10K to overestimation by about 200K. This overestimation is still propagating at the inlet of the horizontal line.

The flow regime is transitional in this zone of the circuit, with a Reynolds number of 2260 at 1000K. The calculation of the heat exchange between the fluid and the wall should not however be a problem, as the evolution of the wall temperature were given as boundary conditions for the problem. In the following sub-sections, we will more concentrate on the consequences of the temperature overestimation on deposition rather than on their exact causes.

In the steam generator start, at level 320 mm, Figure 111, there is again a large dispersion between calculation results and measurements, whereas in the hot leg middle, at level 1500 mm, results become reasonable. Its is suspected that some of the given results were not corresponding to the exact location of the measurement.

8.2.3. Retention in the circuit - overall fractional retention

The overall retention of fission products in the RCS is the most important safety concern and has been looked at in priority. Concerning the time dependence, almost all calculations give deposition kinetics similar to release kinetics, as illustrated in Figure 121 in which are depicted some selected results from various codes. Comparison of the overall retention at the end of the experiment is therefore sufficient, as a first step. Only few elements have been selected for the comparison, taking into account their importance for safety, their specific behaviour, as measured or as calculated, and the quality of the measurements:

- Iodine, the only important fission product not condensed in the hot leg of the circuit;
- Caesium, important volatile FP with a rather high retention above the fuel bundle and being partly re-volatilised just after the end of the release phase;
- Tellurium, important volatile FP, condensed in the hot leg and less retained in the circuit than caesium;
- Molybdenum, with a medium volatility, and able to react with caesium vapours;
- Silver from the control rod, given its importance for iodine chemistry.

8.2.3.1. MELCOR base case calculations

Plots of the overall retention are given in Figure 122 to Figure 126 for the selected elements and the base case calculations.

Concerning iodine, calculated fractional retention ranges from 0.26 to 0.51, with 2 calculations giving 0, and a mean value of 0.38, in excess of the measured one (0.26). For caesium, calculated values range from 0.3 to 0.64, with a mean value of 0.46, very close to the measured one (0.48).

The spreading is larger for tellurium: 0.24 to 0.66, with a mean value of 0.47, larger than the measured one (0.37). The spreading is also rather large for molybdenum: 0.36 to 0.85, with a mean value of 0.59, as measured. Only ten calculations gave results for silver, with a retention ranging from 0.33 to 0.85, with a mean value of 0.56 almost equal to the measured one (0.55).

On the overall, the mean calculated overall retention is rather close to the measured one, but with a rather large spreading, by a little bit more than a factor of 2 between minimum and maximum values. Among the volatile FPs, the largest disagreement is for iodine, whereas it is the only one for which MELCOR predicts correctly the physical state in the hot leg (iodine is measured as a vapour in the hot leg, whilst caesium and tellurium are measured as aerosols). In fact, this reveals that, behind the overall agreement on global retention, discrepancies on the deposition pattern are hidden, as analysed in the next subsection.

8.2.3.2. SOPHAEROS calculations

Although not all the participants used the same version of the code, all the results have been plotted together and compared in Figure 127 to Figure 131.

The trends are very similar to the ones observed for MELCOR. Iodine retention ranges from 0.28 to 0.49, with one result peaking at 0.61 (with probably some specific difficulty), in excess to the measured value (0.26). For caesium, results range from 0.36 to 0.63, with a mean value of 0.48, equal to the measured one (0.48). For tellurium, results range from 0.35 to 0.58, with a mean value of 0.46, slightly larger than the measured one (0.37). Spreading is large for molybdenum, with one result at 0.11 (with probably some calculation problems), and other ranging from 0.35 to 0.52, generally lower than the measurement (0.46). Silver retention ranges from 0.32 to 0.49, with a mean value of 0.44, lower than the measured one (0.55).

The calculated overall retention fraction is generally not too far from the measured one, but with a large scatter in the results, with roughly a factor of 2 between minimum and maximum values. Iodine retention is generally overestimated, this being due in general to a bad prediction of the transported species, as explained later on.

8.2.3.3. ECART, FEAST, IMPACT/SAMPSON and MAAP calculations

There was only one submission for each of these three codes, so that no conclusions can be drawn about a possible user effect, as for MELCOR and SOPHAEROS. The results are summarised in Figure 132.

The trends for ECART are not always the same as for other codes. Iodine fractional retention is underestimated (0.11 instead of 0.26) whereas overall retention compares well for caesium and molybdenum (0.40 and 0.49 instead of 0.48 and 0.46). Silver retention is underestimated (0.24 instead of 0.55).

The fractional retention calculated by FEAST is nearly identical for all the selected elements (0.47 to 0.49), that is reasonable, but the differences in volatility for the elements considered is not well captured, as the code is considering all the elements as aerosols.

IMPACT/SAMPSON gives fractional retentions generally lower than the experiment for volatile fission products: 0.08 for iodine, 0.32 for caesium and 0.17 for tellurium. For less volatile elements, the calculated retention is very close to the experiment: 0.50 vs. 0.46 for molybdenum and 0.0.56 vs. 0.55 for silver. It should be noted that the deposition velocity for adsorption has been

decreased as compared to standard value for all elements but caesium, for which it has been increased. The authors of the calculation state that, without this modification, the deposition was overestimated.

The overall fractional retention calculated by MAAP is always lower than the measured one: 0.1 for iodine, 0.19 for caesium, 0.27 for molybdenum, 0.34 for silver and 0.23 for tellurium. One part of this underestimation is due to the general tendency of all codes to underestimate deposition in the upper plenum above the bundle, as discussed later on. Another part is due to the coarse noding of the steam generator: only one node is used for the rising line of the steam generator (as for power plant applications with MAAP). The mean fluid temperature is therefore underestimated, as well as the temperature difference with the walls, reducing thermophoretic deposition to the walls.

8.2.4. Retention in the circuit - spatial dependence

8.2.4.1. Retention in the upper plenum

As already mentioned, fission product deposition in the FPT1 circuit is mainly concentrated in the two zones where the temperature difference between the fluid and the wall is important, i.e. in the upper plenum just above the fuel bundle and in the rising line of the steam generator. Retention in the other zones (the isothermal ones) is very small. This tendency is generally well captured by the different codes. The observed differences between measurements and calculations for retention in the isothermal zones are therefore not significant in a safety perspective and have not been further analysed.

The comparison was focussed on deposition profile in the three nodes describing the upper plenum and the three nodes describing the rising line of the steam generator, for iodine, caesium, tellurium, molybdenum and silver. The calculations were divided into three batches: MELCOR, SOPHAEROS and other codes. Plots of retained mass in mg/m at the end of the transient are given in Figure 133 to Figure 147.

The general tendency is an underestimation of deposition in the upper plenum and an overestimation in the steam generator. The reasons for discrepancies for deposition in the upper plenum are probably linked to several effects.

Overestimation of the fluid temperature has a different impact for aerosol and vapour species. For rather low volatile elements, such as silver and molybdenum, that nucleate at the inlet of the zone, the condensation zone should be shifted towards the upper locations. This is visible for silver on Figure 133. Calculated deposition are largely underestimated in the first node, and overestimated in the two other ones. Displacement of the condensation zone and increased thermophoretic effects on nucleated particles would explain the observed phenomena. For more volatile elements such as iodine and caesium, the temperature difference could lead to a bad prediction (or assumption for the codes not calculating chemistry) of their speciation. However, we will see later on that this is not the main parameter.

Among the elements selected for comparison, iodine is the only one that was predominantly in a vapour form in the hot leg of the circuit. This implies that deposition in the upper plenum was small, about 60mg/m the first node. Most of MELCOR calculations give lower results, with one giving the right value and two a bit more than 100mg/m. SOPHAEROS results are rather scattered, with results ranging from very few to about 300mg/m. ECART and FEAST give quite reasonable results, whereas MAAP is underestimating the deposits. The reason for overestimation of deposits by certain calculations is probably due to the bad prediction or assumption for iodine speciation: if

iodine is predicted to condense in the upper plenum, deposition by vapour condensation on walls and thermophoresis will be predicted, those two mechanisms having probably only a low importance in this zone during the experiment. For those calculations underestimating the deposition, the ratio between calculation result and experimental measurement is sometimes very large in absolute value. However, as the total iodine deposition in the zone is small, this is not significant on a safety point of view.

A different behaviour was measured for caesium which exhibits a deposition peak at the inlet of the vertical line, due to vapour condensation and thermophoresis, and that is then transported as aerosol with little deposition. The comparison between calculation results and experimental measurements can be seen on Figure 135, Figure 140 and Figure 145. Most of the MELCOR calculations underestimate the deposition in the first node of the upper plenum by more than one decade, with only two giving an underestimation by a factor of roughly two. The explanation for that is the wrong assumption made for caesium speciation in this zone: caesium is assumed to be mostly transported as an hydroxide, therefore remaining a vapour in this zone, and no deposition occurs by vapour condensation on the walls. SOPHAEROS calculations are also generally underestimate the deposition. The reasons are not always the same as for MELCOR, as chemical species are calculated. However, the underestimation of the release of certain semi-volatile elements from the fuel bundle, such as molybdenum, does not allow the integral codes to predict correctly the volatility of caesium in this zone. In the ASTEC V1 calculation for instance, not enough molybdenum is released to convert all caesium to molybdate, resulting in too high a volatility for this element, reducing the deposited fraction.

