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SARNET benchmark on Phébus FPT3 integral experiment on core degradation and fission product behaviour

M. Di Giuli [a,1], T. Haste [a,*], R. Biehler [a,2], L. Bosland [a], L.E. Herranz [b], J. Fontanet [b], E. Beuzet [c], M. Torkhani [c], N. Davidovich [d], W. Klein-Heßling [e], S. Weber [f], S. Dickinson [g], G. Horváth [h], P. Kruse [i], M. Koch [i], S. Paci [j], S.J. Weber [k], M. Salay [l], A. Bujan [m], I. Ivanov [n], P. Kalychev [n], S.B. Kim [o], S. Morandi [p], A. Del Corno [p], M. Kotouč [q], J. Dienstbier [q], H.-C. Kim [r]

[a] IRSN, Cadarache, France
[b] CIEMAT, Madrid, Spain
[c] EDF, Clamart, France
[d] ENEA, Bologna, Italy
[e] GRS, Garching, Germany
[f] GRS, Cologne, Germany
[g] NNL, Didcot, UK
[h] NUBIKI, Budapest, Hungary
[i] RUB, Ruhr-University Bochum, Germany
[j] UNIPI, University of Pisa, Italy
[k] SNL, Albuquerque, USA
[l] USNRC, Washington D.C., USA
[m] VUJE, Trnava, Slovakia
[n] TUS, Technical University of Sofia, Bulgaria
[o] KAERI, Taejon, Republic of Korea
[p] RSE, Milan, Italy
[q] UJV, Rez, Czech Republic
[r] KINS, Taejon, Republic of Korea

Abbreviations: AIM, advanced iodine model; ASTEC, accident source term evaluation code; ATHLET-CD, Analysis of THermal-hydraulics of LEaks and Transients – Core Degradation; BIP, Behaviour of Iodine Project; CEA, Commissariat à l'Énergie Atomique et aux Énergies Alternatives, France; CHIP, experimental programme for chemistry of iodine in the primary circuit; CIEMAT, Centro de Investigaciones Energeticas Medio Ambientales y Tecnologica; CSNI, Committee on Safety of Nuclear Installations; EC, European Commission; EDF, Electricité de France; EPICUR, experimental programme for iodine chemistry under radiation; ENEA, Agenzia nazionale per le nuove tecnologie, l'energia e lo sviluppo economico sostenibile, Italy; ENSI, Eidgenössischen Nuklearsicherheitsinspektorats, Swiss nuclear regulator; EU, European Union; FP, fission product; FPT, Phébus fission products test; GRS, Gesellschaft für Anlagen- und Reaktorsicherheit (gGmbH); HSK, Hauptabteilung Sicherheit Kernenergie, former name of Swiss Nuclear Inspectorate; i.i., initial inventory; IODE, ASTEC module for iodine and ruthenium behaviour in-containment; IOx, iodine oxide; IRSN, Institut de Radioprotection et de Sûreté Nucléaire; ISTP, International Source Term Program; ISP, International Standard Problem; ISTP, International Source Term Project; JAEA, Japanese Atomic Energy Agency, JNES, Japanese Nuclear Energy Society; JRC, Joint Research Centre; KAERI, Korean Atomic Energy Research Institute; KINS, Korean Institute of Nuclear Safety; LWR, light water reactor; MAAP, Modular Accident Analysis Program; MELCOR, methods for estimation of leakages and consequences of releases; MIRE, Mitigation des Rejets à l'Environnement; NNL, National Nuclear Laboratories; NUBIKI, Nuclear Safety Research Institute, Ltd., Nukleáris Biztonsági Kutatóintézet Kft, Hungary; NPP, Nuclear Power Plant; NUGENIA, NUclear GEN II & III Association; OECD, Organisation for Economic Cooperation and Development; Phébus FP, programme to improve the understanding of the phenomena occurring during a core meltdown accident in a light water reactor; PSI, Paul Scherrer Institut; PWR, pressurised water reactor; RI, organic iodide; RSE, Ricerca Sistema Energetico, Italy; RCS, Reactor Coolant System; RUB, Ruhr-University Bochum, Germany; SA, severe accident; SARNET, severe accident research network; SM, structural material; SS, stainless steel; STEM, experimental programme for study of source term and mitigation; ST, source term; THAI, experimental programme for thermal hydraulics and iodine; TMI-2, Three Mile Island Unit 2; TUS, Technical University of Sofia, Bulgaria; UJV, Ústav jaderného výzkumu Řež, Czech nuclear research institute; UNIPI, University of Pisa, Italy; USNRC, United States Nuclear Regulatory Commission; VTT, Technical Research Centre of Finland, Teknologian tutkimuskeskus VTT; VUJE, Výskumný ústav jadrových elektrární, Slovakian Nuclear Power Plant Research Institute.

* Corresponding author at: Institut de Radioprotection et de Sûreté Nucléaire (IRSN), PSN-RES/SAG/LETR – Bât 702, BP 3, F-13115 St-Paul-Lez-Durance Cedex, France. Tel.: +33 4 42 19 95 67; fax: +33 4 42 19 91 67.
E-mail address: tim.haste@irsn.fr (T. Haste).

[1] Att. from ENEA, Bologna, Italy.
[2] Present address: CS-SI, Aix-en-Provence, France.

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ABSTRACT

The importance of computer simulations in the assessment of nuclear plant safety systems has increased dramatically during the last three decades. The systems of interest include existing or proposed systems that operate, for example, normal operation, in design basis accident conditions, and in severe accident scenario beyond the design basis. The role of computer simulations is especially critical if one is interested in the reliability, robustness, or safety of high consequence systems that cannot be physically tested in a fully representative environment. In the European 7th Framework SARNET project, European Commission (EC) co-funded from 2008 to 2013, the Phébus FPT3 experiment was chosen as a code benchmark exercise to assess the status of the various codes used for severe accident analyses in light water reactors.

The aim of the benchmark was to assess the capability of computer codes to model in an integral way the physical processes taking place during a severe accident in a pressurised water reactor (PWR), starting from the initial stages of core degradation, fission product, actinide and structural material release, their transport through the primary circuit up to the behaviour of the released fission products in the containment.

The FPT3 benchmark was well supported, with participation from 16 organisations in 11 countries, using 8 different codes. The temperature history of the fuel bundle and the total hydrogen production were well captured. No code was able to reproduce accurately the final bundle state, using as bulk fuel relocation temperature, the temperature of the first significant material relocation observed during the experiment. The total volatile fission product release was well simulated, but the kinetics were generally overestimated. Concerning the modelling of semi-volatile, low-volatile and structural material release, the models need improvement, notably for Mo and Ru for which a substantial difference between bundle and fuel release was experimentally observed, due to retention in the cooler upper part of the bundle. The retention in the primary circuit was not well predicted, this was due mainly the non-prototypic formation of a boron-rich blockage in the rising line of the FPT3 steam generator, simulated in the circuit as a single external cooled U tube. The deposition mechanism and the volatility of some elements (Te, Cs, I) could be better predicted.

Containment vessel thermal hydraulics, designed in the experiment to be well-mixed, were well calculated. Concerning the containment aerosol depletion rate, only stand-alone cases (in which the input data were derived from experimental data) provided acceptable results, whilst the integral cases (in which the input data came from circuit calculations) tended to largely overestimate the total aerosol airborne mass entering the containment.

The disagreement of the calculated total aerosol airborne mass in the containment vessel with the measured one is due to the combination of a general underestimation of the overall circuit retention and overestimation of fission product and structural material release.

Calculation of iodine chemistry in the containment turned out to be a major challenge. Its quality strongly depends on the correct prediction of chemistry speciation in the integral codes. The major difficulties are related to the presence of high fraction of iodine in gaseous form in the primary circuit during the test, which is not correctly reproduced by the codes. This inability of the codes compromised simulation of the observed iodine behaviour in the containment.

In the benchmark a significant user effect was detected (different results being obtained by different users of the same code) which had to be taken into account in analysing the results. This article reports the benchmark results comparing the main parameters calculated and observed, summarising the results achieved, and identifying the areas in which understanding needs to be improved. Relevant experimental and theoretical work is under way to resolve the issues raised.

1. Introduction

Following the 1979 accident at the Three Mile Island Nuclear Plant, Unit 2 (TMI-2) (Broughton et al., 1989), it was recognised that severe accidents needed further attention, and a worldwide effort has been undertaken to understand more fully severe accident phenomena in nuclear reactors. Development and assessment of the computer codes used for severe accident analysis has taken place on international basis using a wide range of integral and separate-effects experiments. Amongst the integral experiments, those conducted in the international Phébus FP programme has been of major importance. This programme allowed core meltdown accidents in light water reactors to be reproduced as far as possible in representative conditions on a reduced scale. It was initiated in 1988 by the French Institut de Radioprotection et de Sûrete Nucléaire and the Joint Research Centre of the European Commission (von der Hardt et al., 1994). The aim of this programme was to study the degradation phenomena and the behaviour of fission products and structural materials released in the reactor coolant system and the containment (Clément and Zeyen, 2013). The test matrix consisted of five in-reactor tests, performed under different conditions (March and Simondi-Teisseire, 2013). Analysis of these tests has enabled and is continuing to enable better qualitative and quantitative improvements in understanding severe accident phenomena in light water reactors, hence through the use of computer codes enabling better prediction of accident sequences in nuclear plant and reduction in source term uncertainty.

In the frame of the SARNET2 network of excellence under the EC 7th Framework programme (Van Dorsselaere et al., 2015), the last test of the series, Phébus FPT3, was chosen as the basis for a code benchmark. In this exercise, predictions or recalculations of the

main physical parameters with different computer codes were compared with each other and above all with the experimental data, to promote the international exchange of experience amongst the participants in the use of nuclear safety codes. The main objective of the FPT3 benchmark was to assess the capability of computer codes to reproduce in an integral way the physical processes taking place during a severe accident in a PWR, notably as regards the treatment of strongly coupled processes, (i.e. fuel degradation with associated hydrogen production and fission product release, fission product and structural material transport in the primary circuit, aerosol behaviour in the containment and iodine radiochemistry), as identified in the OECD/CSNI International Standard Problem 46 based on Phébus FPT1 (Clément et al., 2005). The organisation of the present benchmark largely follows that of ISP-46.

The FPT3 benchmark has resulted in increased confidence in the validity and accuracy of analytical tools, which are needed to assess the safety of nuclear installations, and improve the ability of the organisations involved, for example (Maurice et al., 2013). It was conducted as an open exercise, with all the relevant experimental data being available to the participants.

The four areas covered by the experiment and therefore by the FPT3 benchmark, are the following (Clément and Zeyen, 2013):

- Fuel degradation, hydrogen and carbonaceous gas generation, release of fission products, actinides, and structural materials ('bundle' phase 1).
- Fission product, actinide and structural material transport in the circuit, in aerosol and gaseous forms ('circuit' phase 2).
- Thermal hydraulics and aerosol physics in the containment ('containment' phase 3).
- Iodine chemistry in the containment ('chemistry' phase 4).

