Progress of ASTEC validation on fission product release and transport in circuits and containment

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Summary

This paper presents an overview of the activities carried out in the framework of the SARNET project by the CIEMAT, INR, JRC/IE, GRS, UJV and VUJE partners involved in the validation of ASTEC on fission product (FP) release and transport experiments simulating severe accident conditions in the reactor circuit and containment.

These activities were mainly devoted to the analysis of the Phébus experiments, FPT0, FPT1 and FPT2, which provided fundamental reference data for the severe accident research. The ELSA, SOPHAEROS, CPA and IODE modules were used respectively for FP release from the bundle, transport in the circuit, containment thermalhydraulics and aerosol behaviour, and finally iodine behaviour in containment. Studies on aerosol behaviour in the STORM experiments and iodine behaviour in the ThAI experiments are also summarized.

In addition, integral ASTEC calculations were performed on the FPT1 and FPT2 Phébus experiments, using all FP modules in a coupled mode.

Together with overview of the progress in the validation of main ASTEC modules, this paper also points out what are the needs for improvement of modelling in the future ASTEC V2 code versions.

A. INTRODUCTION

Since the beginning of the SARNET project in 2004 **[1],** an important activity of validation and assessment of the ASTEC code **[2]** modules related to fission product (FP) release and transport in the reactor circuit and containment was performed by CIEMAT, INR, JRC/IE, GRS, UJV and VUJE. These ASTEC modules included: ELSA (sub-module of DIVA module for in-vessel core degradation) for release of FP and structure materials (SM) from the core; SOPHAEROS for transport of FP vapours and aerosols in the reactor coolant system (RCS); CPA for thermal-hydraulics and aerosol behaviour in containment; and IODE computing the iodine behaviour in the containment.

The validation was mainly done against the Phebus experiments which, due to their integral nature, play a reference role in the research of severe accident phenomena. The Phebus facility (built in a 1:5000 scale) contains all the main components of a reactor unit (reactor core, circuit lines, steam generator and containment). These tests make it possible to analyse experimentally from the degradation of fuel rod bundles and the timing of massive material relocations up to molten pool formation, hydrogen production, and release of FP and their behaviour in the circuit and the containment. Therefore a realistic evaluation of the source term can be obtained.

Five Phebus FP tests have been performed. To study degradation and melting two initial fuel geometries were used: a fuel bundle configuration in four tests (FPT0, FPT1, FPT2 and FPT3) and debris bed geometry in one test (FPT4). Except for the FPT0 test, where fresh fuel was used, all the other tests were run with irradiated fuel (32 GWd/tU). In these tests, various flow rates were imposed in order to study FP release both in highly oxidizing conditions (FPT0, FPT1) and steam-poor conditions (FPT2, FPT3).

Other experiments considered for ASTEC FP models validation were: ThAI at Becker Technologies (Germany) for containment thermal-hydraulics and FP behaviour, in particular aerosols and iodine, and STORM (JRC/Ispra) for thermophoretic deposition and mechanical resuspension in RCS.

This paper summarises this ASTEC validation work done during SARNET: by JRC/IE on ELSA/DIVA vs. Phebus FPT0; by JRC/IE, UJV and VUJE on SOPHAEROS vs. FPT0, FPT1, FPT2 and STORM; by JRC/IE and CIEMAT on CPA vs. FPT0, FPT1 and FPT2; and by CIEMAT and GRS on IODE vs. FPT2 and ThAI. In addition ASTEC full integral calculations were performed by JRC/IE for Phebus FPT2, INR for FPT1 and VUJE for FPT3.

B. Validation of ELSA module

Since the beginning of SARNET a large validation activity has been done at JRC/IE focused on the ELSA module and based on the Phebus FP experiments.

The DIVA/ELSA calculations used the effective melting temperature of fuel (2450 K) instead of the default value (3085 K) following the recommendations from the overall Phebus.FP interpretation **[3]**. The integral release of volatile FPs was well reproduced for Cs, Sb and Te whereas slightly overestimated for Iodine. The detailed analysis of kinetics of FPT0 release of volatiles showed that their calculated release rate is significantly overestimated during the runaway oxidation phase mainly because of melting of the fuel grains.

For the semi-volatile FP, a greater discrepancy with the test results was however observed, especially for Ba.

FPT2 parametric studies showed that the fuel grain size distribution influences the release of volatile and semi-volatile FPs from the grains. Two cases were considered: monodisperse and polydisperse distribution of grain diameters, respectively: same diameter (15 µm) for all fuel grains; definition of 5 different diameters, keeping the same average diameter as for the monodisperse distribution. For volatiles and semi-volatiles, the calculation showed that both distributions give the same integral release (within 3%).