ECART, FEAST, IMPACT/SAMPSON and MAAP also underestimate caesium deposition in this zone.

As a conclusion for this sub-section, it can be said that deposition in the upper plenum is generally underestimated by the codes. The reasons for the differences are multiple. One part is due to the overestimation of the fluid temperature in the line. Another is the wrong assumption or prediction of chemical speciation, this one sometimes coming from an underestimation of the release of some elements from fuel. However, those two reasons cannot explain everything. Indeed, for those elements calculated as nucleating at the inlet of the vertical line, being deposited by vapour condensation on walls and then by thermophoresis of nucleated particles, the underestimation still exists. It is suspected that this is not due to problems in calculating thermophoresis, as models are well validated on separate-effect experiments, and as deposition by thermophoresis in the steam generator are overestimated. However, understanding the detailed reasons for the discrepancies goes beyond the goals of this comparison exercise. This is a work presently achieved in the frame of the Phebus-FP interpretation circles.

8.2.4.2. Retention in the steam generator

All the elements but caesium and iodine enter the steam generator as aerosol particles, and dominant deposition mechanism is thermophoresis. If we first look at elements calculated as aerosol at the steam generator inlet, such as silver and molybdenum, the deposits are overestimated. For calculations underestimating the deposits, this is due to an underestimation of the released fraction of the element from the bundle zone. The shape of deposition profile, a quasi exponential curve is well captured, except by MAAP, but in this simulation, he rising line of the steam generator was described by one single node. On the whole the overestimation is by a factor of 2, or a little more.

For elements often calculated as entering as a vapour but entering as aerosol, such as caesium, the overestimation can be even more in the first node, deposition by vapour deposition on the wall is

also calculated, in addition to thermophoresis. None of the codes is able to calculate the caesium evolution of deposits after the end of the power transient. The measured additional deposition is very likely due to re-vaporisation of caesium from the hot leg of the circuit.

For elements calculated as a vapour, and being a vapour, the deposition profile is quite well captured. However, an overestimation of deposits is still calculated.

The reason for overestimation of deposition by thermophoresis is still unclear. A number of hypotheses have been made in the Phebus-FP interpretation circles. No one has given a clear demonstration at the time being. The usual thermophoresis models are well validated against separate-effect tests, and it was not found up to now how the specificity of Phebus (more representative aerosol population, with high concentration and radioactive material) could affect the deposition process.

8.2.5. Conclusions for circuit phase

Five main conclusions can be given at this stage.

The fluid temperature in the vertical line is often largely overestimated, especially at the inlet. The overestimation of the temperature at the bundle outlet (see analysis of phase 1) is largely contributing to this effect. Whether there are or not other reasons has not been looked at in detail.

There is a general tendency to underestimate the deposited amounts in the upper plenum above the fuel bundle. Although a number of different factors may have played a role, it is suspected that deposition by vapour condensation on walls is underestimated. This point needs further investigations before being confirmed and work on the subject is in progress in Phebus-FP interpretation circles.

Deposition by thermophoresis in the steam generator is overestimated. The same models are generally used for the different codes and have been well validated previously. The reason for the discrepancy is still to be found.

The overall fractional retention in the circuit is generally well predicted, the under-prediction in one part of the circuit compensating the over-prediction in another one. For the MELCOR calculations and the submissions using SOPHAEROS as a transport module, a scatter in the results is observed. Whereas the mean calculated value for the overall retention fraction is not far from the measured one, the ratio between the minimum and the maximum calculated value is about 2.

The volatility of the different elements is not always well calculated. This is the case for caesium, several codes assuming a vapour form in the hot leg, whereas it was mostly condensed during the experiment. No re-volatilisation of caesium from the hot leg deposits is calculated. Concerning iodine, no code is predicting a gaseous fraction in the cold leg, as it is speculated on the basis of early gaseous iodine presence in the containment vessel.

More generally, the reasons for differences in calculated and measured deposited fractions in the circuit need further investigations. These are made in the frame of the Phebus-FP interpretation circles. Understanding the underlying phenomena is necessary before proposing any improvement of deposition models. On a safety perspective, the retention in the circuit for a large break sequence, as simulated in Phebus FPT1, is not so important. It could be in other sequences, for which retention is an important mitigating factor. Understanding of the reasons for the differences between measured and calculated values seems therefore necessary.

8.3. Containment

8.3.1. Introduction

The participation to this phase of the exercise was large, although reduced compared with those to phases 1 and 2.

A total of 11 (i.e. without phase 4) submissions were made using MELCOR. Concerning other integral or semi-integral calculations, 4 were performed with ASTEC, 1 with ATHLET CD/COCOSYS, 1 with MAAP and 1 with IMPACT/SAMPSON. This last one should be regarded more as a stand-alone submission, as it used measured sources to the containment and not calculated ones. There was also 1 semi-integral (circuit plus containment) using ECART, and 2 stand-alone calculations, 1 with CONTAIN and 1 with COCOSYS.

The participants generally used rather a coarse noding, as recommended in the specification report. They however often used more than one volume for the atmosphere, this for practical reasons such as differentiating the deposition on the various surfaces. There was an attempt by one participant to capture multi-dimensional effects by using a very large number of nodes with a lumped parameter code.

A full set of comparison plots is provided in Appendix 9.3.

8.3.2. Containment thermal hydraulics

The study of thermal-hydraulics in the containment was not a major objective of the Phebus-FPT1 experiment, nor is it for the ISP-46 exercise. The Phebus-FP containment model was designed in order to get relatively simple thermal-hydraulic conditions, with sufficiently well-known boundary conditions in order to focus on the study of fission product behaviour, involving both aerosol physics and chemistry. The parameters of the experiment were also defined following the same guidelines.

The present analysis therefore focussed on parameters that may have an impact on fission product behaviour in the containment, especially for aerosol physics. Detailed calculations of thermal-hydraulics using CFD codes have been made in the framework of the Phebus interpretation circles. However, despite the valuable information they provide for the understanding of detailed phenomena, they cannot be really validated against measurements, as local thermal hydraulic parameters are not measured in the Phebus containment. An attempt was made by one participant to get multi-dimensional results using a lumped parameter code with a very refined noding. He concluded that the prediction of mean values of thermal-hydraulic parameters was not better than when using the coarse noding recommended in the specification report. The comparison work was therefore restricted to the following parameters: average gas temperature, absolute pressure, steam condensation rate and average relative humidity.

The volumetric average gas temperature for base and best-estimate cases is plotted in Figure 150 and Figure 151. The calculated results approach well the measurement, with a scatter of about 2.5K, The calculations giving more different results should not be regarded as representative of code capabilities, but more of user effect. The result is satisfactory.

The absolute gas pressure is plotted in Figure 148 and Figure 149. Most of the results approach the measured values by ± 0.01 MPa during the periods of interest (aerosol injection and depletion phases. The result is satisfactory.

The condensation rate is also well calculated, as it can be seen in Figure 154 and Figure 155. Significant differences with the measurements are only seen for one calculation when the condensation rate is small, so with little impact on aerosol physics, as the diffusiophoresis deposition velocity is proportional to the condensation rate.

There is more scatter in the volumetric average humidity ratio, Figure 152 and Figure 153, the maximum calculated values ranging from about 75 to 95%. These values are not high enough to induce bulk condensation of steam nor important hygroscopic effects, given the fact that most elements present in aerosol particles are not soluble. The results are therefore judged satisfactory.

In general, the results of thermal-hydraulics calculations for the FPT1 experiment are close enough to the measurements. The small differences that can be observed are not expected to have a significant impact on aerosol physics. Some of them, especially at the end of the transient, are partly due to the fact that some participants did not take correctly into account the draw-off flows for sampling of the containment's atmosphere. However, the present conclusion cannot be extrapolated to all reactor situations. First of all, the Phebus containment model is simple, with a homogeneous well mixed atmosphere. Secondly, the relative humidity is moderate; should it have been higher, the observed differences between some calculations and the measurements might have had important consequences, such as reaching or not conditions for bulk steam condensation.

8.3.3. Containment aerosol physics

8.3.3.1. Airborne aerosol mass evolution

The most relevant parameter for aerosol physics in the containment is the airborne aerosol mass. It is given for base and best cases in Figure 160 and Figure 161. A large variation in calculation-results can be observed, with peak values ranging from less than 5 to 90g for the whole set of calculations. An early peak is present in some calculations, in disagreement with the experimental data. This is due to too high a burst release of cadmium at the time of control rod failure.

The best estimate calculations give much better results, as it can be seen in Figure 161. Indeed the differences between other calculation results and experimental data mainly result from an integral effect. We have seen in the analysis of phase 1 that many codes are underestimating or even not calculating the release of a number of structural elements, that are accounting for most of the mass released into the containment. Caesium, for instance, which has a high fission yield and is almost completely released represents only about 5% of the total mass in the containment.