The emphasis was on integral calculation (all phases) and on the use of the codes as in plant studies i.e. using standard models/options as far as possible, representing the facility in a similar level of detail.

2. Schedule and participation

The benchmark started in February 2011, with a time scale of 2.5 years. A key event was the finalisation of the Phébus FPT3 Final Report (Payot et al., 2011) in July 2011, thus making the detailed results in final form available to all the benchmark participants. The issue of a draft version of the Specification Report in advance of the first meeting in March 2011 allowed time for comments, which were taken into account in the final version. The most intensive phases were preparation of the specifications (6 months), participants' calculations and submission of their results (1 year), and the coordinators analysis of the results and draft of the Comparison Report (7 months). Submissions were received from 16 organisations in 11 countries. The latter comprised Bulgaria, Czech Republic, France, Germany, Hungary, Italy, Korea, Slovakia, Spain, UK and USA. The participating organisation included utilities, regulators and their technical support organisations and research institutes, thus providing a good range of backgrounds to the technical work.

Eight different codes were used: ASTEC (Chatelard et al., 2014a, 2014b; Bosland et al., 2010), ATHLET-CD (Trambauer et al., 2011), COCOSYS/AIM (Allelein et al., 2008; Weber and Funke, 2009), ECART (Parozzi and Paci, 2006), INSPECT/IODAIR (Dickinson and Sims, 2000), MAAP4 (Rahn, 2010), MELCOR (Gauntt et al., 2005) and RAIM (Oh et al., 2011; Kim and Cho, 2012). Three of these eight codes are integral codes (ASTEC, MAAP4 and MELCOR), covering all aspects of severe accidents from initiating event through to release of FPs from the containment, with ASTEC providing the most detailed treatment and MAAP the fastest, based on simplified physics, well suited to probabilistic safety studies by industry in which a large number of cases need to be run. MELCOR has an intermediate level of detail, providing engineering-level modelling for severe accidents in light water reactor nuclear power plants. An iodine pool model is implemented to predict iodine in the containment, whilst the capability to model gaseous iodine chemical behaviour is rather limited, e.g. in the circuit. ATHLET-CD provides detailed models of core degradation and of fission product release and transport; COCOSYS calculates detailed thermal hydraulic behaviour in the containment, whilst AIM is a detailed iodine chemistry model. ECART is a specialised thermal hydraulic aerosol physics code, whilst INSPECT/IODAIR gives a detailed mechanistic treatment of iodine chemistry in the containment. RAIM is based on the semi-empirical IMOD methodology for iodine chemistry in the containment sump (Wren et al., 1999), and is used in conjunction with MELCOR. An integral calculation was also performed using ATHLET-CD and COCOSYS/AIM coupled together, see Table 1. For the base case, 23 calculations were received, with 3 for the optional best-estimate version. Of the base case calculations, 5 were integral (defined as including calculations for 3 or 4 phases).

3. Description of the Phébus FPT3 test

The in-reactor integral Phébus FP test studied bundle degradation, release, transport and deposition of fission products, structural and control rod materials in the model primary circuit and containment building, under steam rich or steam-poor atmospheres, and under low pressures (~0.2 MPa), with specific attention to the behaviour of fission products, Fig. 1 (Grégoire and Payot, 2009). The experimental facility scenario and objectives of the series have been extensively presented in literature, for example (Schwarz et al., 1999).

The FPT3 test studied especially the impact of the boron carbide control rod on the fuel degradation and FP speciation and transport in steam poor condition. The FPT3 test sequence (Haste et al., 2010)

Table 1
Summary of submissions for the Phébus FPT3 benchmark.

Organisation	Code	Phase	Country
CIEMAT	ASTEC v2.02	3	Spain
EDF	MAAP 4.07	1	France
ENEA	MELCOR 1.8.5	1,2	Italy
ENEA	ASTEC v2.0	1,2	Italy
GRS	ATHLET/COCOSYS coupled	A	Germany
GRS	ATHLET-CD 2.2B	1,2	Germany
GRS	COCOSYS V2.4beta	3,4	Germany
IRSN	ASTEC v2.0 rev1 p2 beta	A	France
IRSN	ASTEC v2.0 rev2 p2/IODE*	4	France
NNL	INSPECT2k/IODAIR-v3	4	United Kingdom
NUBIKI	MELCOR 1.8.6YT	3	Hungary
RUB	ATHLET-CD2.2A	1,2	Germany
UNIPI	ASTEC v2.0 rev.2	1,3	Italy
UNIPI	MELCOR 1.8.5	1,3	Italy
USNRC	MELCOR 2.1	1	United States
VUJE	ASTEC v2.0 rev2 p1	A	Slovakia
TUS	ASTEC v.2.0	3,4	Bulgaria
KAERI	MELCOR 1.8.6 YT	1,2,3	Republic of Korea
RSE	ECART	3	Italy
RSE	MELCOR 1.8.6 YN	3	Italy
UJV	ASTEC v2.0 rev1 p2 beta	A	Czech Republic
UJV	ASTEC v2.0 rev1 p2 beta	3	Czech Republic
UJV	ASTEC v2.0 rev1 p2 beta	4	Czech Republic
UJV	MELCOR 1.8.6 YV patch 3481	1,2,3	Czech Republic
UJV	MELCOR 1.8.6 YV patch 3481	3	Czech Republic
KINS	MELCOR 1.8.5/RAIM	4	Republic of Korea

Phase: 1–4 = bundle, circuit, containment, chemistry respectively; A = all (full integral calculation); 26 calculations in all.
* Improved version intended for ASTEC v2.1.

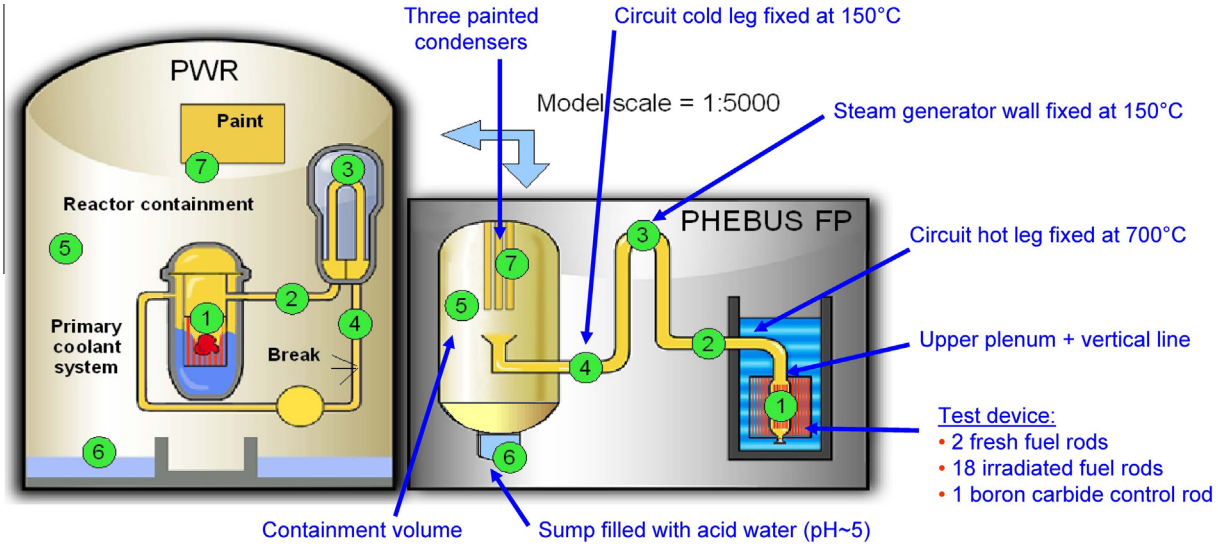

Fig. 1. Simplified layout of the Phébus FPT3 test train showing relationship with a LWR (Grégoire and Payot, 2009).

involved heating of the bundle through a succession of power ramps and plateaux, leading to an oxidation runaway, further ramps and plateaux leading to fuel melting and relocation, with the degradation phase being terminated by reactor shutdown at 17,370 s after the beginning of the heating phase, Fig. 2. At the end of this phase the total amount of hydrogen released was 120 ± 6 g (1 standard deviation), whilst the gas release coming from the B_4C oxidation corresponds to 16 g of carbon dioxide and 17 g of carbon monoxide. The release fraction of the main volatile FPs ranges between 64% for Cs to around 80% of the initial bundle inventory (i.i.) for I and Te, whilst the semi and low volatile FP releases show a wider spread. A remarkable feature of the experiment was the substantial fraction of volatilised materials (Cs, Ag, Mo, Ru, and Ba) which re-deposited on the intact upper part of the fuel rods (Grégoire and Haste, 2013).

The released material was swept by the coolant flow from the bundle through the experimental circuit; deposition of aerosol and vapour in some parts of the circuit was measured, as well as the flow rates of the different elements in the cold and hot legs. The deposition took place in the zones where thermal gradients were important, just above the fuel bundle and in the rising line of the steam generator. In this last zone, the mass deposited was enhanced by the formation of a boron-rich blockage, not prototypic in a reactor case (Haste et al., 2012a). The transported material was injected into 10 m^3 vessel, simulating the containment building of a nuclear power plant. The 37 h aerosol phase started at 22,500 s when the containment was isolated. Airborne aerosols were deposited mainly by gravitational settling on the lower surface of the vessel. After about 51 h from the beginning of the transient, the aerosols deposited on the containment floor were washed out into the sump water. The 2 days chemistry phase started at the end of the washing phase; it was devoted to the analysis of iodine chemistry under conditions representative of LWR severe accidents, emphasising iodine speciation. An important objective of the experiment was to study the iodine behaviour in the containment vessel, in particular the amount and speciation – inorganic versus organic – of volatile iodine in the atmosphere. Another remarkable feature of the experiment was the very high iodine gas fraction