The sensitivity of the FP and SM release to the fuel relocation temperature was also examined. The release of low-volatile FPs was very sensitive to the relocation temperature: the higher the fuel relocation temperature, the higher the total release of semi-volatiles and non-volatiles FP, but the lower the total release of the volatiles FP.

C. Validation of SOPHAEROS module

C.1 Validation against Phebus FPT0, FPT1 and FPT2

For the entire circuit analysis **[3]** using SOPHAEROS it was found by JRC/IE that the total mass retention of all considered FP/SM before point C (i.e. before SG) was significantly underestimated (factor 0.5 – 0.3) and, on the other hand, it was significantly overestimated in the steam generator U-tube (FPT0: factor ~1.8, FPT1: factor ~2.5, see green column in **Fig.1**).

Due to the compensating effect, the retention for the entire circuit was predicted nearly perfectly, an overestimation by a factor lower than ~1.2 being obtained.

Several hints have been given to explain the underestimated deposition in the bundle upper plenum and vertical hot leg. One is the effect of developing laminar flow, with a velocity profile far from the parabolic one, since codes such as SOPHAEROS routinely apply heat and mass transfer correlations suitable for developed gas flows **[4]**. Another explanation could be the fact that, according to calculation, a large amount of aerosols was formed in the upper plenum and at the entry to the vertical section and that the aerosol particle size farther in the circuit was underestimated. Small size aerosol probably behaved differently in the analysis and contributed to the overestimation of deposits in the SG tube, obviously caused by thermophoresis.

Another support to this idea comes from FPT2 calculations that exhibit much better results with the same geometry data and aerosol parameters as FPT1. This was indicated by overall deposition (see red column in **Fig. 2**), but also by repartition of deposits between the vertical line and the SG tube. Looking for the reasons of better agreement for FPT2, faster vapour condensation on aerosol was found yielding also larger particles than in FPT1, mainly because the much smaller gas flow was cooled more efficiently by walls in the upper plenum or SG tube.

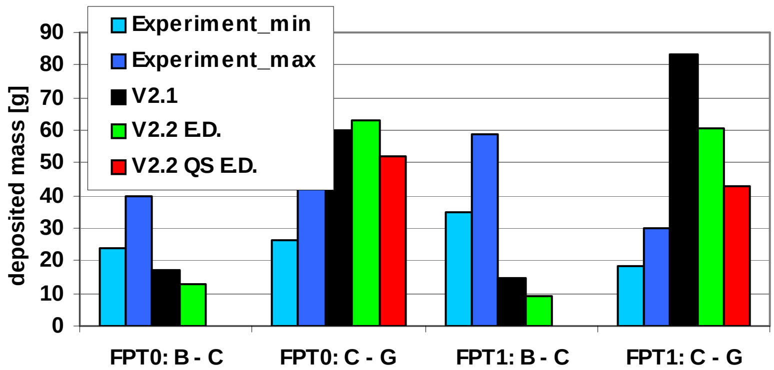

Fig. 1 SOPHAEROS and Phebus FPT0-FPT1 deposited masses before SG (B–C) and in SG (C–G) at test end (ED = extended MDB, QSED = imposing release measurements at point C)

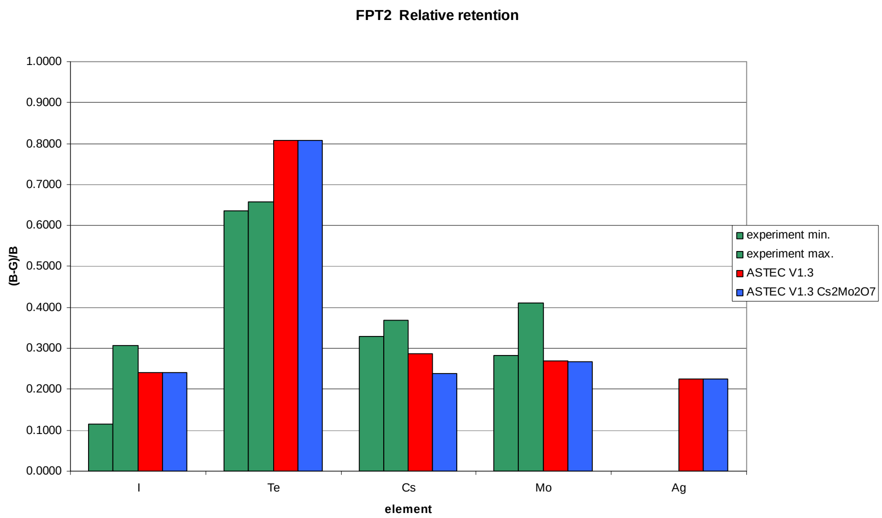

Fig. 2 SOPHAEROS results and Phebus FPT2 FP deposited fractions in circuit

Concerning the overestimation of the deposition in the SG tube, this overestimation is considerably reduced when FP and SM mass flow rates at point C correspond to the measured values (so called "quasi-separated" SG analyses). The predicted deposited masses are mainly due to thermophoresis and are still overestimated by a factor of 1.5 – 1.8 (see red column in **Fig. 1)**. The model to calculate the thermophoretic velocity is based on the Talbot formula, where the Nusselt number is calculated using the Dittus-Boelter correlation. This correlation is valid if the difference between the gas and wall temperature is less than 350K and this is not fully the case for the Phebus SG hot leg tube: it decreases from ~500 K to ~100 K in the first 2.5 m from the inlet of the SG tube, where a dominant overestimation of deposition is calculated (note that ~80% of predicted deposited mass is due to thermophoresis and ~20% due to FP/SM vapour condensation at the wall).