The main aerosol depletion processes during the experiment were gravitational settling and diffusiophoresis on the wet condensers, with deposition on other surfaces representing only few % of the total deposition. At the end of aerosol injection, at about 17000s, and before the end of steam condensation, at about 20000s, the measured overall deposition velocity, including all phenomena, predominantly diffusiophoresis and settling, is fairly constant. This is the same after the containment isolation. This can be seen on the plots in logarithmic scale of airborne mass (in Figure 162 and Figure 163, dotted bold line). This allows an easy comparison of the overall aerosol depletion rate by looking at the slope of airborne mass on a logarithmic scale. For best estimate cases (Figure 163), the results are satisfactory. This is also the case for most of the base cases

(Figure 162), except for some MELCOR submissions which underestimate the depletion rate. This is not a general feature of MELCOR calculations. This disagreements seems to be correlated to an underestimation of the aerodynamic median mass diameter, as illustrated in Figure 156 at about 23000s.

8.3.3.2. Deposition processes

The evolution of the total mass deposited on the wet condensers and settled on the containment floor is given in Figure 164 and Figure 165, and Figure 170 and Figure 171 respectively. One can see that deposition on the wet condensers is decreasing at the end of the transient for the COCOSYS and some MELCOR calculations. This is due to the implementation in these codes of a model allowing drainage of deposited aerosols with the condensate flow. It is not clear from the output given by the participants where the material is drained, in the sump (as it should be), or on the containment floor (as it seems to be for some when looking at the curve of settled mass). The current official version of ASTEC V1 does not have a similar model; however, one was recently implemented in the V1 version by GRS. The results obtained are given in Appendix 10.3.

Most of the codes cannot simulate the washing of the hemispherical floor that took place at the end of the aerosol phase. Most of people who made integral calculations including the chemistry phase have overcome this difficulty by injecting all the settled material into the sump water since the beginning of the transient, obtaining the right concentration of fission products in sump water for chemistry calculations.

It is thus difficult to assess quantitatively the quality of results, as regards the partition of deposits between diffusiophoresis and gravitational settling. On a qualitative point of view, one may remark that this partition has some variability. This can be seen in the figures for best estimate cases. The two MELCOR calculations without draining tend to overestimate the ratio diffusiophoresis/settling, whereas the CONTAIN one gives satisfactory results. The same variability seems to exist for the other submissions. Models for diffusiophoresis and gravitational settling are well-established and have been validated extensively. Whether the observed variability is simply a user effect or is due to other reasons is difficult to find out. An example of possible error is what was reported by the ASTEC developers during the final workshop: they found two bugs in the coding of the diffusiophoresis model, made the necessary corrections and obtained good results afterwards.

The deposition on the dry part of the condensers, Figure 166 and Figure 167, is generally largely underestimated. This point is of low importance, as the amount deposited is small.

The deposition on the outer walls of the vessel is generally underestimated, Figure 168 and Figure 169, with the noticeable exception of the CONTAIN and some MELCOR calculations. Whether this results from a better quality of the calculations or not is not obvious, as previous studies, in the framework of interpretation, had shown that deposition on the walls in Phebus experiments could hardly be reproduced using standard models. However, this is not significant in a safety perspective, as the deposition on the outer walls is small.

8.3.3.3. Aerosol characteristics

Concerning aerosol characteristics such as aerodynamic median mass diameter (AMMD), Figure 156 and Figure 157, and geometric standard deviation (GSD), Figure 158 and Figure 159, the scatter is large, and the differences with the measured values often significant. For the diameter, about one half of the calculations give a reasonable value at the time of the measurement, and the other half exhibits an underestimation. As said before, there is some correlation between the

underestimation of aerodynamic median mass diameter and underestimation of depletion rate. Concerning geometric standard deviation, the larger scatter (if we except the beginning of the transient when the concentration is negligible) occurs during the period where concentration is maximum (15000 to 20000s). It then decreases with the concentration. During the period of maximum concentration, some extremely high values, approaching 3 are reached. Such a result does not look physical. It should be noticed that these two variables are not always standard outputs in the codes. They often have to be calculated "by hand", and this might generate errors.

Other aerosol characteristics, influencing their behaviour and being input parameters for the models, such as shape factor and density, were not measured in the Phebus experiments. Some participants provided information on the values used for these parameters. They were generally reasonable and defendable on a physical basis. However, at least in one case, an unrealistic value (12440 kg/m^3) was used for the aerosol density (to fit the total airborne mass, to compensate for the lack of structural release models). Attention should be paid in the definition of reasonable recommended values in the guidelines for code users.

8.3.4. Conclusions for the containment phase

The conclusions of the analysis of the containment phase are two-fold.

For thermal hydraulic aspects, the situation is satisfactory, with very few differences between calculation results and experimental data. In addition, these differences had probably only a weak influence on aerosol physics calculations. However, one should be cautious in making extrapolation to reactor scale, as thermal hydraulics of the Phebus containment model are rather simple, with a single rather well-mixed volume for the gas phase. Other ISPs provide a more challenging environment for assessing containment thermal hydraulic modelling, with conditions more relevant to reactor situations.

The situation is still satisfactory, but more contrasted, for aerosol physics.

- The evolution of the aerosol airborne mass largely depends on the quality of structural material release calculations, for integral submissions. A large number of calculations underestimate this release, and therefore do not allow a correct prediction of the airborne mass in the containment;
- However, the overall aerosol depletion rate evolution is generally well captured, despite an underestimation for certain calculations. These underestimations seem to be correlated with an underestimation of the aerosol aerodynamic median mass diameter. It is likely that this is more due to user effects than to code deficiencies;
- The above-mentioned last two conclusions should not be extrapolated without caution to reactor situations. It seems that, due to the limited height of the Phebus containment model, aerosol agglomeration processes played a less important role than expected for actual reactor containments;
- No clear conclusions have been drawn concerning the relative importance of the two main depletion processes in the experiment (diffusiophoresis and gravitational settling), because of the rather large variability in .calculation results. The reasons for this variability are probably multiple; in one case, bugs were found in the original submission. It is recommended that code developers look again at the validation work already done, paying special attention at experiments where both deposition mechanisms are important.

8.4. Chemistry

8.4.1. Introduction

There are fewer submissions for phase 4 of the exercise than for the other phases. The calculations can be divided in two groups:

- Stand-alone base cases calculations using INSPECT-96 (submission AE1 by AEA-T) and IMPAIR3 (submission EC3 by JRC). In addition to the base case, JRC submitted a best-estimate calculation EC3BE.
- Integral calculations using ASTEC V0.4 (submission GR3 by GRS), ASTEC V1 (submission IP1 by IRSN), ATHLET-CD/SOPHAEROS/COCOSYS (submission GR4 by GRS), IMPACT-SAMPSON (submission NP1 by NUPEC), MAAP EDF 4.04c (submission EF1 by EDF), MELCOR 1.8.5 (submissions NR1 by NRI and UM1 by UPM). In addition to the base case, UPM submitted a best-estimate calculation UM1BE. It should also be noticed that the NP1 submission is not really integral, as the release to the containment is not coming from the NP1 circuit calculations. For that reason, it should be more considered as a stand-alone calculation in the comparison.

One important feature for the integral calculations is that the circuit calculations do not calculate any gaseous iodine release from the circuit to the containment as inferred from experimental data. However, MAAP-EDF allows specifying a gaseous iodine fraction released to the containment and this possibility was used by EDF. IRSN did the same for an additional submission IP3 but this is not a standard option of the code at the time being.

Several codes had difficulties to simulate the washing phase of the containment floor at 250000s. From the results, it seems that those which could not make the simulation injected settled iodine-bearing particles into the sump from the beginning of the transient.

8.4.2. Overview of results

8.4.2.1. Gaseous iodine amount in the atmosphere

Calculations with a source of gaseous iodine from the circuit

The total amount of gaseous iodine (molecular + organic) in the atmosphere is displayed in Figure 172 for calculations AE1, EC3, EC3BE, EF1, NP1 and IP3. Note that EC3BE and IP3 are not base cases. For the base cases, as regards containment phenomena. EF1 and NP1 are very close to the experimental values during the quasi steady state before and after washing. AE1 overestimates the concentration by a factor of about 3. EC3 underestimates it by a factor of about 30, while EC3BE matches the experimental data nearly perfectly. In all these calculations, the washing phase is simulated and results in an increase of the gaseous iodine concentration.

The ratio between the amount of organic iodine and the overall gaseous amount is given in Figure 175. The experimental data are given only after the washing phase, as the measurements performed before were less reliable, the Maypacks suffering from a lack of selectivity. There is a large dispersion between the results. In EF1, organic iodine is largely predominant during the whole transient, while for AE1 its fraction is always small. EC3 calculations show a rather constant proportion of organic iodide (about 50%) during the two quasi steady-states periods. For NP1 and IP3, the proportion is always increasing during the same periods. It should be noticed that the

decrease of the proportion of organic iodine during the washing phase is due to a temporary production of I_2 by radiolysis in the sump. This effect cannot be seen in IP3, as the washing is not simulated in the calculation.