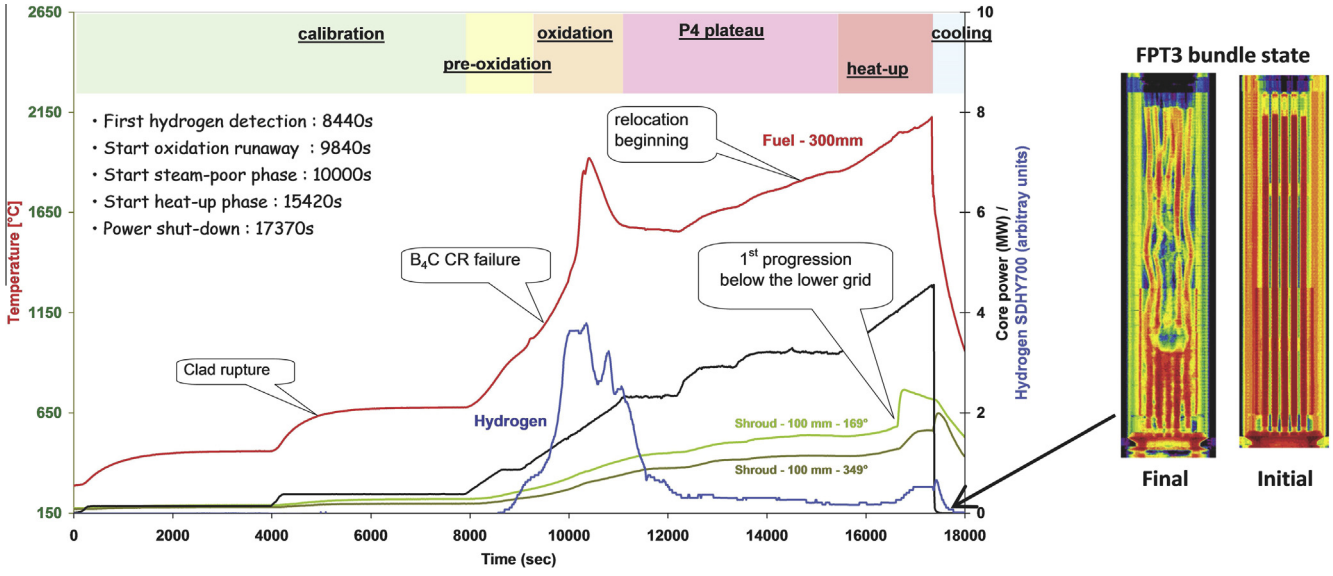

Fig. 2. Schematic test sequence for Phébus FPT3, with bundle initial and final states (adapted from Payot et al., 2011).

(~90%) entering the containment during the transient, which determines the iodine behaviour in the short term in the containment atmosphere. In the long term the gaseous inorganic iodine release from the deposited aerosols radiolytic destruction becomes the main inorganic gaseous iodine contribution in the gaseous phase whereas the gaseous organic iodides contribution comes mainly from the radiolytic reaction of I_2 with paints, leading to the formation of organic iodides (RI), (Simondi-Teissiere et al., 2013) .

4. Representation of the facility

A noding scheme was recommended in the specification report (Bieliauskas and Haste, 2011). In this scheme, the bundle is divided into 11 axial nodes whilst the number of radial rings is being left free as the number of thermal hydraulic flow channels. The minimum numbers of nodes recommended for the circuit was 12, in order to obtain an adequate calculation of deposition. For the containment model 14 nodes were suggested, but also 5 nodes could be used. This constituted the mandatory 'base case' calculation, in which it was intended that the participants would use code options as for a plant study. This nodalisation scheme proposed is representative for plant studies, and appeared adequate for assessment of the models relevant to the source term calculation. A more detailed 'best-estimate' sensitivity study could also optionally be performed. For this case, the noding density was increased by typically a factor 2 or more at the choice of the user, and code options could be chosen to give a better match between calculated and observed results.

5. Analysis of results

The results were analysed in detail, comparing the results amongst each other and with FPT3 experimental data. There was considerable scatter amongst the results obtained from each code by different users, the 'user effect', as noted for example in the SARNET benchmark based on the THAI experiments Iod-11 and Iod-12 (Weber et al., 2013; Haste et al., 2014). To minimise this effect, representative cases were selected where necessary, taking into account the quality of key output variables, completeness and accuracy of the technical reports, and including code developers where possible. This analysis led to an assessment of the main models in each of the four areas considered. The results are subdivided according to the four phases mentioned above. The best estimate cases simulations were plotted together with those of the base cases, given that the differences observed are not particularly significant. The impact of the results on research programmes is considered in an Appendix to this paper.

5.1. Bundle phase

The physical phenomena occurred in this phase are strictly related on the bundle thermal behaviour. Indeed the bundle degradation process is a critical factor in the progression of a severe accident. This process provides also the initial conditions for subsequent phenomena within of the primary circuit and the containment vessel. This is the reason why a correct prediction of the fuel rod temperatures is essential for an accurate calculation of the bundle degradation and fission product release; similar remarks also apply to the control rod degradation for structural material release that forms the large part by mass of the aerosols transported into the circuit. Most of the participants assumed a reduction of the input nuclear power by about 10% and an increase of the shroud thermal conductivity, both within the experimental uncertainties. With these assumptions, the thermal behaviour of the fuel rods is rather well reproduced by the codes. The comparison between measured fresh fuel temperatures and calculated results are illustrated in Figs. 3 and 4 for an axial elevation of 500 mm and 300 mm respectively. The appreciable discrepancies, during the thermal calibration of the bundle (until 7920 s) are mainly due to the lower input power selected for the simulation during this phase, whilst throughout the degradation phase a generally good overall agreement is observed up to the shutdown of the nuclear power at 17,370 s.

The total hydrogen production, which took account of the hydrogen generated by the boron carbide control rod oxidation were well captured. The results given by different code simulations are consistent with the experimental value (120 ± 6 g); the beginning of the run-away phase is rather well described, whilst the steam starvation duration tends to be in general overestimated,

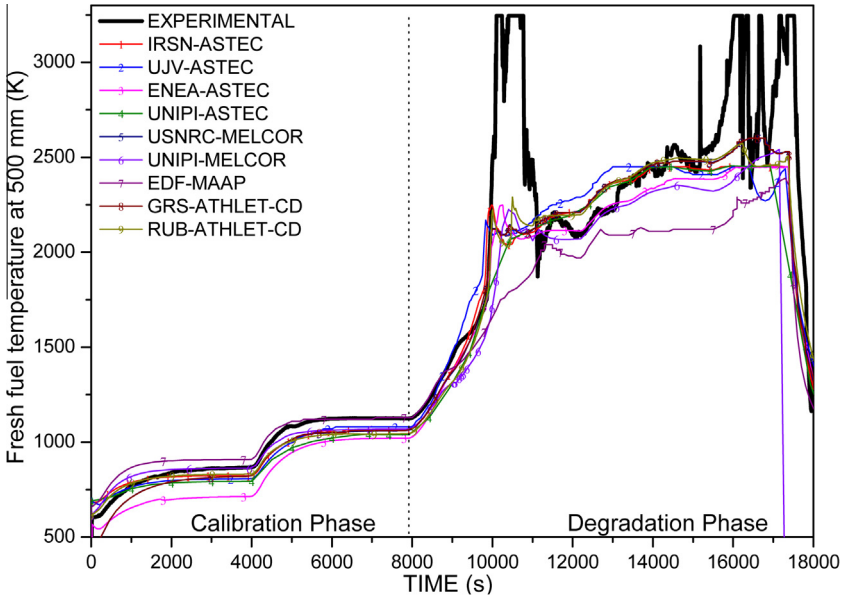

Fig. 3. Fresh fuel temperature at 500 mm axial elevation.

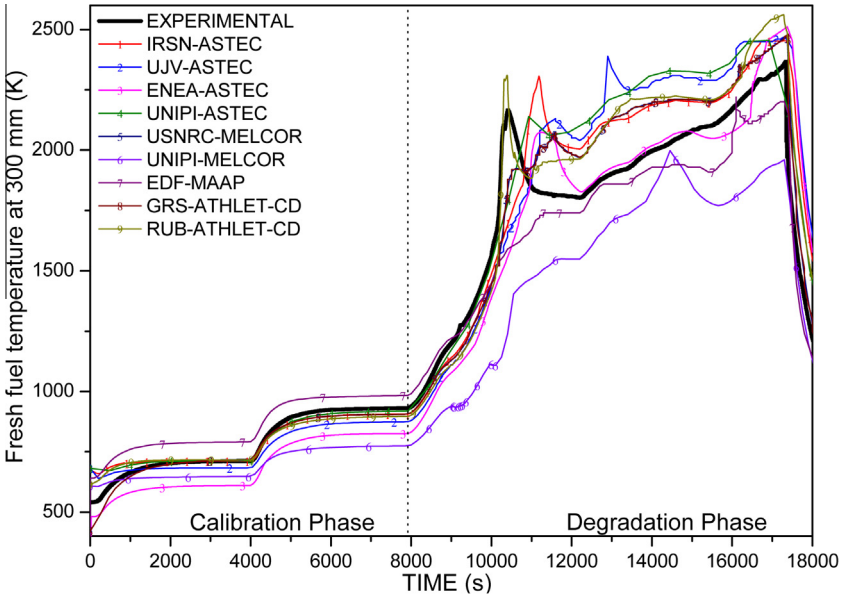

Fig. 4. Fresh fuel temperature at 300 mm axial elevation.

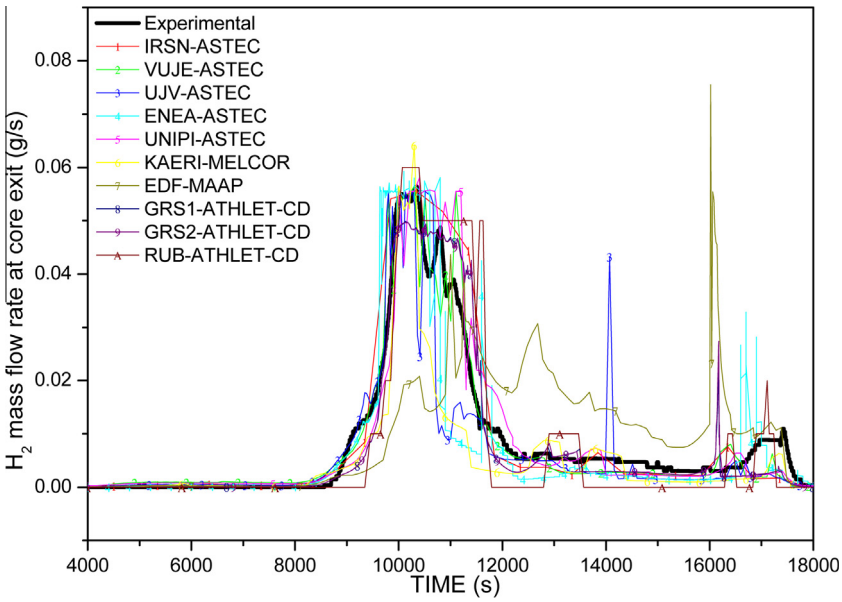

Fig. 5. Hydrogen mass flow rate.

Figs. 5 and 6. As it is possible to see in Fig. 5, the code results show steam starvation for the bundle after 10,200 s.

Although the bundle temperature evolution is quite well calculated, there are still great difficulties to reproduce the final degradation state of the bundle, Fig. 7. The FPT3 test is the only test of the Phébus FP programme which used a B_4C control rod. The suspected effects of spreading molten materials of the control rod towards fuel rods of the bundle and the B_4C-SS (boron carbide-stainless steel) eutectic formation and liquid B_4C-SS-Zr relocation, are not accounted for in the codes, these phenomena cannot be neglected to simulate the observed bundle degradation behaviour.