The calculated velocity of thermophoretic deposition for wall-to-fluid temperature differences greater than 200 K can considerably decrease when using near-wall temperature instead of the gas bulk temperature at which the carrier fluid properties used in the Talbot formula are calculated (current SOPHAEROS approach). Another suggested model improvement can be the consideration of the 2-D temperature and velocity profile by adding the radial dimension (especially in turbulent flow and under large wall-to-bulk temperature conditions) and the coupling of this profile with the appropriate chemistry to reduce significantly the thermophoretic deposition in the SG hot leg tube. Perhaps a simplified approach of the 2-D temperature and velocity calculations could be developed **[5].**

Concerning the release of the highly volatile iodine form into the Phebus containment (i.e. in gaseous or vapour form at 150 ºC), the results obtained with the application of the extended MDB (Material Data Bank) are in relatively good agreement with the experimental observations **(Fig.1).** But relatively small changes in the Cd release kinetics can have a significant influence on these results **[4]**. The sensitivity study performed on the Cd release kinetics showed that if no Cd is available in the circuit during the significant iodine release, a relative large amount of volatile iodine is formed and reaches the containment. While the Cd impact in the volatile iodine production in equilibrium chemistry calculations was clearly evidenced, in parallel rate-limited vapour chemistry is currently under investigation **[6]**.

A specific effort was done by UJV in explaining the test results by FP speciation focussing on iodine **[7] [8]**. The strong overestimation of iodine (CdI_2) condensation in the SG tube and the relatively good results for iodine in ISP-46 cast light on the iodine chemistry and its connection with caesium-molybdenum chemistry. In ISP-46, all FP sources used by UJV were taken from a MELCOR integral calculation, where the Mo release was underestimated by a factor of 4. Most iodine in that case was in the form of CsI. When using the Mo source derived from measurement, Cs became consumed in the circuit by molybdic acid, H_2MoO_4. Iodine was in the form of HI which reacted with Cd vapour forming mostly CdI_2 at the entry to the SG tube. Different explanations are suggested in **[9], [4]** based on part of HI surviving chemical reactions in the SG tube – intermittent release of Cd and including the kinetic of chemical reactions instead of assuming equilibrium conditions. Another hypothesis could be (based in Cs-Mo chemistry) that CsI should be more important if not the main iodine species instead of CdI_2. This could be especially the case if polymolybdates would be formed. Indeed, in some chemical literature, spontaneous change of mono-molybdates to poly-molybdates is mentioned, though not particularly for Cs and Rb **[10]**.

By applying the above ideas (except the last one), the FPT1 calculation yields a large release of HI to the containment while the observed fraction of volatile iodine was within 1% of the inventory. Sensitivity calculations were performed in order to decrease CdI_2 condensation in SG: 1) artificially decreasing of the saturation pressure of H_2MoO_4 in order to favour CsI formation. 2) using, in the condensation equation, the temperature near the wall instead of the bulk temperature 3) using Cs and Rb bi-molybdates instead of mono-molybdates. But even with these options the deposition of iodine is still too high, though any of these changes, when used alone, suppressed strongly the iodine deposition in the SG tube.

As a matter of fact, potential Bi(poly)-molybdates $Cs_2Mo_2O_7$ and $Rb_2Mo_2O_7$ together with kinetics limitations in the chemical reactions seem to be the best explanation to be considered for both reducing the iodine condensation in the SG and the amount of volatile iodine persisting at low temperature. The effect of shift from CdI_2 to CsI chemistry does not much suppress the volatile HI in the hot leg (less than by the factor of two) while HI is consumed almost completely either by Cs or Cd in the SG tube. It should be noted, however, that the shift to CsI slightly (the shift is not incomplete) contradicts the experimental finding that CsI is not the main iodine species in the hot leg **[11]**.

For iodine in FPT2, also the different timing of Mo versus Cs release plays a role: Mo is released with some delay. Thus, there is less H_2MoO_4 at the time of massive Cs release and CsI is predicted to prevail over CdI_2 at the circuit exit during the hydrogen-rich phase. It was also found that, due to cold wall temperature upstream the SG entry, CdI_2 condensation is suppressed in the SG tube comparing to FPT1. A supplementary calculation was performed (see blue column in **Fig. 2)** where Cs_2MoO_4 and Rb_2MoO_4 were replaced in the database by bi-molybdates $Cs_2Mo_2O_7$ and $Rb_2Mo_2O_7$. The effect in FPT2 is negligible, especially for iodine.