Calculations without a source of gaseous iodine from the circuit

The total amount of gaseous iodine (molecular + organic) in the atmosphere is displayed in Figure 173 for calculations NR1, UM1 and UM1BE, and in Figure 174 for GR3, GR4 and IP1. The two base cases using MELCOR, UM1 and NR1 give very high gaseous iodine concentrations, with differences with experimental values peaking at more than 2 orders of magnitude for NR1. In UM1BE, the fraction of silver allows to react with iodine was increased from 10^{-6} (default value) to 10^{-2}. This leads to more reasonable values. One should however be cautious about this result, as 0.43g of iodine (the injected mass was 0.53g) are neither as vapour in the atmosphere, nor dissolved in the sump, nor deposited on the walls, nor as AgI, CH_3I, HIO^-, IO_3^-, I_2O_2, I_2OH, I_3^-,OI^- in the aqueous phase. The amount of organic iodide is always negligible or zero in the three MELCOR calculations.

IP1 calculation with ASTEC V1 gives very low concentrations of gaseous iodine, about three orders of magnitudes lower than the experiment. This is simply explained by the absence of gaseous iodine injection from the circuit. Results of IP3 with gaseous iodine injection give values about two orders of magnitudes higher. GR3 calculation gives a very low molecular iodine concentration, but an organic iodine concentration very close to the measurement. For GR4, the molecular iodine gives values close to the measured one for total gaseous iodine, with much lower organic iodide. In both cases, gaseous iodine is produced by radiolytic processes in sump water, as not enough silver is released to the containment for those calculations. This is analysed in the next sub-section.

8.4.2.2. Iodine behaviour in the liquid phase

The chemistry in the liquid phase is dominated by the reaction of silver with iodine. The dominant species in the liquid phase is then silver iodide that has a very low solubility. Once the reaction is nearly complete, the sump water can no more act as a source for volatile iodine.

The evolution of silver iodide mass in the sump water is given in Figure 176. Note that UM1 results are not plotted because the calculated mass of AgI is zero. All the other calculations give rather high amount of AgI at the end of the transient, with the exception of GR3 and GR4. Concerning the kinetics of AgI formation, there are two groups of calculations: for AE1, EC3, EF1, NR1, the kinetics is very rapid. It is slower for IP1 (id. IP3), NP1 and GR3. The stepwise increase at 250000s can only be seen for those calculations which simulate the washing phase.

For calculations in which silver iodide is largely predominant, the concentration in other species is always very small. The calculated speciation depends on the degree of detail of the modelling. As an example, the calculated amount in moles of the various species calculated by various codes at the end of the transient is given in the following table.

	AgI	I_2	I^-	HOI	IO_3^-	Organic	Other species
AE1 INSPECT	$4.56\ 10^{-3}$	$6.79\ 10^{-9}$	$1.03\ 10^{-6}$	$2.86\ 10^{-6}$	$9.28\ 10^{-5}$	$7.09\ 10^{-9}$	$3.07\ 10^{-7}$
IP1 ASTEC	$3.73\ 10^{-3}$	$4.44\ 10^{-10}$	$5.82\ 10^{-4}$	$5.06\ 10^{-11}$	3.4010^{-8}	$6.65\ 10^{-11}$	
EC3 IMPAIR	$4.70\ 10^{-3}$	$1.45\ 10^{-11}$	2.5010^{-10}	$4.56\ 10^{-6}$	$9.18\ 10^{-7}$	$2.94\ 10^{-10}$	
NR1 MELCOR	$6.09\ 10^{-4}$	$7.24\ 10^{-5}$	$5.91\ 10^{-3}$	$4.14\ 10^{-8}$	$4.60\ 10^{-17}$	0	
NP1 IMPACT	$2.21\ 10^{-3}$	$2.02\ 10^{-11}$	$1.96\ 10^{-5}$	$7.45\ 10^{-11}$	$8.68\ 10^{-12}$		

8.4.3. Discussion

Calculations with a source of gaseous iodine from the circuit

In all the set of calculations, the reaction between silver and iodine in the sump is modelled, and there is always enough silver to efficiently trap iodine, except temporarily during the washing phase. The reactions with the surfaces are therefore the dominant mechanisms in determining the gaseous iodine concentrations. Not all the participants have indicated the adsorption/desorption rates they have used. The available information is given below.

	INSPECT AE1		IMPAIR3 EC3		IMPAIR3 EC3BE		ASTEC IP3		IMPACT NP1
Surface	$Vdep/m.s^{-1}$	$Kdes/s^{-1}$	$Vdep/m.s^{-1}$	$Kdes/s^{-1}$	$Vdep/m.s^{-1}$	$Kdes/s^{-1}$	$Vdep/m.s^{-1}$	$Kdes/s^{-1}$	Vdep
Paint in gas phase	$5\ 10^{-4}$	$5\ 10^{-5}$	$1.3\ 10^{-3}$	$6.6\ 10^{-8}$	$1.3\ 10^{-3}$	10^{-5}	10^{-4}	$4.5\ 10^{-6}$	Decreased value /standard
Steel in gas phase	$9.4\ 10^{-5}$	$6\ 10^{-4}$	$2.0\ 10^{-5}$	0	0	0	10^{-5}	10^{-6}	

In addition, the RI formation rate at the painted condensers was increased by a factor of 25 in EC3BE to account for the deposition of iodine-bearing aerosols, which could constitute an extra iodine source for RI formation.

Another way to make comparisons is to look at the calculated deposits on painted surfaces that have the largest impact on gaseous iodine concentration. They are plotted on Figure 177 and Figure 178 together with the experimental value at the end of the experiment. Note that this value includes all forms of iodine, adsorbed or deposited as aerosols.

The NP1 results largely exceed the experimental value. The differences between the maximum deposited value and the deposited values just before the washing and at the end of the transient are respectively 0.26 and 0.58 mg. This corresponds roughly to $4.5\ 10^{-6}$ moles. This rather large desorption is probably the main factor explaining both the calculated gaseous iodine concentration and the continuous increase of the proportion of organic iodine during the 2 quasi steady-state phases. Why the deposited value is so high remains unclear at the time being.

Among the other calculations, the highest deposited amount is found in EF1. The maximum is reached at 71600s and the difference between this value and the value at the end of the transient is 0.41 mg, i.e. 3.2 10^{-6} moles. This would explain the high calculated organic iodine concentration.

Concerning IMPAIR3, the effect of the modifications made for the best-estimate case are clearly visible. There are less deposits on the paints, and the desorption is more important.

The models in ASTEC/IODE and IMPAIR are rather similar for the phenomena concerned.

Calculations without a source of gaseous iodine from the circuit

Among the 9 integral MELCOR calculations, only 2 have provided results for the iodine chemistry in the containment. This is due to a number of reasons, for instance the difficulties to release and transport silver to the containment.

The results obtained in the IP1 submission can be easily explained by comparison with IP3. In fact the amount of silver transported to the containment is large enough in the calculation to trap rapidly the iodine and only a small amount of gaseous iodine is produced by radiolysis in the liquid phase. As there is no other source of gaseous iodine, the concentration in the gas phase is consistently small. This is not the case for GR3 submission, for which the amount of silver reaching the containment is only 0.18% of the inventory. This is not enough to trap iodine efficiently. Gaseous iodine is then produced by radiolysis and further converted to organic iodine. By coincidence, the amount of gaseous iodine produced compensates for the lack of gaseous iodine injected from the circuit. In GR4, the release of silver is not sufficient to trap efficiently iodine as silver iodide in the sump water. However, the production of gaseous iodine by radiolytic processes is again important.

Speciation in liquid phase

During most of the transient, the calculated concentration of I_2 in the sump is always very small compared to the concentration of AgI, except for UM1 case where it is only one decade lower. This low concentration and the rather limited mass make iodine chemistry in the sump largely unimportant in determining the gaseous iodine concentration. The sometimes-large differences in speciation between the different calculations are therefore not meaningful.

The low kinetics of AgI formation in certain calculations (Figure 176) can be due to several factors. If we compare for instance the IP1 calculation (slow kinetics) and the AE1 (fast kinetics), one can see that:

- For IP1, 7.17g of silver are injected, into the containment, compared to 0.63 g of iodine. If 10% are oxidised and react with iodine, there is only a small excess of reactive silver versus iodine. AE1 being a stand-alone calculation, it uses measured values, resulting in a large excess of oxidised silver;
- .Another important parameter is the specific surface of silver particles. In IP1, it is 100 m^2/kg, whereas in AE1 the input for the silver particles diameter leads to 645 m^2/kg.

These two simple comparisons show that, even when the modelling is derived from the same experimental data set, the choice of values for the input parameters may influence the results.

8.4.4. Conclusions for iodine chemistry in the containment

8.4.4.1. Modelling aspects

The dominant phenomena for iodine chemistry in the containment during the FPT1 test were:

- The fraction of iodine exiting the circuit as a gas;
- The rapid trapping of iodine by silver in the sump water, resulting in a low influence of liquid phase chemistry on the gaseous iodine concentration in the atmosphere;
- The interaction of iodine with painted surfaces, including adsorption, desorption and organic release;
- The destruction of iodine species in the atmosphere by radiolytic processes.

All of those influence deeply the gaseous iodine concentration in the containment's atmosphere, which is the most important safety-related parameter. When looking at Figure 173 and Figure 174, depicting the measured and calculated gaseous iodine concentration, one may conclude that several codes have a very good predicting capability. When looking at details, the reality is more contrasted.