The need for further code developments of the early phase of core degradation is recognised for the absorber rod material behaviour (Repetto et al., 2010). Therefore extensive programmes of separate-effect experiments have been performed, such as ISTP/BECARRE at Cadarache by IRSN (Clément and Zeyen, 2005; Dominguez and Drouan, 2014) under the International Source Term project and BOX, LAVA and QUENCH-SR at the Karlsruhe Institute of Technology (KIT), (Steinbrück, 2010) to enable a better understanding of B_4C oxidation and interactions with cladding materials. As regards the control rod, the cumulative boron release is illustrated in Fig. 8. The results show a wide spread, mainly due to the model adopted by the users notably for MELCOR, nevertheless the boron cumulative releases predicted by the ASTEC and ATHLET-CD codes are within a range of ±10%, even if the calculated kinetic of releases do not match the experimental data.

The carbon gas speciation (CH_4, CO, CO_2) following the B_4C oxidation needs attention. The CH_4 production was correctly calculated as being low, but the fact that CO production is favoured in steam-poor periods (<~11,000 s) and CO_2 in steam-rich

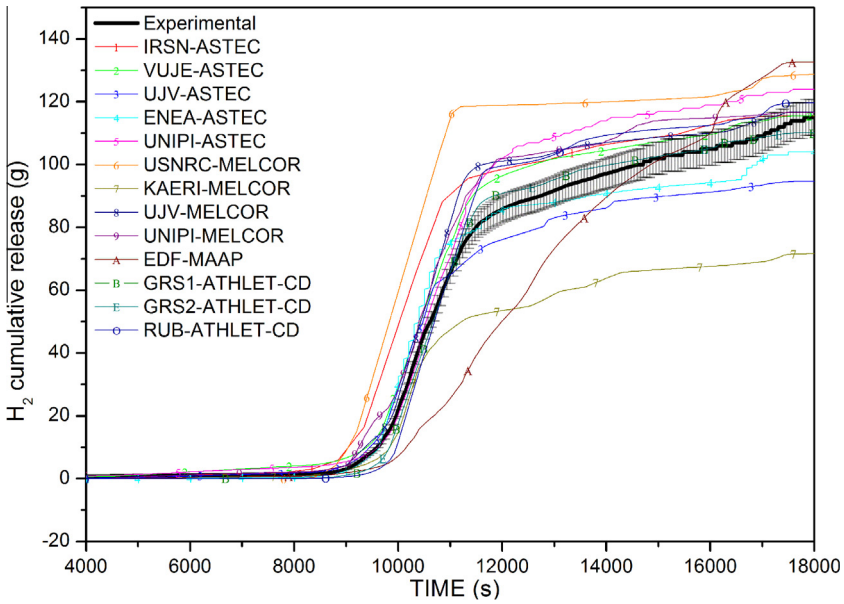

Fig. 6. Hydrogen integrated production.

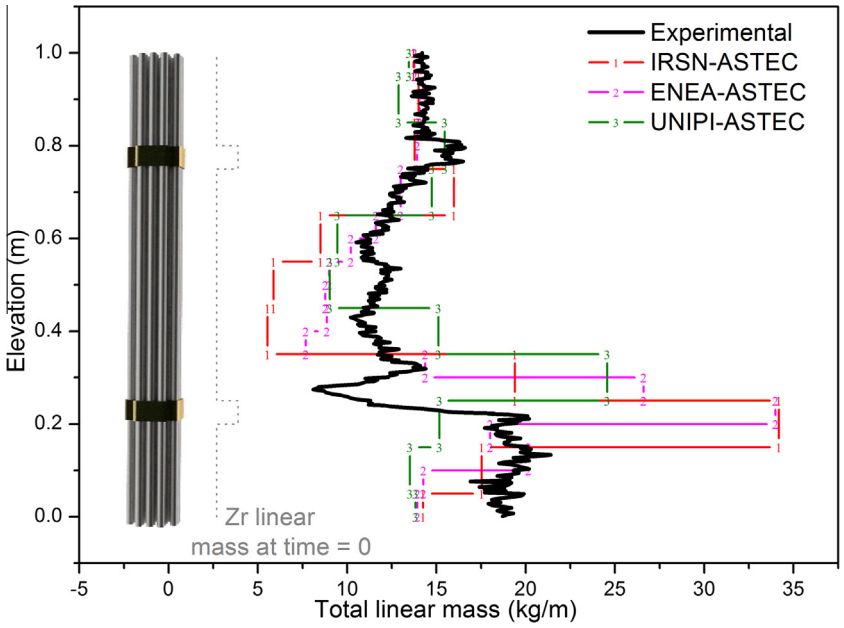

Fig. 7. Bundle final linear axial mass distribution.

(>~11,000 s) periods is not well captured. The calculated releases for carbonaceous gases are illustrated in Figs. 9 and 10 for CO and CO_2 respectively. The wide scatter in results indicates that the current models need improvement

The ASTEC code, unlike the other integral codes; does not discern CO from CO_2 because of the parametric simplified semi-empirical approach which has been adopted.

The FP release from intact fuel followed by the release from the in-core molten pool depends mainly on temperature and oxygen potential but also on various physical and chemical processes that occur within the fuel matrix and in the surrounding gaseous atmosphere. In the FPT3 test, the main fission products were basically classified according to the results from the VERCORS programme (Ducros et al., 2013). The results from VERCORS and Phébus FP were found to be mainly consistent. The resulting classification is the following:

- Noble gases: Xe, Kr.
- Highly volatile fission products: I, Cs, Rb, Te, Sb, Ag.
- Semi-volatile/low volatile fission products: Mo, Ba/Ru.

In this experiment, the silver is released only as a fission product; whilst in the previous Phébus tests, the Ag release was dominated from that coming from the Ag/In/Cd control rod there present.

Concerning the bundle release, all the experimental data were used for cross-checking, for statistical treatment, and for overall

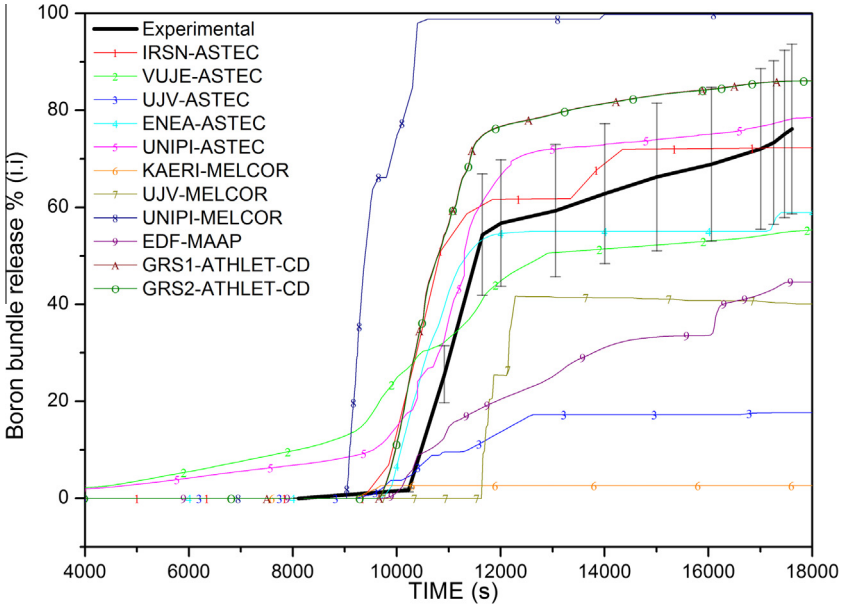

Fig. 8. Boron release from the bundle.

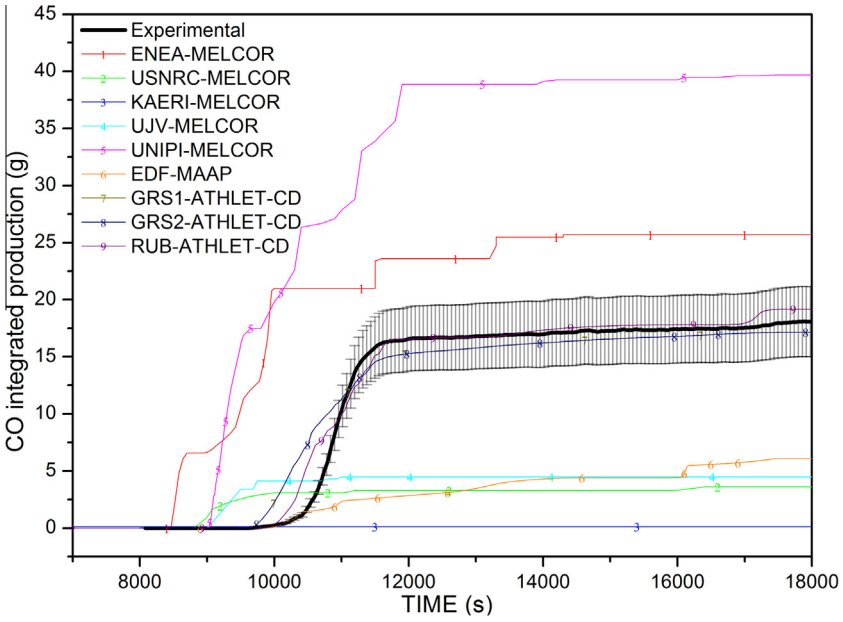

Fig. 9. Carbon monoxide integrated production.

accuracy estimation. As a result the measured data fall within an estimated error band of ±16% for gamma emitters (I, Te, Cs, Ag, Ru, Ba) and ±20% for Mo.

An important feature in noted in the FPT3 post-test analysis was the significant deposition of several elements on the upper part of the fuel rods, see Table 2. The lower coolant flow, along with the moderate bundle degradation in the test, favoured these depositions. In order to take into account this phenomenon the reference value used in the benchmark for Mo, Ba, Ru and Cs elements was the fuel release (bundle release + deposition in the bundle upper part).