In FPT1 and FPT2, tellurium deposition due to chemisorption of SnTe on Inconel is extremely overestimated **[4]**. This would mean that the SnTe was not the main Te species as calculated by the code. Another explanation also exists, the high chemisorption velocity is correct, but saturation was reached at the wall surface, which is not accounted for in the code.

C.2 Validation against the STORM experiments

JRC/IE has applied SOPHAEROS to the STORM aerosol deposition-resuspension experiments performed at JRC/Ispra which dealt with the deposition and resuspension of aerosol particles in pipes **[12]**. The gas velocities at which the resuspension phenomenon was studied were in the range between 60 m/s and 140 m/s, i.e. much larger than in Phébus tests. Anyway re-suspension of deposits was measured during the inerting phase of Phebus for low gas velocities. For the analyses both the “Force-Balance” (FB) and “Rock’N Roll” (RnR) models were used.

Four computational analyses were carried out for each STORM resuspension test such as SR09, SR10, SR11, SR12 and SR13 by using the SOPHAEROS module of the ASTEC V1.3R0 code in stand-alone mode. The modelling options used in the calculation are as follows: “Force-Balance” model with the default value of cohesive force coefficient ($1.0 \cdot 10^{-6}$ N/m) (“FB1” results), or with a value 10 times higher (“FB2”); “Rock’n Roll” model with maximum time step set of 1 s. (“RnR1”) or 30 s. (“RnR2”).

As **Fig. 3** shows, the FB model of mechanical resuspension with the default value of the cohesive coefficient (FB1) over-estimates the final resuspended fraction for the entire analyzed STORM tests. The FB model gives substantially better agreement with the estimated final resuspended fractions if the value of the default cohesive coefficient is increased by a factor of 10 (FB2); however, remarkable over-estimation for SR12 and SR13 still remains. It should be pointed out that according to the FB model the resuspension is a continuous process and therefore the calculated resuspended mass significantly depends not only on the carrier fluid velocity during resuspension phase, but also on the duration of these phase (one or several steps). This is, however, in contradiction with the experimental measurements.

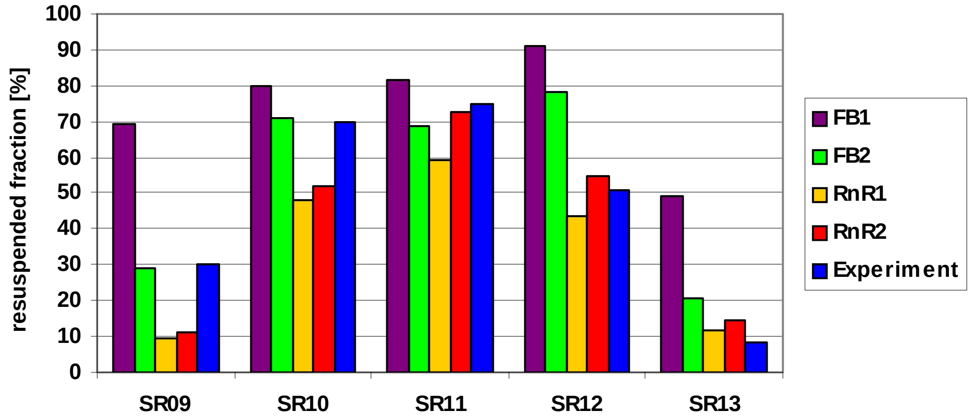

Fig. 3 Comparison of SOPHAEROS and measured total resuspended fractions on STORM

The STORM SR09 to SR12 resuspension tests showed that the majority (>99 %) of the deposited mass is resuspended in a very short time interval (5 s to 25 s) just after the increase of the carrier fluid mass flow rate, which means that, in reality, the resuspended mass (fraction) only partly or negligibly depends on the duration of resuspension step, when the gas flow velocity is kept at a constant value. The RnR model significantly underestimates the final resuspended fraction for the SR09 and SR10 tests, in which the resuspension phase was simulated in one step by increasing the carrier fluid velocity from ~20 m/s to ~54 m/s (SR09) and to ~83 m/s (SR10). On the other hand this underestimation of the final (total) resuspended fraction is small or negligible (even slightly over-estimated for SR13),. Also, in the RnR model, 99 % of the fraction is resuspended in a very short time. For SR11 and SR12 tests, both SOPHAEROS "Rock'n Roll" calculations (RnR1 and RnR2) over-estimate the resuspended fraction during the first (SR12) and the first two resuspension steps (SR11) whereas the situation becomes the opposite during the later steps, and this has a compensating effect on the final resuspended fraction.