The first phenomenon (iodine transport in the circuit) is discussed in the following sub-section, as it deals with integral aspects. Concerning the second one (Ag-I reactions), one may conclude that the implemented models are generally good enough in the case of the ISP-46. However, there are some differences in the kinetics of the reaction that may play a role in other accident sequences for which silver is not so much in excess as compared with iodine. Nevertheless, such uncertainties are overwhelmed by those related to the amount of silver reaching the containment and its propensity to react with iodine, as discussed in the next sub-section.

The last two phenomena determine the quasi steady-state level in gaseous iodine concentration measured in the experiment; before and after the washing phase. The analysis reported above show that, for codes giving good results, there are large discrepancies in the values of influential parameters that are used, mainly adsorption/desorption rates on/from painted surfaces. On the basis of Phebus experimental results, it is not possible to determine which set of parameters is the most relevant. Such a statement is consistent with the lessons learnt from ISP41 follow-up phase1; In the final report of this exercise, it was concluded: "*The largest source of the discrepancies between code predictions appears to be the different sub-models in each code for the formation and destruction of organic iodides. Although the current ISP exercise identified the organic iodide sub-models as contributing significantly to the discrepancy between the code predictions, parametric calculations cannot tell us which (if any) of the sub-models are correct, and what the range of user-defined input parameters for each of the sub-models could be."* It is expected that the final step of ISP 41, that will be a code comparison against four intermediate scale experiments, will provide code users with optimum values for the user-defined input parameters in their iodine behaviour codes.

8.4.4.2. Integral aspects

The calculations of iodine chemistry use the results of release, transport and aerosol behaviour in the containment. There is therefore a risk of propagation of errors when estimating the gaseous iodine concentration in the containment's atmosphere, that is a key factor for safety studies. We will examine successively the various factors having an influence on the final result.

Concerning iodine release from fuel, all calculations give good results for the overall amount. For the kinetics, there are some overestimations of release at the beginning of the transient, especially with models based on CORSOR. However, the kinetics in the containment being much smaller, this has a negligible influence on the final result.

A more important point is the release of silver from the control rod. The results here are very contrasted, ranging from rarely good to very poor. While some show quite good agreement with the data, most disagree regarding both the total amount and the time dependence. A few codes have good models, calculating the vapour pressure of silver and the associated release. However, there is a strong link with the degradation of the control rod, which needs to be accurately calculated. The corresponding models are generally accurate enough for core degradation purposes. Indeed, once the liquid Ag-In-Cd flows down from the cladding and the guide tube, it rapidly relocates to cold regions of the core to form partial metallic blockages. These blockages are quite well predicted by the degradation codes, and this is the important matter for the subject, and a very precise timing is not important. However, for release purposes, the time during which liquid Ag-In-Cd stays in the hot regions of the core and the temperature of the melt have a great importance. It would probably therefore be worthwhile to refine the degradation models of Ag-In-Cd control rods, to help improve the calculation of the structural materials aerosol release.

Concerning the transport of iodine and silver-bearing aerosols in the primary circuit, predictions seem to be accurate enough. Even if there are uncertainties in aerosol retention in the primary circuit, they are much smaller than those associated to chemical processes in the containment.

Much more important is the question of transport of gaseous iodine in the primary circuit. None of the codes is able to reproduce what was experimentally observed, even those having a detailed chemistry modelling. Indeed, those models are based on equilibrium thermochemistry, and it is suspected that non-equilibrium effects may have played a role. At the time being, this is just a speculation, and new experiments are needed to solve the issue, and provide kinetic data, if kinetic effects are confirmed to be important. As the impact of gaseous iodine injection into the containment from the primary circuit is very important, it would be worthwhile, in the absence of a validated model, to allow the users to specify the fraction of iodine transported as a gas. This would, at least, allow the possibility of performing sensitivity studies.

Thermal-hydraulics and aerosol physics in the containment are sufficiently well known, as far as their impact on iodine chemistry is concerned for the ISP-46 application. However, a number of Phebus-specific or generic features can hardly be reproduced by certain codes. This especially the case for the entrainment of deposited iodine-bearing aerosols by water, either due to steam condensation (generic feature), or when washing the bottom of the containment vessel (Phebus-specific).

Iodine chemistry calculations have to be fed with a number of other boundary conditions, such as mass transfer coefficients from the sump to the atmosphere, water pH evolution, fraction of oxidised silver (oxidised silver reacts efficiently with iodine), and dose rate. These points were not really addressed in the ISP-46 exercise, as the data were provided in the specification report. However, from the knowledge of the authors, it is not sure that all these parameters are sufficiently well predicted by integral calculations for making precise enough chemistry calculations.

8.5. Overall integral aspects

This section considers integral aspects from the point of view of the two 'key signatures' of severe accident analysis as defined in the MELCOR peer review[19], namely the bundle final state (relevant to in-vessel retention) and the potential source term to the environment in case of containment failure. As the thermal hydraulics in the experiment are relatively simple, not including the two-phase conditions that would be found in the core and primary curcuit following the initiating event, and in the initial stages of heatup, it follow that no conclusions can be drawn regarding the propagation of uncertainties in thermal hydraulic modelling into the rest of a plant calculation.

8.5.1. Bundle state

The nodalisation scheme proposed for the bundle phase of the ISP, designed to be representative of plant studies, appeared to be adequate for assessment of the models for core degradation (although it may not be so for interpretation of the experiments). There were no strong differences between the base and the best-estimate cases, model quality and parameter choice had the stronger influence on the calculated outcome. Good agreement for the final state could be obtained with suitable adjustment of bulk fuel relocation temperature, but this is unlikely to be representative for similar tests, for example for Phebus FPT0 and FPT2, and for PBF SFD1.4, so plant studies need sensitivity calculations to this parameter with the modelling in its current state. No study has yet been performed on the progression to the core final state (fewer data are available; also there was lack of time). Results need to be compared with those of other experiments to give conclusions of general validity, and further efforts in this area are encouraged.

Furthermore, in the time available, it was not possible to examine in detail differences in parameter choice (e.g., control rod failure temperature, oxide shell breach criterion, Zircaloy oxidation correlation), to make specific recommendations on such choices, or to explore fully the consistency with previous ISPs. It would be beneficial to perform such work, and the Appendices provide the data required for such an analysis.

8.5.2. Source term

The nodalisation scheme proposed for the ISP, designed to be representative of plant studies, appeared adequate for assessment of the models relevant to the source term calculation (although it may not be so for interpretation of experiments, e.g. for the rising line and steam generator hot leg, where there are large temperature gradients). There are no strong differences between base and best-estimate cases; model quality and parameter choice had the stronger influence. Release from the bundle is not generally sensitive to the choice of nodalisation. Simple nodalisation for the containment appeared adequate, but the thermal hydraulics in ISP-46 are relatively simple so this result cannot be extrapolated to plant studies (similar remarks apply to the thermal hydraulics in the bundle and circuit, where uncertainties relating to two-phase flow modelling, typical of the early stages of plant transients, are not addressed as being out of scope of the Phebus FP series).

Accuracy of containment calculations in integral treatments is sensitive, often highly, to results of previous stages (propagation of uncertainties):

- calculation of fission product release from the bundle, and of the structural materials Ag, In, Cd and Sn, affects transport in all the subsequent stages, note that the kinetics of release are as important as the total amount;

- temperatures at the entrance to the circuit, which strongly influence the deposition;
- for those codes which calculate the chemistry, the speciation is influenced by the calculated release;
- release of structural materials is often under-calculated or not calculated; this results in under-calculation of total mass of aerosols, but there is weak impact on overall retention in the RCS and depletion in the containment;
- iodine speciation and physical form in the circuit is poorly predicted; no code reproduced the observed gaseous iodine fraction in the RCS.

Given these limitations, it is hard for an integral calculation to predict well the containment chemistry, however detailed the modelling of its phenomena; uncertainty on iodine release from fuel, aerosol transport in RCS and behaviour in containment is overwhelmed by uncertainties in chemistry. This has implications on the conduct of plant assessments, for example it may be the best strategy to use the chemistry codes in stand-alone mode to determine bounding cases and sensitivities, rather than as part of an integral calculation.

8.5.3. Other remarks

On general integral aspects, attention should be paid in determining the priorities for code improvement on finding the weakest link(s) in the chain of calculations which contribute most to uncertainty in the assessment of risk ("cost-benefit" approach; is it a model itself or the input to it?).

8.6. Computing aspects

8.6.1. Computer usage and timings

Participants were asked to provide details of the computer systems that they used for their work, and also to perform a standard benchmark ('Linpack') so that the computational efficiency could be measured. The results of this exercise are given in Appendix 5.