Concerning the high volatile fission products; the total amounts released predicted by the codes are in agreement with experimental data, but generally the kinetics of release are too quick, see Fig. 11 for iodine, and only the caesium release tends to be overestimated, see Fig. 12. The release of medium and low volatiles needs attention. The predicted results for molybdenum disagree with the measured data, showing a general tendency to overestimate the cumulative release. As seen in Fig. 13, the bundle and the fuel release show a large discrepancy, 23% and 53% respectively, thus approximately 30% of the Mo initial inventory is deposited in the upper part of the bundle; revaporisation of these deposits is possible later. Most of the codes cannot compute deposition in the upper part of the bundle, which affects strongly the total bundle release, in particular for Mo, Ru and Ba, but also for the volatile Cs. Models that consider this phenomenon are necessary. MELCOR

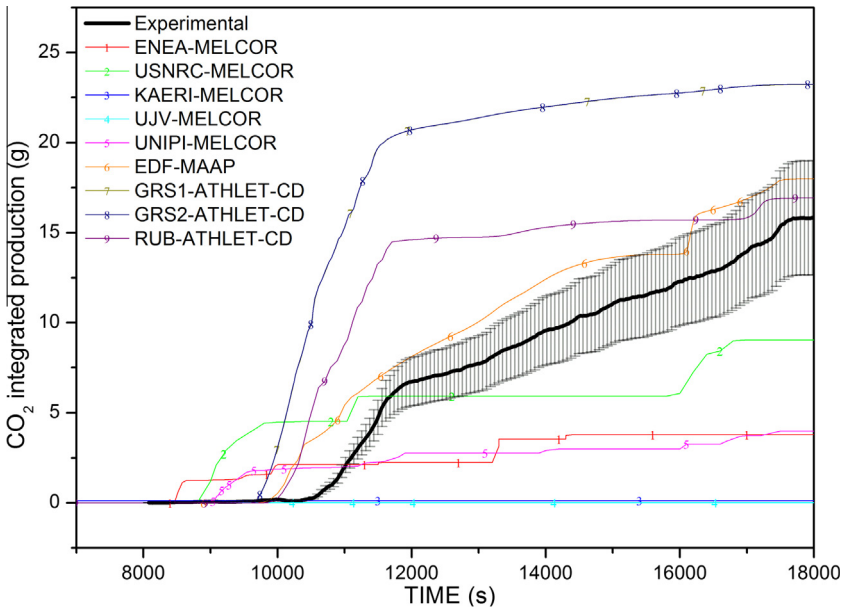

Fig. 10. Carbon dioxide integrated production.

Table 2
Release of fission products, actinides and structural materials in the Phébus FPT3 experiments.

Released element	Bundle release (% initial inventory)	Deposition in the bundle upper part (% initial inventory)	Fuel release (% initial inventory)
Noble gases			
Kr	72	0	72
Xe	84	0	84
Volatiles			
Cs	64	9	73
I	79	1	80
Te	80	1	81
Sb	40	n.d	40
Ag	70	27	97
Rb	35	n.d	35
Cd	>40	n.d	>40
Semi/low volatiles			
Mo	23	30	53
Ba	6	5	11
Ru	1	7	8
Sr	0.05	n.d.	0.05
La	>0.059	n.d.	>0.059
Ce	0.28	n.d.	0.28
Actinides			
U	>0.011	n.d.	>0.011
Pu	>0.0009	n.d.	>0.0009
Control rods and structural materials			
B	78	n.d.	
Sn	>29	n.d.	

n.d. = not detected.

is the only code which can discriminate between the bundle and fuel release, but no participant provided this parameter. Concerning Ba and Ru, the calculated releases vary greatly, ranging from quite good to very poor agreement with the data.

The good predictions of hydrogen production as well as the total amount of high volatile FPs released are important from the point of view of reactor safety. The semi-volatile and low-volatile results are mainly consistent concerning the total amount released, but no code can predict correctly the release of all of these elements (Di Giuli et al., 2013). The release models could be improved; because a correct prediction is of extreme importance, either due to their radio-toxicity and influence on the residual power, or by their propensity to react with other fission products. The same considerations apply for structural materials, although they have no direct radiological significance, they potentially react with fission products, and their source terms are therefore necessary for accurate calculation of chemistry and transport in the circuit. Furthermore, the structural materials also form the bulk of the aerosol mass, affecting the aerosol concentration and the agglomeration processes. The user influence on predicted results can be noticed in most of the MELCOR cases, whilst ASTEC and ATHLET-CD submissions show only small differences amongst themselves.

5.2. Circuit phase

The injected steam flow swept FPs and structural materials from the degrading fuel bundle through the circuit into the containment vessel. They were quantified by online instruments and by post-test analyses of the samples collected during the test. The experimental results have shown that all condensable FPs are transported through the simulated primary circuit in aerosol form, except iodine and cadmium that were detected mainly in gaseous form (Haste et al., 2013). On their way through the primary circuit, the aerosols tend to deposit mainly where the temperature of the wall and fluid decrease strongly or where the flow is diverted: above the bundle, in the so-called upper plenum and vertical line and in the upstream part of the steam generator tube.

The analyses of FP and structural material transport in the Phébus FPT3 tests for the entire circuit with the integral codes showed that the total deposited mass is underestimated on average by a factor 1.5, as shown in Fig. 14. A remarkable feature of the FPT3 test was the large deposition of boron-containing material between the hot leg and cold legs, with the potential of forming a partial blockage in the circuit (Haste et al., 2012a). This is an artefact of the experiment and not typical of reactor conditions. The main effect of this phenomenon was the reduction of the tube section, and the increase of the deposition surfaces, both effects enhance the FP retention in the circuit zones involved, notably in

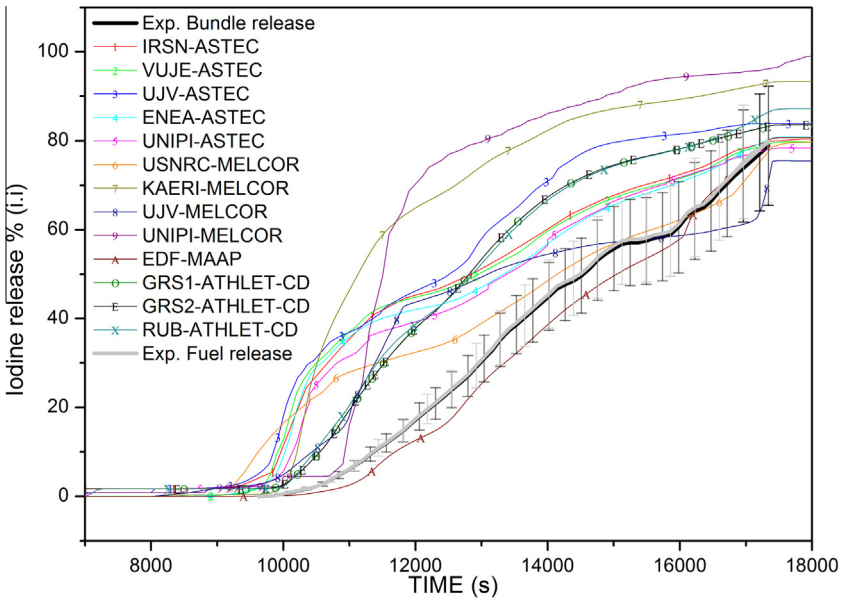

Fig. 11. Iodine release from the fuel and bundle.

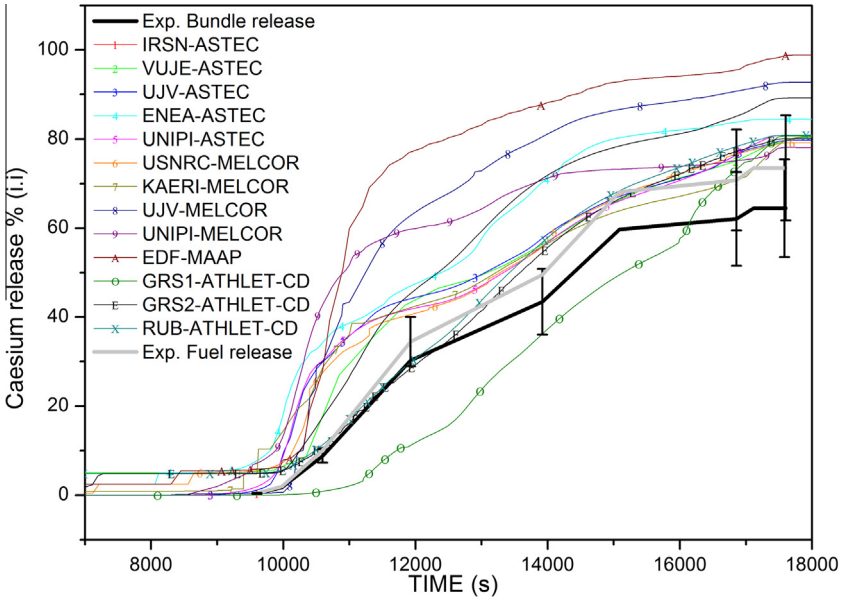

Fig. 12. Caesium release from the fuel and bundle.

upstream of the SG. No code could reproduced these conditions and thus, the submitted results tend to underestimate the overall mass retention in the circuit. The boron deposition in the primary circuit is not considered so important regarding plant safety assessment. In a commercial PWR, the number of SG tubes is around 5000, and it is very unlikely that the boron contained in the water and in the control rods would form blockages in all the tubes at once. In the Phébus FPT3 facility using only a single tube this phenomenon is more important and for a correct analysis of the results it would be necessary to take the boron-rich blockage effect into account. Nevertheless, further difficulties were also observed in capturing the thermophoretic deposition in the upper plenum for elements as Cs and Te, see Fig. 15, despite that the steam temperatures along the circuit were well predicted by most of the contributions. These discrepancies are mainly due to the wrong prediction or assumption of the chemical form of the FPs, and therefore their volatility. However, this is also not enough to explain the differences in the upper plenum. As regards molybdenum, the general overestimation of its bundle release led the Mo calculated total deposition along the circuit to be in agreement with that measured.

It is worth noting that work is already in progress to improve FP transport and deposition modelling in various codes. Regarding speciation, account is taken of the importance of caesium molybdates, whilst borates are also being considered. Similarly, in MELCOR 2.1, caesium molybdate has been introduced as the default fission product class for Cs (Ross et al., 2014; Herranz et al., 2015).

5.3. Iodine behaviour in the circuit

The Phébus FPT3 test clearly provided new insights into the iodine transport through the primary circuit during a core

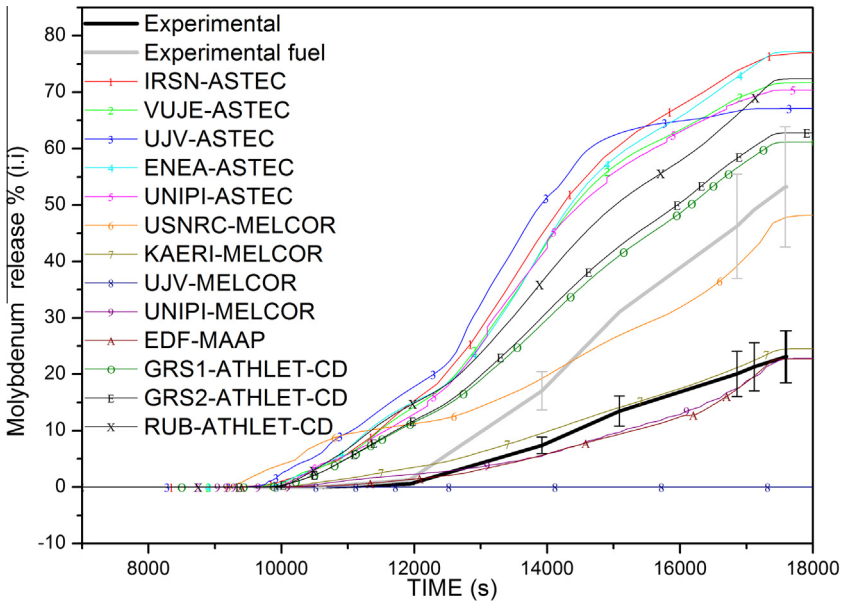

Fig. 13. Molybdenum release from the fuel and bundle.