As a conclusion, the two ASTEC V1 models encompass the measurements of the final resuspended fraction but there is the need of further improvement of the aerosol mechanical resuspension model.

D. VALIDATION OF THE CPA MODULE

For the CPA calculations JRC/IE analysed the aerosol behaviour in the containment **[13]** of the Phebus FPT1 using the ASTEC V1.2 version. First it was shown that after the steam condensation phase, good calculated results (suspended aerosol mass versus time, number mean geometric diameter versus time) could be obtained only when the average density of aerosol particles was set to 7000 kg/m3. This value is a little higher than the estimates of Phebus experts. More recently, the IRSN investigations with recent ASTEC versions, using density lower values, gave an acceptable agreement.

In CPA, the gas velocity field was simulated by means of a user-defined network of flow resistances and making use of a reference flow pattern taken from a CFD calculation **[14]**. A sensitivity study showed that the developed gas circulation comprising two loops slightly increases the maximum concentration of suspended aerosols and can slow down to some extent the decrease of suspended mass. In the final stage of the transient, the suspended mass decreases nearly exponentially but it is about 20 % higher when the developed gas circulation is modelled in the calculation). Further effects of the developed circulation are that the final aerosol mass settling on the elliptic bottom slightly increases, while the final mass transported to the wet condensers decreases a little.

The CIEMAT thermal-hydraulic simulation of Phebus FPT2 can be considered satisfactory **[18]**. Nevertheless, a slight discrepancy in relative humidity has been studied in depth (**Fig. 4**). Even though during most of the transient the code predictions followed closely the experimental trends of steam condensation rate, no experimental data were available for the first 2000 s (the time interval in which those differences built-up). Through a sensitivity analysis it was shown that such discrepancy could be well due to the uncertainties on the experimental measurements of surface temperature of wet condensers, since just 1K change could notably reduce the data/estimates gap.

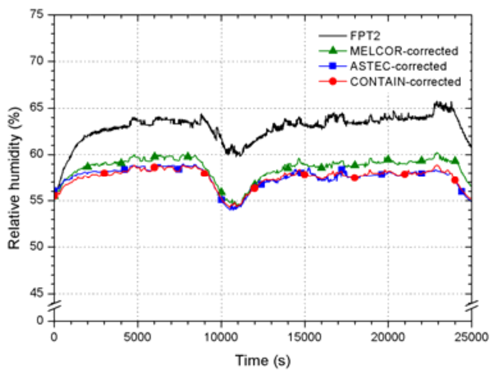

Fig. 4 Relative humidity versus time in the FPT2 test

Major assumptions have been made in FPT2 aerosol modelling. Aerosol injection has been modelled by considering three components: Iodine (I), Caesium (Cs) and a mixture including the rest of compounds observed in aerosol particles. Their input rates have been estimated from the IRSN data at the point G filters **[15]**. Aerosol density has been approximated to be 6350 kg/m3. This value has been obtained as a mass average based on assuming specific chemical forms of the elements that made up aerosol particles. The Mass Mean Diameter (MMD) of the particle has been assumed to be 1.11 µm (with a GSD around 1.9). This particle size has been taken from previous Phebus interpretation work **[16]**. Preliminary size measurements from impactors in FPT2 suggest that aerosol size distributions were similar to those in FPT1 test **[17]**. The large under-saturation state of the atmosphere does not allow considering the hygroscopic behaviour of the aerosol particles.

Overall evolution of airborne aerosols is predicted reasonably well, as shown in **Fig. 5** in the case of iodine. Nonetheless, the maximum concentration and the decay rate deviate slightly from measurements. Consistently with data, sedimentation is predicted to be the dominant aerosol removal mechanism of aerosols from the vessel atmosphere. However, ASTEC, like the other used codes (MELCOR and CONTAIN) fail to remove particles on vessel walls, as experimentally measured. Sensitivity studies carried out on particles size, shape and density indicate that uncertainties on those variables cannot justify the magnitude of the deviation found.

At the time the calculations have been conducted, no experimental data on time history of aerosol mass deposition were available. **Table 1** shows the mass distribution at the end of the aerosol phase (samplings have not considered), and a comparison with other codes. Particle growth is a little faster in CPA than in CONTAIN, and this different size evolution leads to the sedimentation over-prediction in CPA. A more accurate description of surfaces and the fitting of the sump temperature led to better agreement. Another explanation of the sedimentation over-prediction could be well due to the high density estimated for aerosol particles. Indeed, in recent ASTEC/CPA FPT2 calculations, IRSN has recommended lower values for aerosol density and higher values for MMD than CIEMAT ones.