The computer details listed in A5.1 show that a range of systems were used, both Unix and PC-based. The timings of the benchmark range from 1 to 116s (about 75% response from participants). Total timings were mainly consistent with the length of transient analysed, with the best-estimate cases taking ~1.5 to ~6 times longer than the base cases, reflecting the more detailed modelling. Bundle phase absolute timings, Figure 179, varied from 10^3 to 10^6s; the groupings are clarified if results normalised by the Linpack time, but many data are not available. Detailed points are:

- IMPACT/SAMPSON takes the longest time (as in ISP-45);
- MAAP4 was almost the fastest in absolute terms for an integral calculation, but the Linpack timing was not provided so the efficiency could not be determined;
- MELCOR timings were intermediate, with a spread in efficiency range of about 5:1 (perhaps surprisingly large, the fastest MELCOR calculation reflects its coarse noding);
- there was no obvious difference between MELCOR (engineering-level) and SCDAPSIM (detailed-level) codes, this may reflect recent efforts in improving the numerical scheme in the latter code, for example smoothing out mismatches in value and slope of heat transfer correlations across flow regime boundaries;

- codes slow down in the oxidation excursion phase, as expected;
- the Linpack benchmark did not give as great a degree of normalisation as expected.

It appears unlikely that computing time would be a limiting factor in the analyses, with the possible exception of IMPACT/SAMPSON.

Bundle phase timesteps, Figure 180, show a wide range even in the same part of the transient (ICARE 100s, SCDAPSIM 0.05s, for the plateau 3000-7000s), but with a tendency to shorten the timestep in the excursion phase, consistent with the overall CPU timing (note: the plotting frequency may obscure oscillations here). Similar trends seen in the circuit and containment data, with ASTEC taking the longest timesteps and MELCOR the shortest (SCDAPSIM does not calculate this phase). Some codes (some ASTEC versions, ICARE) did not give CPU timings - such information can be useful, along with the timestep, to indicate where the calculation could be having numerical problems indicating a need for input deck or code changes.

The MELCOR code gives information on split of times amongst its modules. In submission PS1, Figure 181, the degradation package COR is the largest contributor (but the thermal hydraulic timing CVH, almost the same as radionuclide package RN2, may be slow compared with a plant transient, as the thermal hydraulics in the Phebus bundle are relatively simple). However in contribution CS1, Figure 182, there is greater time spent in RN transport modelling.

Little evidence of timestep convergence studies, which are normally considered essential in this type of analysis, was found in the participants' technical reports. However, this may have been assumed in some instances. Plotting the CPU usage and timestep variation can give useful information on convergence behaviour and can aid efficient use of the code, so having this information available for plotting is useful (but is not available for all codes).

8.6.2. Platform dependencies

Participants were also asked about computer/compiler effects and portability issues. Little information was reported here as most participants used only one computer. MELCOR participant PS1 reported differences between Unix and PC results and also compiler options in the degradation part, leading to different relocation sequences, this is consistent with other users' experience in other cases. ASTEC management reported platform differences for version V0 resulting from the ESCADRE degradation package, but this is eliminated in V1 where the DIVA package is used (similar to ICARE) . ICARE was believed to show virtually no platform dependence. In addition, the SCDAPSIM developers have reported that their code shows no platform dependence either.

The presence of platform dependence has implications on code assessment, and use for plant studies. The presence of these effects confounds genuine sensitivities arising from parameter variations, and should therefore be mitigated as far as possible, preferably eliminated entirely. It is not normally clear which, if any, of the results from the same case run on different machines produced the 'right' results. Further discussion is beyond the scope of the present report, but it is noted that the issue has been addressed for thermal hydraulic codes [20]. It would be beneficial if this study was extended to the severe accident area.

8.6.3. Conclusions

- CPU time and timestep information should be available for plotting, to help optimise code use;

- Platform dependence should be eliminated as far as possible, but in the meantime, developers should provide detailed guidance on coping with the effect (e.g. performing all runs in a given application with the same load module on the same kind of machine);
- The earlier CSNI review on computer/compiler dependencies for thermal hydraulic codes could be usefully extended to the severe accident area;
- The Linpack benchmark did not give perfect normalisation amongst platforms, and so may need updating;
- Although not strictly speaking a conclusion only from this ISP, it is worth reminding that temporal and spatial convergence studies should always be performed for major code applications.

8.7.Code assessment aspects

8.7.1. Discussion

In general, detailed comparison of calculated results with experimental data requires provision of a graphics dump file so that the analysis can be carried out off line, and that new variables can be plotted without re-doing the whole calculation. On-line visualisation on its own appears insufficient. Comprehensive graph plotting facilities are needed to aid such analysis, these are nowadays almost universally available.

The variables requested for comparison are intended to quantify key phenomena in accident sequence modelling, e.g. as identified in the CSNI Code Validation Matrix for core degradation[21 22]. It follows that these outputs should be available as standard options, but this was not always the case, giving extra work for users and scope for error. In some cases also, different timebases were used for different variables in the code, requiring conversion programs so all could be plotted together. Again, this difference is something that should be avoided. In other cases, it was noted that there were inconsistencies in variables available as plot and control variables, with some being available in one case and not in another, and/or different formats for the input specification being defined for these quantities. This presents another opportunity for tidying of the code specification.

In other cases, consistency checks (plotting together variables that are physically linked, such as hydrogen rate vs. oxidation heat, gas temperature change up the bundle vs. convective heat loss) showed unexpected discrepancies, similar remarks apply to checking of rate of change stored heat against bundle heatup rate.

It was also noted that mass was not always conserved globally, so that structural material release as aerosol to the circuit was not subtracted from the bundle inventory (by contrast, fission product decay heat is usually tracked).

Regarding the output relevant for code assessment:

- bundle temporal variables are normally readily available (temperatures, pressure, hydrogen production, fission product release, etc.);
- bundle energy balance, not all quantities are always available;
- bundle spatial variables, often some items are missing such as U and Zr reacted, especially if relocated; additional output should be provided for the parameters requested in the ISP ;

- circuit temporal and spatial variables are normally available;
- containment thermal-hydraulics variables are normally available;
- aerosol physics temporal variables: there is need for some attention to the definition of diameters (AMMD, geometric mean/median diameters, etc.).

As checking the mass and energy balance should be a feature of major applications, it follows that the relevant quantities should be readily available for plotting. Similarly, all output quantities needed for code assessment (the present list makes a good starting point), should be available as otherwise much extra work is needed to make a good validation. This seems essential if the good practice of running each new code version for a standard set of cases is followed, for example the 'non-regression' testing performed by the ICARE/CATHARE team. Including experimental quantities as control variables in the input decks for experiments can aid this kind of work, but it is realised that this cannot be done for everything as the input decks could become unreasonably large.

8.7.2. Conclusions

- Provisions should be made for direct output in a graphics dump file of the output physical quantities requested for the ISP as mentioned above, if not already available – in the meantime developers should provide users with detailed guidelines on how to extract the required data from what exists now (to avoid post-processing errors and possible misinterpretation);
- Temporal variables should all be referred to the same timebase;
- Where control function and plot variables are used, these should be consistent both in range and in syntax;
- Provision should be considered for including some experimental data as plot variables in the input decks used for assessment of the code against major experiments, as this can save on subsequent post-processing.

9. Implications for plant studies

The major objective of the ISP-46 exercise is to assess the capability of codes to model in an integrated way the physical processes taking place during a severe accident. To determine whether this objective had been reached, it is necessary to discuss adequacy of codes and models, and the role of users' experience. 'Plant studies' is a generic term, and, when making a judgement on the quality of a plant study, one has to keep in mind its purpose. For example:

- a vendor may have to demonstrate that the engineering features chosen satisfy the demands of the customer;
- a utility may need to demonstrate that its plant meets the regulatory requirements;
- a technical support organisation may want to explore domains not covered by the licensees;
- a regulatory body may ask for a proof of the quality of calculation tools and results.

Although the physical basis is the same for the different studies, the implications depend on the purpose of the study, so that the required degree of conservatism may vary.

Regarding adequacy of models and codes, the ISP has identified a number of necessary improvements in codes and models, of which the most important are:

- better estimation of structural material release, especially for control rod elements, and of semi- and low-volatile release;
- possibility to take into account the presence of gaseous iodine in the reactor coolant system (RCS);
- definition of optimum parameters for iodine chemistry codes.

As not all necessary improvements can be achieved in a short term, users have to be well aware of the validation status of codes and must take into account their limitations when performing plant studies.

Regarding users' experience, ideally, calculations for an ISP should be done with the same degree of quality as calculations for a safety file. Unfortunately, limited resources available for participation in an ISP can introduce some "distortion". Sometimes, work is done by an inexperienced user, without adequate support from experienced staff, and, often, checking procedures are not as tight as for power plant studies. Nevertheless, it must be acknowledged that all ISP-46 participants did their best.

Some 'user effect' is visible in ISP-46, as it was in previous ones. The fact that the data in the numerical files were sometimes not consistent with the technical report figures suggests that detailed checking was not always carried out. Whether or not the observed user effect can be transposed to power plant studies is difficult to answer, because:

- the degree of experience of users is generally unknown, and can just be inferred from the quality of obtained results, by comparison with those obtained by users with recognised experience;
- the amount of effort devoted to the ISP, especially for checking and peer review, is also generally unknown.

The user effect in plant studies cannot be ruled out, and a major objective is to limit its consequences on the quality of the study. This could be achieved by:

- checking that previous training has been efficient;
- using adequate procedures for controlling the results and peer reviewing, involving experienced specialists in the field;
- checking that enough support is provided by code developers when necessary.