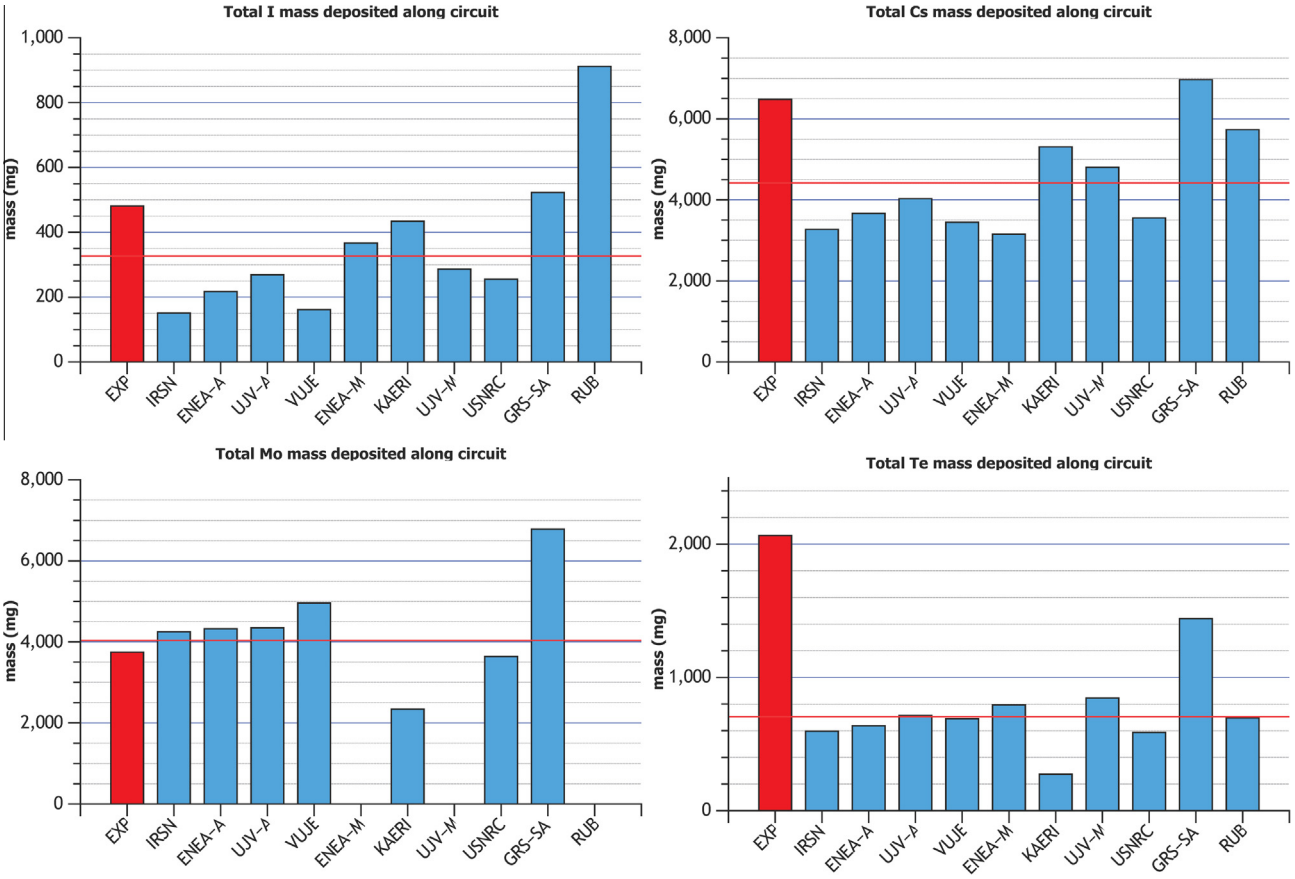

Fig. 14. Overall mass retention of the fission products I, Cs, Te, Mo in the circuit.

meltdown accident for the iodine vapour speciation and for the transport of fractions of gaseous iodine into the containment. The circuit measurements for iodine were made with a total mass balance of only 68.1%, this lack of mass balance made difficult a detailed comparison between experimental data and calculated results. Generally, the iodine mass retention factor of the circuit has been underectimated on average by 40%. The measured gaseous iodine fraction entering the containment was about 95%,

the highest amongst the Phébus FP tests carried out, whilst the submitted results predicted values around 2%. This discrepancy has proved that the codes using models based on equilibrium thermochemistry and/or user-defined fixed speciation are not able to predict the chemistry phenomena occurring during this kind of transient, where it is suspected that non-equilibrium effects played a fundamental role, as indicated by existing studies for iodine (Herranz et al., 2015). In order to improve the modelling of iodine chemistry in the primary circuit, particularly concerning the kinetics, new modelling of kinetic limitations regarding iodine reactions is in progress in the ASTEC/SOPHAEROS module.

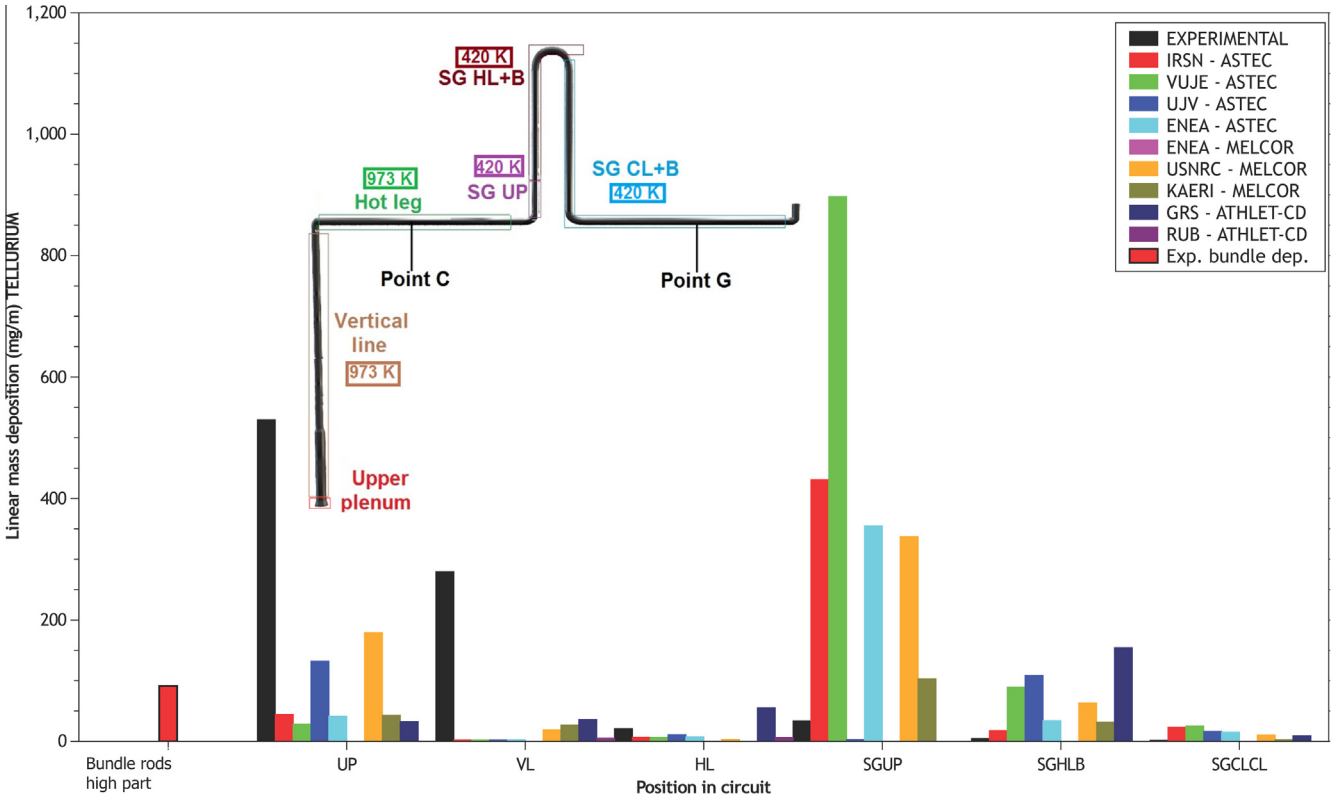

Fig. 15. Tellurium linear mass deposition along the circuit.

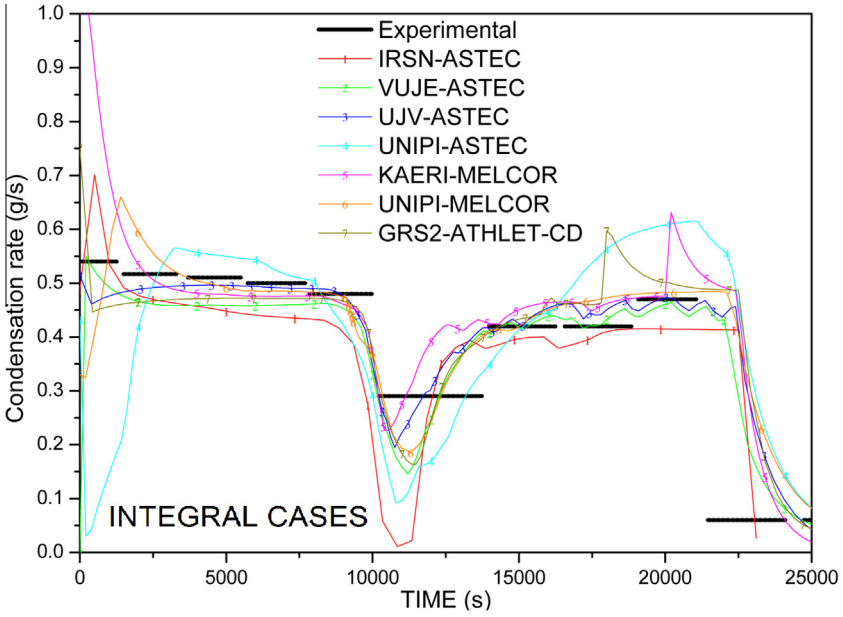

Fig. 16. Containment condensation rate, integral cases.