	FPT2	CPA	MELCOR	CONTAIN
Floor and sump	75%	88.1 %	84.5 %	83.4 %
Wet condensers	15%	11.6 %	14.1%	14.2 %
Walls	10%	0.3 %	1.4 %	2.4 %

Table 1 Final mass distribution

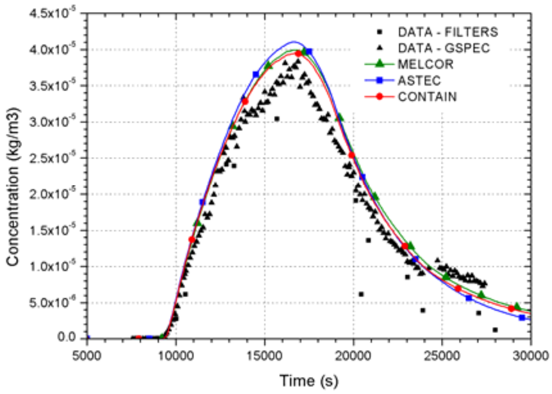

Fig. 5: Containment Iodine evolution during the FPT2 test in form of aerosols

E. VALIDATION OF THE IODE MODULE

E.1. Validation on Phebus FPT2

The chemistry phase of the Phebus FPT2 experiment has been analysed by CIEMAT using the IODE module of the ASTEC V1.2 code **[18]**. The main objective was to understand the potential phenomena responsible for the iodine chemical behaviour under conditions prevailing in the FPT2 test (i.e., an alkaline, evaporating sump).

The input deck was based on available experimental data. However, some data were missing at the time this study was conducted, so that some approximations and hypotheses were made. Several cases have been modelled to assess those assumptions and to explore different factors that could have played a role in the scenario. A simple proposal of the chemical scenario was done in the base case and checked by comparing predictions to data.

Calculations showed no major differences with respect to data. The results indicated that assumptions concerning pH and the amount of oxidized silver are not responsible for the slight discrepancies. Other factors like adsorption/desorption onto/from surfaces would have largely over-predicted gaseous iodine depletion. However, unlike MELCOR predictions, IODE module is even capable of capturing the iodine evolution in the gas phase when the radiolytic oxidation of gaseous I_2 is considered (**Fig. 6**).

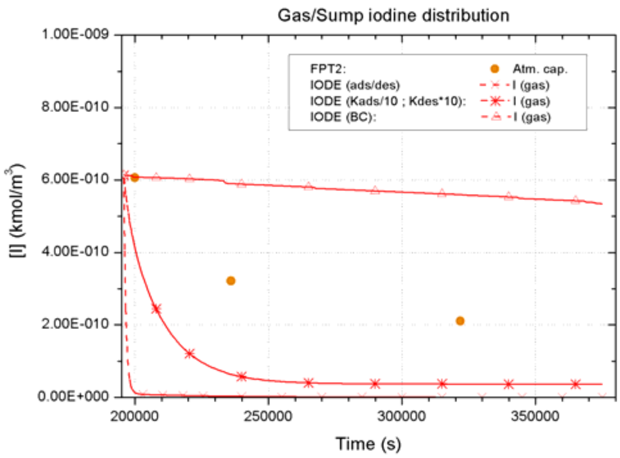

Fig. 6: Phebus FPT2 gas iodine concentration. ASTEC simulation including gas phase

These results seem to indicate that, during the chemistry phase, dissolved iodine remained in the aqueous phase but in the form of an ionic highly oxidized species, IO_3- (i.e., AgI was not formed quantitatively during the chemistry phase). As for the gaseous iodine evolution, the results suggest focusing the attention on phenomena related to gaseous iodine oxidation and on adsorption/desorption processes.

E.2. Validation on ThAI

Post-test GRS calculations were performed with IODE module of ASTEC V1.2 rev1 on large-scale ThAI tests in order to validate the iodine multi-compartment transport and modelling behaviour **[19]**. The objective of the ThAI program (Thermal hydraulics, Aerosols, Iodine) is to generate a database for the validation of codes in the area of containment thermal hydraulics and the behaviour of FP, in particular aerosols and iodine. In the tests Iod-10, Iod-11 and Iod-12 in the 60m^3 facility of Becker Technologies (Eschborn, Germany), the transport and deposition behaviour of gaseous molecular iodine (I_2) was investigated in 5-compartment geometry with a sump under typical severe accident conditions. Each test included a phase with stratified atmosphere followed by transition into a well-mixed phase.

Qualitatively, the distribution of I_2 in the vessel is calculated correctly for all tests, especially the concentration differences of several orders between the compartments in the stratification phases that are well simulated. The significantly slower or incomplete homogenisation of I_2 as compared to the helium behaviour in the vessel during the mixing phase is also well reproduced. The code demonstrates clearly how the steel walls act as an intermediate storage for I_2 due to temporary adsorption and desorption processes.