To summarise, severe accident codes are difficult to handle, and their validation is not complete. Consequently:

- they must not be used as "black boxes", i.e. their results have to be interpreted, according to the goal of the study for which they are used;
- extensive training of new users should be mandatory;
- efficient and effective quality assurance procedures must be used for reactor studies.

In conclusion, users should not automatically trust the results of their calculations. A critical analysis should always be undertaken, to see if the results seem consistent and reasonable. This may be termed a ‘reality check’.

10. Feedback from code developers

10.1. Introduction

Each code developer of integral codes, used by more than one organisation in the ISP, was asked to summarise at the final workshop their findings from the exercise. These are compiled in Appendix 8 with contributions for ASTEC, ATHLET-CD, ICARE/CATHARE, MELCOR and SCDAPSIM. The main outcomes are summarised in the following. People interested in more details are invited to go to the appendix.

10.2. Fuel degradation

There is a consensus that results are satisfactory for the thermal response of the fuel bundle and the fuel relocation provided that:

- there is a small adjustment of bundle power or shroud thermal conductivity;
- the onset of fuel relocation takes place well below 2800K.

The implications of the low fuel relocation temperature for plant studies and the needed code improvements are not the same for all developers. From their analysis of FPT1 and PBF SFD-1.4, SCDAPSIM developers consider a different behaviour for low and high pressure sequences. They intend to keep the code as it is for high pressure, and to introduce modifications for low pressure. MELCOR developers intend to change the default treatment for melt relocation based on FPT1 and other Phebus tests. ATHLET-CD developers point out the fact that they use the same model parameters for plant applications than for Phebus and QUENCH post-test calculations. They are in a process of improving the melt relocation crust re-melt models. ASTEC and ICARE/CATHARE developers recommend to use the same default options for reactor applications. They are working on code improvement, validating and numerically optimising a model based on the use of the U-Zr-O phase diagram.

There is a consensus that hydrogen production is fairly well reproduced. However, ATHLET-CD developers are working on the use of Cathcart/Prater/Courtright oxidation model instead of the commonly used Urbanic/Heidrick one.

Recommendations were made by ATHLET-CD and ICARE/CATHARE developers about the nodalisation of the fuel bundle. They go in the direction of a recommended finer axial meshing than quoted in the specification report for the base case.

10.3. Fission product release

ASTEC and ATHLET-CD developers conclude that the release of volatile species is well described by their codes. MELCOR developers point out the fact that CORSOR captures well the release fraction but overestimates the initial release rate. They plan to improve that by using the ORNL-Booth diffusion coefficients.

Improvements are planned in ASTEC (ELSA) and MELCOR for a better prediction of the release of certain semi-volatile elements. Improvements are also in hand in ASTEC (ELSA) for structural material release. They also plan to incorporate or improve models for the release of structural material. A review of the release kinetics of medium-volatile species under various oxidation conditions is planned by ATHLET-CD developers. They will also improve the model for absorber rod material release, considering the saturation pressure of species and a correct link to the relocation model.

10.4. Transport in the circuit

ASTEC developers think that results are globally satisfactory. However, they point out the questions of the underestimation of deposits in the upper plenum, and of the overestimation in the steam generator. They also mentioned the influence of too high a calculated temperature at the bundle exit and the influence of the calculated source on the transport, taking molybdenum as an example.

MELCOR developers conclude that overall deposition of fission products in the circuit is reasonably correct. They attribute the too low deposition in the upper plenum to re-vaporisation of deposits in this region. They intend to use the caesium molybdate vapour pressure in the future to overcome the difficulty. In general, they think that models appear adequate for predicting consequences in full plant analysis.

ATHLET-CD is coupled with SOPHAEROS for the fission product and aerosol transport calculations. The ATHLET-CD developers think that the calculated aerosol deposition is in fair agreement with the experimental data. They expect however a better simulation of fission product transport with the implementation of the current SOPHAEROS version used in ASTEC and the improvement of the absorber material release.

10.5. Thermal-hydraulic and aerosol behaviour in the containment

ASTEC developers think that results are globally satisfactory. They observe a good agreement for steam condensation, pressure and relative humidity evolutions, as well as for the overall decrease of the airborne concentration. They indicate that the difficulties in predicting the partition of deposits between diffusiophoresis and gravitational settling, in the original submissions, was due to two bugs in coding of diffusiophoresis velocity. Corrections were made and led to an excellent agreement. They will introduce a model for fission product mass transfer to the sump by washing (see Appendix 10.3 for more details). They propose to improve the coupling between the transport module (SOPHAEROS) and the containment one (CPA) in making SOPHAEROS automatically calculate the containment zone connected to the break to get the right nucleation of species injected as vapours at the break.

MELCOR developers consider that many analyses using their code performed reasonably well, for instance for depletion rate, but that the partition of settling vs. diffusiophoresis may need some improvement.

10.6. Iodine chemistry in the containment

The ASTEC developers think that the results are globally unsatisfactory. Integral calculations (no stand-alone calculation was performed) suffer from the lack of gaseous iodine injection at the break, the calculated concentrations of organic and inorganic iodine in the gas phase are too low. They observe that the calculations are however self-consistent: the trapping of iodine by silver is well reproduced leading to low concentration in the gas phase in the absence of injection from the circuit. They will propose a user-defined source (% of iodine source under gaseous form), waiting for better knowledge of this phenomenon. They will also introduce a calculation of dose rate in the gas phase, that is presently neglected in the code.

The MELCOR developers consider that almost all analyses suffer from the low silver release, owing to the lack of a model in the code. They indicate that iodine modelling requires the implementation of such a model and improvements to the treatment of organic species.

10.7. General considerations

The ASTEC developers observe that the users did not solicit the development team very much. This could be an indication of the quality of the code documentation; however IRSN and GRS are aware of some necessary improvements. They observed that they have neglected or forgotten to transfer some improvements performed in individual modules to the coupled version of the code; They made the same observation for some updated recommended "default values" issued from the qualification of individual modules. They insist on the importance of the cumulative error effect on source term evaluation when performing integral calculations.

The ATHLET-CD developers indicate that the same code limitations as observed in the ISP-46 are valid for the reactor calculations. They insist on the strong need for education and training of code users. They think that the knowledge embedded in the codes cannot replace the proper education of engineers to make useful calculations and correct interpretation of the results. They add that to get familiar with a code by trial and error takes more time than well-organised training. They propose candidates for possible follow-up exercises and recommend that a special attention is given to experiments typical of BWRs.

The ICARE/CATHARE developers have found only few differences between their four participants' input decks. They observed consistent results amongst all the code users. They think that the fairly good agreement for the best-estimate cases show that the use of default options and the proper choice of a few selected user parameters is enough to obtain good results. They indicate that most conclusions about abilities and deficiencies of the code after the ISP-46 exercise are confirmed by the analysis of a large number of other integral tests. They think that, for reactor applications, a few models rely on user parameters which may be different from the FPT1 case.

The MELCOR developers indicate at first that a reasonable prediction of the bundle thermal response is essential before any other insights from the experiment can be determined. They think that the ISP-46 exercise was extremely valuable in assessing and advancing the code models.

Indeed, the evaluation of ISP participants' results will be ongoing, with the aim of code improvement. The models of the next MELCOR version, 1.8.6, for core degradation, fission product release and containment behaviour will be modified based on ISP-46 and Phebus results.

They SCDAPSIM developers were strongly involved in the ISP-46 exercise; they provided a reference input deck and gave technical advice to the participants. They reviewed the input and the results. They analysed the user effects and the experimental and modelling uncertainties. They identified the problem areas (training, model use, code deficiencies). They compared the analyses of PBF SFD 1-4 and Phebus FPT1. They re-evaluated the reduced system pressure transients with temperature near 2500K to determine the impact of early collapse of fuel and formation of molten pool below 2800 K. They are proceeding to interim temporary changes for low pressure for low pressure scenarios in the code. In the future a fuel failure model at low pressure will be added.

10.8. Concluding remarks

The code development teams have taken a positive attitude towards the outcome of the ISP, and are taking steps to plan, develop and implement new and revised models to remedy problem areas identified in the exercise. Similar remarks apply to the major code MAAP4, which was used in an in-house modified form by EDF, and to the new NUPEC code IMPACT/SAMPSON. There is general agreement on the areas that need improving, while the details of the modelling envisaged naturally vary from one development team to another. As illustrated in Appendix 10, some of the improvements have already been carried out. It would be interesting to compare the results before and after these improvements have been made, in the framework of an assessment programme that takes into account the results of other integral tests under different conditions.

11. Conclusions

This ISP has given rise to a substantial number of detailed conclusions and recommendations for each of the four phases, and on integral, code assessment. computing and plant calculations aspects. These are given at the end of the individual sections. A summary of the most important points is given below.

Phase1: Bundle

- Modelling of the fuel temperatures and hydrogen production is adequate;
- The outlet gas temperature is generally calculated too high, with an impact on circuit transport calculations;
- The core final state is well calculated in the best calculations;
- The integrated fission product release for volatile species is well calculated, but usually with too high a rate at low temperatures (later models show better agreement);
- There is a wide scatter in the release for semi-volatiles and low-volatiles, indicating the need for model improvement;
- The calculation of structural material release (tin from the cladding, absorber materials from the control rod) is inadequate and substantial model development is necessary.