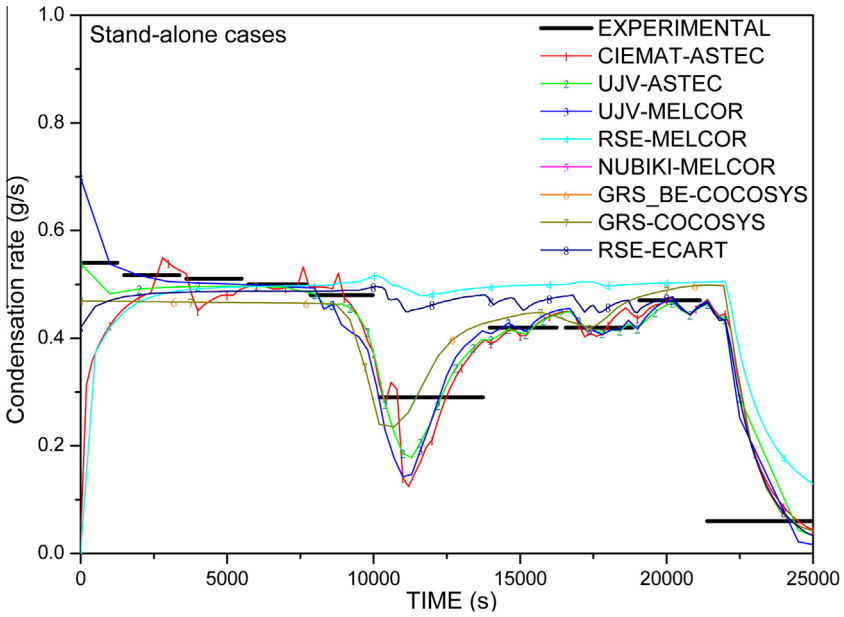

Fig. 17. Containment condensation rate, stand-alone cases.

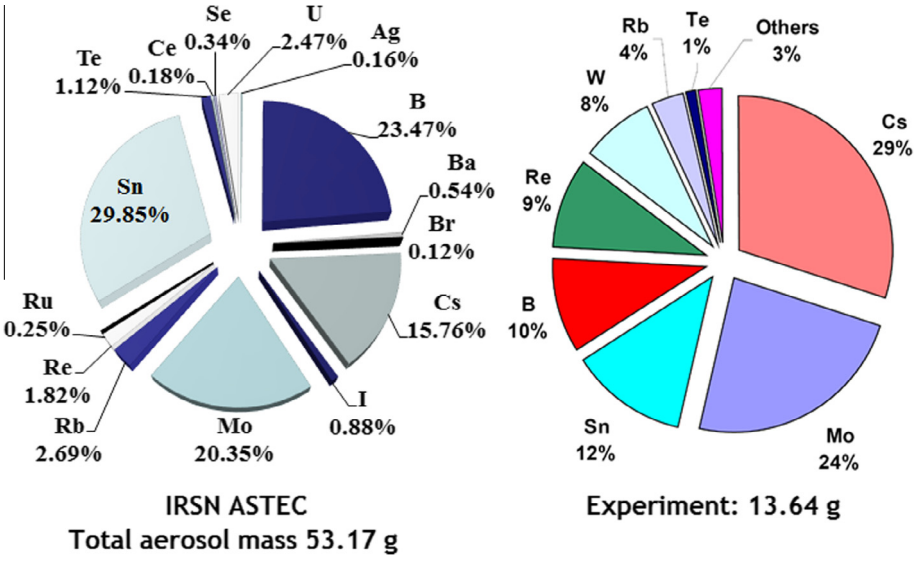

Fig. 18. Aerosol speciation and mass entering the containment.

5.4. Containment phase

The study of the thermal hydraulics in the containment is not a major objective of the Phebus-FPT3 experiment. The Phébus FP containment model was designed in order to get relatively simple (well-mixed) thermal hydraulic conditions, with sufficiently well-known boundary conditions in order to focus on the study of fission products behaviour, involving both aerosol physics and chemistry. The prediction of the thermal hydraulic parameters in the containment as temperature, pressure, condensation rate, humidity, etc. was in general satisfactory and, the small differences observed had probably only a weak influence on aerosol physics calculations, see Figs. 16 and 17 for the condensation rate for the integral and stand-alone cases respectively. In the case of the stand-alone calculation the boundary conditions come from the experimental data, thus the composition, physical form (aerosol, gas) and mass flow rate entering the containment as a function of time along with the measured temperatures inside the containment are provided to the participants as input data.

The evolution of the aerosol airborne mass largely depends on the quality of structural material (SM) and FP (Cs, Mo) release and transport calculations, for the integral submissions. All the integral calculations tend to underestimate the total structural material and FP deposition in the circuit and to overestimate the Mo and Cs releases, this combination (along with the boron blockage effect mentioned above) does not allow a correct prediction of the total airborne mass entering the containment, making the calculated integral results unreliable, Fig. 18.

Figs. 19 and 20 show the aerosol airborne mass inside the containment atmosphere during the transient, for the integral and

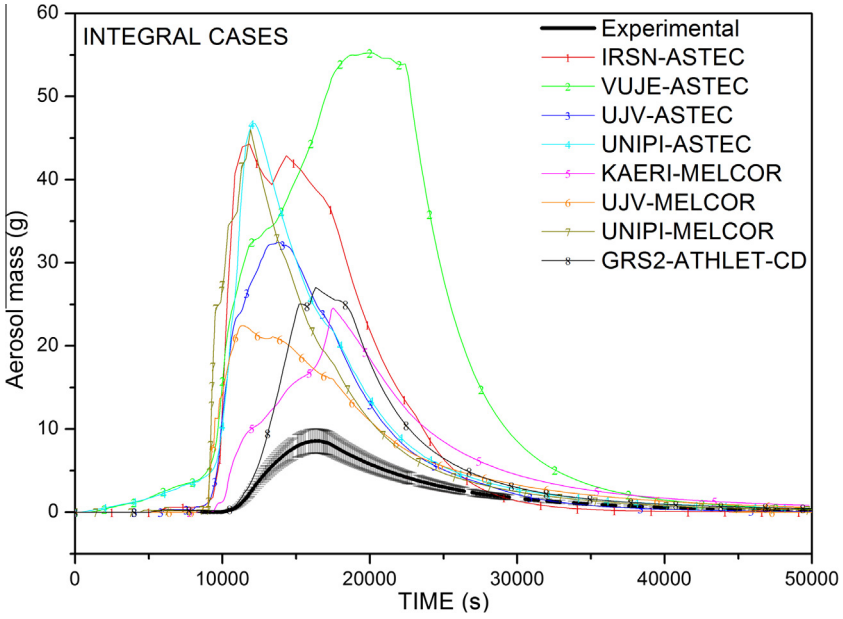

Fig. 19. Total aerosol airborne mass in the containment, integral cases.

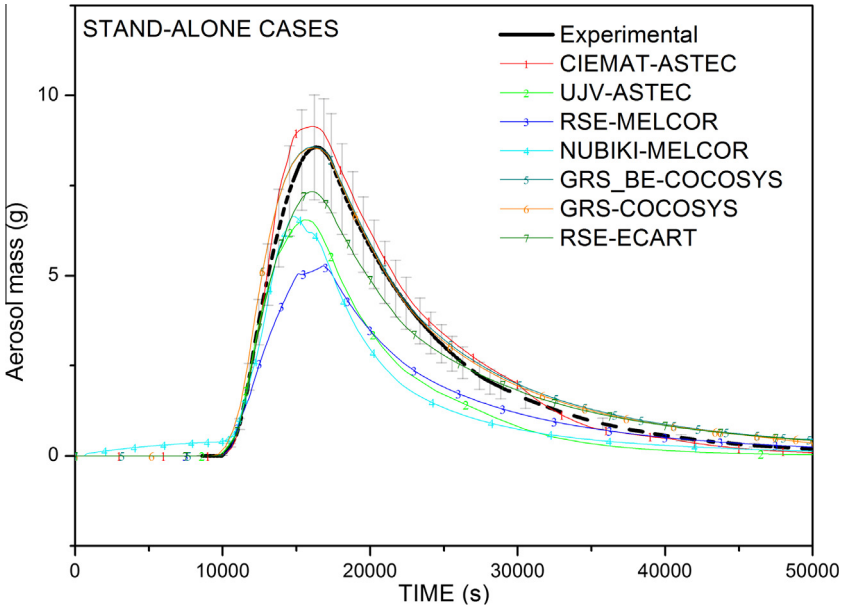

Fig. 20. Total aerosol airborne mass in the containment, stand-alone cases.

stand-alone cases respectively. For the stand-alone calculation (using as input the experimental data), there is less than a factor 2 between the experimental data and calculated aerosol concentration. Regarding the integral calculations, there is a significant overestimation of the total aerosol mass entering the containment (up to a factor 5), the higher concentration of aerosol leads to more agglomeration in the containment and to an overestimation of the depletion rate up to a factor 3. Given this discrepancy, no clear conclusion could be drawn on the relative importance of the main depletion processes in the experiment (diffusiophoresis and gravitational settling) for the integral cases; the results predict a greater deposited mass by gravitational settling than by diffusiophoresis at least 7 times greater, as against about 2 times greater in the data. This merits further investigation.

5.5. Chemistry phase

The dominant phenomena for iodine chemistry in the containment during FPT3 test were:

- The fraction of iodine exiting the circuit in the gaseous phase.
- The interaction of iodine with painted surfaces, including adsorption, desorption, and organic iodide formation and destruction.

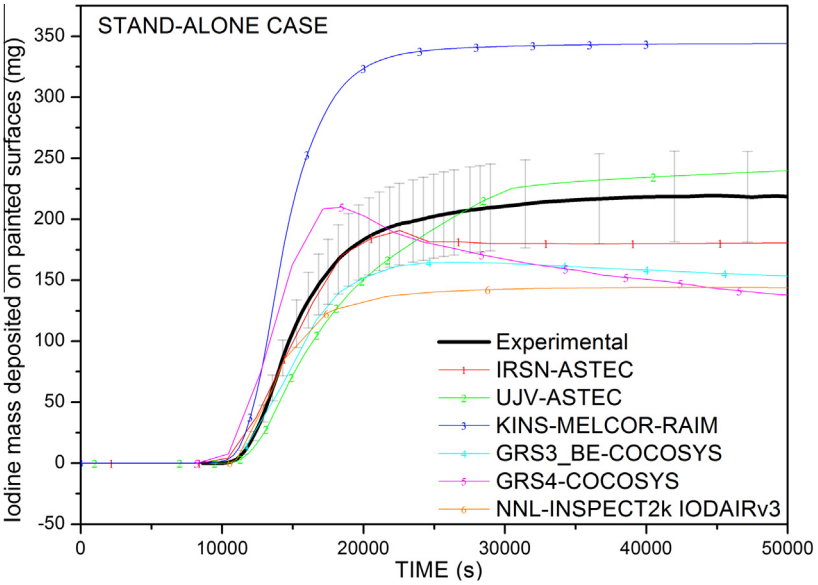

Fig. 21. Iodine mass deposited on painted surfaces in the containment, stand-alone cases.