Quantitatively, the agreement between calculated and measured gaseous I_2 concentrations is good at dry conditions (Iod-10). However, ASTEC overestimates the gaseous I_2 concentrations when the relative humidity is high, with or without wall condensation as given in the tests Iod-11 and Iod-12. The most likely reason is a slow reaction of deposited I_2 to the non-volatile FeI_2 on the steel surfaces, which has not been modelled yet. The comparison with results of COCOSYS GRS containment on these three ThAI tests was also performed. The agreement on the thermal-hydraulics is good.

The overall agreement on iodine results is acceptable. Indeed, the iodine modules differ between the codes: COCOSYS-AIM default I_2 adsorption/desorption models have been developed with data from earlier ThAI tests. The IODE I_2 default adsorption/desorption models have been derived from literature data partly on laboratory-scale experiments.

F. FPT1 AND FPT2 INTEGRAL CALCULATIONS

Note that only the FP results of these integral calculations are described in this chapter.

A full integral calculation on the Phebus FPT2 test was performed in JRC/IE using ASTEC V1.3 code version. The analysis of FP release and transport for FPT2 was carried out for the whole duration of the test, until and after the washing phase.

Concerning the release of FP and SM elements from the bundle, a general statement about over or underestimation cannot be done, because an element-by-element comparison would be needed. The Cs and I total release was correctly reproduced but the kinetics was overestimated of about the same factor (1.4).

The excessive release of semi and low-volatile elements, as calculated at bundle outlet, causes their deposition in the circuit to be overestimated (~factor of 2). For the transport of iodine in aerosol (solid) state, Cs and Cd play the most important role. In gas state, in transport of iodine the Mo and Sn play the most important role. Mo is fission product; Sn is the main alloying element of zirconium cladding.

For the containment the integral calculation shows that gaseous iodine release happens only when the core temperature is at about 2300 K or higher, at some locations during the late bundle phase. 60% of iodine initial bundle inventory (i.b.i.) is transported to the containment with solid aerosols; additionally, 2% of i.b.i. is transported in gaseous form (I_2MoO_2, I_4Sn, I_2Sn, HI...) Altogether 62% of i.b.i is released to containment while the total measured mass of iodine in the FPT2 containment is 57% of i.b.i. A total aerosol mass of 56 g was calculated as released to the containment against the 50 g measured.

The IODE module deals only with I_2 and ICH_3 as gaseous iodine, however the calculated I_2 (gas) concentration was six orders of magnitude lower than the other gaseous forms with Mo, Sn and H. Most part of iodine after the washing phase was located in the sump. The total calculated iodine mass in the sump was 45.9% of i.b.i. against 46.4% of i.b.i. measured.

INR performed also an integral calculation with ASTEC V1.3 rev2 but on FPT1. The overall conclusions are similar to the JRC ones above.

Some attention was paid to FP release. The results for indium release are closer to the measured ones than with previous ASTEC versions. Since the cadmium is known to be highly volatile, its release was not very much affected by the new model, but mostly by the axial temperature distribution: even if the simulated release began earlier than the experimental one, the curve shape is in better agreement with the experiment, but the final release fraction is still by 25% greater than the measured one. For the tin component of Zircaloy, the results are in better agreement with the experiment than the previous versions, reproducing all 3 experimental points and also leading to a smaller (i.e. closer to the measurement) final release fraction. The Sn release is still calculated to begin too early (5500 s earlier than it really occurred in the experiment). The release rate of semi-volatile FPs was underestimated for ruthenium, but overestimated for molybdenum and barium.

G. CONCLUSIONS

G.1 ELSA module

The ELSA validation vs. the Phebus experiments showed that the best agreement with experimental data was obtained for the release of volatile FP, like Cs, Sb, I and Te. For the semi-volatile FP, a great discrepancy with the test results was obtained, especially for Ba (overestimation). A strong impact of the fuel relocation temperature was observed on the release of low-volatile FP.

The main model improvements on FP release that were done in successive ASTEC V1 versions concern semi-volatile FP and SIC but new improvements are under way for ASTEC V2.0. Models also were added to for all SM (Fe, Ni, Cr...). The results of the INR FPT1 integral calculation have shown a better agreement on Indium, Cadmium (both from control rods) and on Sn than with previous versions.

G.2 SOPHAEROS module

The validation performed at JRC/IE and UJV on SOPHAEROS has improved the understanding of the modelling of the transport of FP vapours and aerosols in the RCS including the chemical interactions of vapours. The RCS iodine chemistry led IRSN to review in 2006 the MDB gas databank and to launch studies on kinetics of iodine chemistry within the framework of the ISTP program (CHIP project) **[20]**. The results evidenced Cs_2MoO_4 as a major species in Cs chemistry and support the fact that some chemical reactions can occur also in the circuit where the temperature is much lower than in the core. It was shown, as previously evidenced**,** that relatively small changes in the considered Cd release kinetics could have a significant influence on iodine release. The role of molybdic acid was clearly evidenced while the potential formation of poly-molybdates which may impact the iodine speciation as well still has to be checked

The studies showed an overestimation by 1.5 to 1.8 of deposits in the SG, despite a slight improvement with respect to the previous code versions. Some hints have been given on the origin of this overestimation, in particular linked to the thermophoresis model. Other explanations can be the underestimation of deposition, especially of small size aerosol, in the volumes at bundle exit, due to the complex geometry in this location.