Phase 2: Circuit deposition and transport

- The fluid temperature in the vertical line is often largely overestimated, especially at the inlet - overestimation of the temperature at the bundle outlet largely contributes to this effect;
- There is a general tendency to underestimate the deposited amounts in the upper plenum above the fuel bundle - it is suspected that deposition by vapour condensation on walls is underestimated;
- Deposition by thermophoresis in the steam generator is overestimated although the same models are generally used for the different codes and have been well validated previously - the reason for the discrepancy is still to be found;
- The overall fractional retention in the circuit is generally well predicted, the under-prediction in one part of the circuit compensating the over-prediction in another one;
- The volatility of the different elements is not always well calculated,for example for caesium and for iodine (no code is predicts a gaseous fraction in the cold leg, as it is speculated on the basis of early gaseous iodine presence in the containment vessel).

Phase 3: Containment thermal hydraulics and aerosol physics

- For thermal hydraulic aspects, the situation is satisfactory, however one should be cautious in making extrapolation to reactor scale, as thermal hydraulics of the containment here are simple compared with reactor situations;
- A large number of integral calculations underestimate the structural material release, and therefore do not allow a correct prediction of the airborne mass in the containment;
- The overall aerosol depletion rate evolution is generally well captured, underestimations in some cases seem to be correlated with an underestimation of the aerosol aerodynamic median mass diameter (likely that this is more due to user effects than to code deficiencies);
- These last two conclusions should not be extrapolated without caution to reactor situations, as it seems that, due to the limited height of the containment, aerosol agglomeration processes played a less important role than expected for actual reactor containments;
- No clear conclusions could be drawn on the relative importance of the two main depletion processes in the experiment (diffusiophoresis and gravitational settling), because of the rather large variability in calculation results.

Phase 4: Containment chemistry

- The implemented models for Ag-I reactions are good enough for FPT1, but this cannot be necessarily extended to cases where the Ag is not so much in excess with respect to I;
- It is recommended that a facility be introduced to input into codes the fraction of gaseous iodine released into the containment, as no reliable model currently exists;
- Even doing so, there are still some difficulties in predicting the gaseous iodine concentration within one order of magnitude;
- There is considerable uncertainty regarding the modelling of organic iodine reactions, and there is no consensus on optimum values for the user-defined input parameters such as adsorption velocity and desorption rate on/from painted surfaces;
- Progress is expected from the analysis of more simple experiments, as is done in the ISP-41 follow-up exercises;

- Overall, the results are very contrasted, ranging from unreliable to very good (but with some tuning).

Integral aspects

- Accuracy of containment calculations in integral treatments is sensitive, often highly, to results of previous stages (propagation of uncertainties):
  - calculation of fission product release from the bundle, and of the structural materials Ag, In, Cd and Sn, affects transport in all the subsequent stages, the kinetics of release are as important as the total amount;
  - temperatures at the entrance to the circuit, which strongly influence the deposition;
  - for those codes which calculate the chemistry, the speciation is influenced by the calculated release;
  - release of structural materials is often under-calculated or not calculated; this results in under-calculation of total mass of aerosols, but there is weak impact on overall retention in the RCS and depletion in the containment;
  - iodine speciation and physical form in the circuit is poorly predicted; no code reproduced the observed gaseous iodine fraction in the RCS.
- Given these limitations, it is hard for an integral calculation to predict well the containment chemistry, however detailed the modelling of its phenomena; uncertainty on iodine release from fuel, aerosol transport in RCS and behaviour in containment is overwhelmed by uncertainties in chemistry.
- This has implications on the conduct of plant assessments, for example it may be the best strategy to use the chemistry codes in stand-alone mode to determine bounding cases and sensitivities, rather than as part of an integral calculation.

Computing aspects

- Platform dependence should be eliminated as far as possible, but in the meantime, developers should provide detailed guidance on coping with the effect (e.g. performing all runs in a given application with the same load module on the same kind of machine);
- The earlier CSNI review on computer/compiler dependencies for thermal hydraulic codes could be usefully extended to the severe accident area;
- Although not strictly speaking a conclusion only from this ISP, it is worth reminding that temporal and spatial convergence studies should always be performed for major code applications.

Code assessment aspects

- Provision should be made for direct output in a graphics dump file of the output physical quantities requested for this ISP, as these are the most relevant to assessing the modelling of the key physical phenomena – in the meantime developers should provide users with detailed guidelines on how to extract the required data from what exists now.

Implications for plant studies

- As not all the necessary model improvements identified above can be achieved in a short term, users have to be well aware of the validation status of codes and must take into account their limitations when performing plant studies.
- Some 'user effect' is visible in ISP-46, as it was in previous ones, and the analysis suggests that detailed checking was not always carried out - whether or not the observed user effect can be transposed to power plant studies is difficult to answer, because:
  - the degree of experience of users is generally unknown, and can just be inferred from the quality of obtained results, by comparison with those obtained by users with recognised experience;
  - the amount of effort devoted to the ISP, especially for checking and peer review, is also generally unknown.
- The user effect in plant studies cannot be ruled out, and a major objective is to limit its consequences on the quality of the study. This could be achieved by:
  - checking that previous training has been efficient;
  - using adequate procedures for controlling the results and peer reviewing, involving experienced specialists in the field;
  - checking that enough support is provided by code developers when necessary.
- To summarise, severe accident codes are difficult to handle, and their validation is not complete. Consequently:
  - they must not be used as "black boxes", i.e. their results have to be interpreted, according to the goal of the study for which they are used;
  - extensive training of new users should be mandatory;
  - efficient and effective quality assurance procedures must be used for reactor studies.
- In conclusion, users should not automatically trust the results of their calculations. A critical analysis should always be undertaken, to see if the results seem consistent and reasonable. This may be termed a 'reality check'.

12. Acknowledgements

The exercise was carried out under the auspices of the OECD/CSNI GAMA working group, and the authors gratefully acknowledge the tireless efforts of its Secretary, J Royen, in assistance with managing the ISP, organisation of the meetings, accurate minuting of the discussions, and for his contribution to the Preface of this report. The authors would also like to thank the European Commission, a major sponsor of the Phebus FP programme, for the help provided in the organisation of this ISP under the EC Nuclear Fission Safety 5th Framework Thematic Network 'THENPHEBISP', contract number FIKS-CT-2001-20151, including financial support of the coordinators and many European partners. Special thanks go to the Commission officer A Zurita. The hospitality of EC-JRC Petten in hosting the second and the fourth Workshops is gratefully recognised.

The technical contributions from the following persons are gratefully acknowledged.

Summaries of the codes used: ASTEC, by J-P van Dorsselaere (IRSN Cadarache, France); ATHLET-CD, by K Trambauer and W Erdmann (GRS Garching and GRS Cologne, Germany); COCOSYS, by W Klein-Heßling (GRS Cologne); CONTAIN, see below; ECART, by S Paci (University of Pisa, Italy); FEAST, by J Barrett (HMS Sultan, UK); ICARE/CATHARE, by F Fichot (IRSN Cadarache, France); IMPACT/SAMPSON, by T Ikeda (NUPEC, Japan); IMPAIR, by E Krausmann (EC-JRC Petten, the Netherlands); INSPECT, by S Dickinson (AEA Technology, Winfrith, UK); MAAP4, by S Marguet (EDF Clamart, France); MELCOR, see below; SCDAP/RELAP5, by W Sengpiel (FZ Karlsruhe, Germany), and see below; SCDAPSIM, by C Allison and J K Hohorst (ISS Idaho Falls, USA); SOPHAEROS, by M Kissane (IRSN Cadarache, France).

Material for the USNRC-sponsored codes CONTAIN, MELCOR and SCDAP/RELAP5 was adapted from the NUREG reports as referenced in Appendix 6.

Feedback from code developers ; ASTEC, by W Plumecocq, J-P van Dorsselaere and P Giordano (IRSN Cadarache, France); ATHLET-CD, by K Trambauer (GRS Garching, Germany); ICARE/CATHARE, by F Fichot and G Repetto (IRSN Cadarache, France); MELCOR, by D Powers and R Gauntt (Sandia NL, USA); SCDAPSIM, by C Allison and J K Hohorst (ISS Idaho Falls, USA).

The contribution of sub-contractors G Carpi and A Commandé from CS-SI allowed us to keep the analysis work on schedule by providing semi-automatic procedures for plotting calculation results for a large number of cases. We are also grateful to K Fischer of Battelle Ingenieurtechnik GmbH (now Becker Technologies) for kindly supplying the Linpack computing benchmark.

The coordinators warmly thank all the participants for their diligence, enthusiasm and helpful feedback throughout the course of the ISP. W Hering of FZ Karlsruhe provided valuable advice based on his experience in co-ordinating ISP-45. The assistance of P Giordano and M Kissane (IRSN Cadarache) for their reviews of the documentation and helpful comments is much appreciated. Finally, one of us (TJH) gratefully acknowledges the hospitality of IRSN/DRS Cadarache in the course of this work.

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