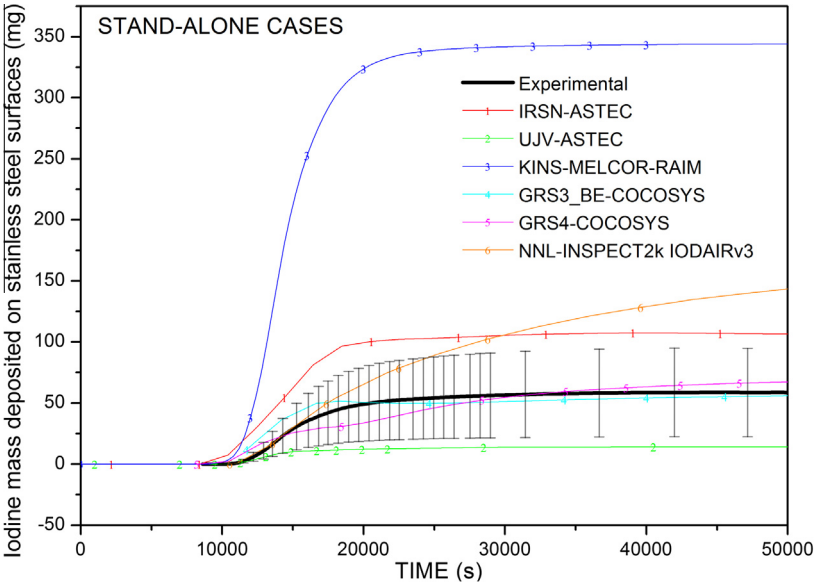

Fig. 22. Iodine mass deposited on stainless steel surfaces in the containment, stand-alone cases.

- The destruction of iodine species in the atmosphere by radiolytic processes, leading to iodine oxide aerosol formation (Bosland et al., 2008, 2010, 2011).

All of these have a strong influence on the gaseous iodine concentration in the containment atmosphere, which is one of the most important safety-related parameters. For the integral cases, the first phenomenon is very difficult to predict, because 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 atmosphere that is a key factor for safety studies. Iodine interaction with painted surfaces and the destruction by radiolytic processes determine the quasi steady-state level in gaseous iodine concentration measured in the experiment before and after the washing phase. Regarding the transport of gaseous iodine in the primary circuit, none of the codes is able to reproduce what was experimentally observed, even those having chemistry modelling. Given this difficulty in predicting the iodine source to the containment in the integral cases, only the stand-alone cases with iodine source input based on the test data were analysed.

The iodine deposition on painted surfaces, 54% containment inventory, was well predicted, Fig. 21, as well as the iodine deposited on stainless steel surfaces, Fig. 22, whilst there were greater discrepancies with the organic iodine fraction in the gas phase, Fig. 23 (from iodine interactions with paint in the long term) with a tendency to overestimation in the long term. The organic iodide (RI) is more difficult to remove by containment sprays or by filtration than I_2, in any case the results are conservative. Inorganic iodine was rather better predicted than organic iodine, Fig. 24. Overall, the behaviour of gaseous iodine in the containment,

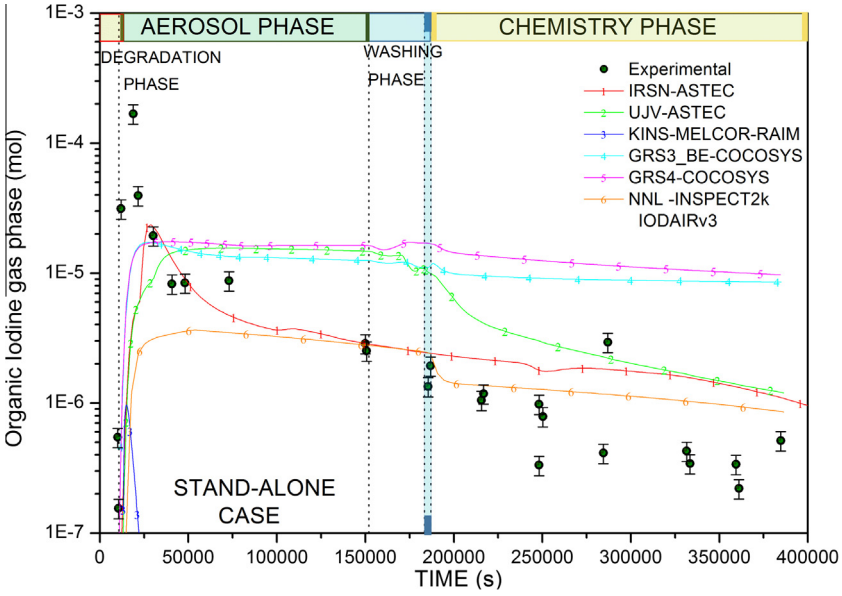

Fig. 23. Organic iodine mass in containment atmosphere gas phase.

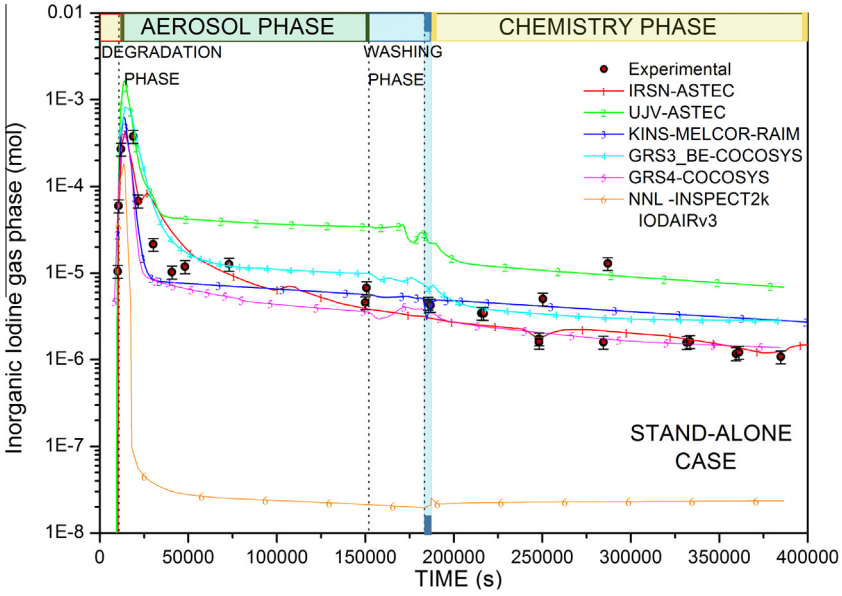

Fig. 24. Inorganic iodine mass in containment atmosphere gas phase.

assuming that its predominant form entering the containment is inorganic, is quite satisfactorily reproduced in the better code calculations.

6. Conclusion

The SARNET benchmark on Phébus FPT3 has provided many insights on the ability of severe accident codes to calculate the different phases of an accident sequence in an integral manner. A significant 'user effect' as observed (i.e. different users calculating different results with the same code), as seen also for example in the SARNET benchmark based on THAI experiments Iod-11 and Iod-12, and this was taken into account in analysing the results.

Several areas where code improvements are recommended have been identified, the main ones involve:

- Improvement in models taking into account the boron-stainless steel–zirconium interactions during core degradation.
- A better estimation of structural material release, especially for tin from Zircaloy cladding, and of semi/low volatile fission product release.
- The possibility to take into account the presence of gaseous iodine in the RCS.

The areas identified where modelling improvements are recommended have been or are being covered by relevant experimental programmes, which can form the basis for such code developments, e.g. for kinetics of iodine reactions in the primary circuit, see the Appendix to this paper. When these have been completed, new benchmarks based on Phébus FP data (e.g. comparing predictions on FPT1, FPT2 and FPT3 under the same modelling assumptions) and on THAI (e.g. on THAI-Iod30 where painted surfaces

were introduced) are planned to assess this progress using independent data, and to see what further research needs to be done, for example under the aegis of the NUGENIA Association (www.nugenia.org). In formulating these benchmarks, the need to account for user effects as noted here and in the THAI Iod-11/Iod-12 benchmark will be carefully considered.

Acknowledgments

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Appendix A. Impact on future research programmes

In order to gain more understanding about severe accident phenomena and to improve code models, international experimental programmes have been/are being carried out. For the effects studied in FPT3, and more generally in Phébus FP, the most relevant are:

- BECARRE experiments (2005–2010) performed by IRSN (Dominguez and Drouan, 2014) in the framework of the International Source Term Program (ISTP) (Clément and Zeyen, 2005), devoted to boron carbide effects on core degradation, as well as corresponding tests carried out at Karlsruhe Institute of Technology (BOX, LAVA, QUENCH-SR) under the German national programme (Steinbrück, 2010).
- VERDON series (Ducros et al., 2013), being performed by CEA under ISTP, and the completed VERCORS series (Pontillon et al., 2010) also by CEA, which study/studied fission product (FP) release and transport.
- CHIP program being performed by IRSN along with smaller scale circuit tests (Haste et al., 2012b; Gouello et al., 2013), the first series being completed under ISTP, to provide data on the physico-chemical transformations of iodine in the primary circuit, including kinetics, for example considering the systems {Mo, Cs, I, O, H} and {B, Cs, I, O, H}.
- EPICUR experiments, performed by IRSN under ISTP (Haste et al., 2012b) and continuing under the OECD/STEM project (www.oecd-nea.org/nsd), OECD/BIP projects on behaviour of iodine in the containment (Glowa et al., 2013), and the earlier PARIS project (Bosland et al., 2008, 2011), completed by AREVA in collaboration with IRSN to provide experimental data on the physicochemical transformations of iodine (formation and destruction of volatile iodine species) under irradiation in the reactor containment (Guilbert et al., 2008). Particular importance is accorded to the absorption/desorption of iodine on painted surfaces under irradiation (Bosland et al., 2014), to the stability under radiation of deposited iodide aerosols and to gas phase iodine oxidation reactions (Dickinson et al., 2014).
- THAI experiments, performed by Becker Technologies and their predecessors under German national funding (Weber et al., 2010a,b) then/now under OECD projects (www.oecd-nea.org/nsd), on the effects of thermal hydraulics on iodine behaviour and on iodine interactions with surfaces and aerosols in the containment.

These concern source term, with the exception of the first. Other priority research areas identified in SARNET indicated in the review of (Klein-Heßling et al., 2014), such as reflood behaviour, in-vessel melt retention generally, and ex-vessel phenomena such as molten-core concrete interactions, are out of scope here, as these issues are not addressed in the Phébus FP programme. Examples regarding how all available data are taken into account regarding code validation and development are given in (Chatelard et al., 2014b) for the ASTEC code, a similar approach is adopted elsewhere for the other codes considered.

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