The validation performed at JRC/IE vs. the STORM experiments (SR09 – SR13) showed an overestimation of aerosol deposits, with thermophoresis as dominant deposition process, but comparable to the literature results. The overestimation is below 30% except for SR11 (50%) where the highest fluid–to–wall temperature difference was applied. Further examinations of the thermal hydraulic uncertainties are required. Discrepancies remain on aerosol mechanical resuspension at high carrier gas velocity (above 90 m/s); with the existing empirical model of resuspension, acceptable results could be only obtained by modifying artificially the cohesive force coefficient.

Investigations on the more adequate way to simulate aerosols deposition in the complex geometry such as the core/bundle upper plenum must go on.

Suggestions for further model improvements are:

- In a first priority, rate-limited vapour chemistry models (i.e. non-equilibrium chemistry models under current investigation in IRSN **[6]**;
- Simplified approach of the 2-D temperature and velocity profile by adding the radial dimension (especially in turbulent flow and under large wall-to-bulk temperature conditions); coupling of this profile with the appropriate chemistry model to reduce significantly the overestimation of the thermophoretic deposition in the SG;
- Checking the influence of reference temperature for calculation of fluid properties in the Talbot formula, used to calculate the velocity of thermophoretic deposition **[21]**;
- Further improvement of aerosol mechanical resuspension (under investigation in SARNET).

G.3 CPA module

The CPA validation performed by JRC/IE and CIEMAT vs. the Phebus experiments showed how the lumped-parameter concept is useful for the interpretation of the thermal-hydraulic parameter changes and aerosol transport in the containment. However, the analyses pointed out that it is necessary to use adequate nodalization and boundary conditions to qualitatively describe the continuum flows in the investigated domain. The overall thermal-hydraulic simulation can be considered satisfactory. The aerosol behaviour in containment is predicted rather accurately: Cs and I airborne concentrations are in good agreement with data.. CPA predicts that the main depletion mechanism is sedimentation on the floor. However it over-predicts the sedimentation rate whereas it under predicts the deposition by diffusiophoresis on the wet condensers and it hardly foresees, like all codes, any deposition on containment wall. This over-prediction could be due to the estimate of a too high density for aerosols.

G.4 IODE module

The investigations on the IODE module performed by CIEMAT based on Phébus FPT2 showed that most of the iodine is retained as ionic species in the sump. According to calculations, iodine oxide dominates the iodine gas phase concentration in the long term. Adsorption and desorption could have played a role in the chemistry phase, but current models largely over predict gaseous iodine depletion.. Consideration of gas radiation chemistry provides a potential explanation of gaseous iodine evolution. IODE results show no major differences with respect to Phebus FPT2 data. The module is even able to capture the iodine evolution in the gas phase when the radiolytic oxidation of gaseous I_2 is considered.

Analyses using IODE module performed by GRS on ThAI experiments contributed to the validation of adsorption/desorption models in multi-compartment large-scale experiments. Qualitatively, the distribution of I_2 in the vessel is calculated correctly for all tests, especially the concentration differences of several orders between the compartments in the stratification phases. The significantly slower or incomplete homogenisation of I_2 as compared to the helium behaviour in the vessel during the mixing phase is also well reproduced.

In general, the agreement is good at dry conditions but improvements should be made for conditions where the relative humidity is high, since ASTEC overestimates there the gaseous I_2 concentrations.

G.5 Integral Phebus calculations

The capability to perform a fully realistic integral calculation using ASTEC code is confirmed by the two integral FPT1 and FPT2 calculations, respectively performed by INR and JRC/IE. The integral mode allowed checking the consistency among the main code modules. A few FP results are shortly commented below.

The SIC rod degradation model implemented in ASTEC V1.3 rev2 led to results closer to the experimental values, in terms of the events timing and release kinetics evolution. The kinetics of release of volatile FPs was overestimated: for instance, the iodine release was simulated to begin earlier than in the experiment, but both the curve shape and the final release fraction are in good agreement with the measurements. Release of semi- and low-volatile FP from the bundle is in general overestimated. This is likely one of the explanations for the overestimation of deposition in the circuit for most species.

But, despite some discrepancies on FP release and deposition, overall good results were obtained on aerosol mass to containment and iodine mass in the sump. More analyses are needed to confirm these integral calculation results including benchmarking with other codes.

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