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# Fission product modelling in ASTEC

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**Abstract:** Modelling fission product (FP) behaviour during severe light-water reactor accidents covers a considerable diversity of phenomena such as solid-state diffusion, high temperature chemistry, aerosol physics and radioiodine chemistry. Over a number of years IPSN developed computer codes for modelling FP behaviour where, now, improved versions of these are included in the integral code ASTEC, jointly developed by GRS and IPSN. Whereas ASTEC models a whole accident sequence, this paper describes just its FP modules: ELSA for release from the core, SOPHAEROS for radionuclide transport in the reactor coolant system and IODE for radioiodine behaviour in the containment building. The approaches used aim to provide reliable indications of FP behaviour without excessive calculation times. This said, the degree to which modelling is simplified to render calculations faster must be compatible with the level of confidence required in the predictions.

Based on results of validation campaigns of the FP models in ASTEC V0 and in the context of needs arising from analyses for probabilistic safety assessments, further essential modelling improvements are being made for integration in ASTEC V1. Recent enhancement of ELSA has improved prediction of semi-volatile FP (e.g., Ba, Sr, Mo, etc.) release from solid fuel and included release models for degraded-core geometries and control rod materials. Enhancement of SOPHAEROS concerns improved numerical efficiency, addition of a new, comprehensive thermochemistry database and inclusion of a pool scrubbing module. As for IODE, developments focus on the formation of organic iodine due to paints and gas-phase destruction mechanisms of organic iodides. Beyond the above developments, principal areas are identified where improvements are still required.

## 1. INTRODUCTION

Nuclear power plant safety studies include very low probability events, that may lead to severe accidents. Accident scenarios, involving breach of the reactor coolant system (RCS) and, in some scenarios, loss of safety systems, are analyzed for potential emissions of radionuclides to the environment. Thus, modelling of radionuclide behaviour in the diverse conditions of an accident is an essential feature of evaluating the masses and physico-chemical forms of released radionuclides, the so-called source term. This modelling entails coverage of a multiplicity of phenomena including fields such as solid-state diffusion, high temperature chemistry, thermal hydraulics, nucleation, aerosol physics, bubble hydrodynamics and radioiodine chemistry.

Over a number of years IPSN developed computer codes modelling radionuclide behaviour in severe light-water reactor accidents for inclusion in the integral severe-accident code ESCADRE. Now, improved versions of these codes are included in the integral code ASTEC [1,2], jointly developed by GRS and IPSN. While an integral code aims to model a whole accident sequence by taking account of all major phenomena that can occur, the impact of emergency systems included, this paper focuses on the modelling required for dealing with radionuclide behaviour. The status and current developments are presented for the main ASTEC modules concerned: ELSA for releases from the reactor core, SOPHAEROS for radionuclide transport in the RCS and IODE for radioiodine behaviour in the reactor containment building. We note that modelling of radionuclide decay and activity in the

RCS, containment and environment (ASTEC module ISODOP) and aerosol behaviour and FP distribution among different media - "hosting" - in the containment (ASTEC module CPA, also dealing with containment thermal hydraulics) are not described in this paper. The semi-empirical and mechanistic approaches used in the ELSA, SOPHAEROS and IODE modules are described while it is stressed that the objective is to provide reliable indications of radionuclide behaviour within a reasonable calculation time, i.e. the modelling embodied by the codes must be suited to routine use in reactor analyses. This said, the degree to which modelling is simplified to render calculations faster must be compatible with the range of conditions to be covered and the level of confidence required in the predictions.

The modelling required for the different situations encountered in a severe accident are outlined below along with a summary of the validation studies that have been performed. In conclusion, the main areas where improvements are still required are indicated.

## 2. IN-VESSEL RELEASE

Radionuclide release, particularly release of fission products (FPs) from solid fuel, involves intricate processes which lead to significant calculational complexity when modelled fully. However, the need here comprises adequate coverage of a range of configurations leading to release while minimizing recourse to onerous models. In ASTEC, release is dealt with by the ELSA code where the modelling principal is to simplify considerably by only taking account of limiting phenomena governing release in typical accident conditions. Particularly in relation to solid fuel, this simplification can obviate much physical insight into release processes and requires that caution be exercised if atypical conditions (e.g. fast temperature transients) are examined.

Release from intact fuel is the only configuration dealt with by ELSA in the current version of ASTEC, V0, others being modelled by applying CORSOR correlations. ASTEC V1, due for release in 2002, will use the latest version of ELSA, v2.0, which models release from a full range of degraded-core configurations and *Ag-In-Cd* control rods. The modelling in ELSA v2.0 is described below by separating requirements in terms of solid fuel, liquefied fuel and other materials. Detailed overviews of the models in ELSA v2.0 are given in [3] for intact fuel and [4] for other configurations; where references are given in the individual subsections below, these provide more comprehensive descriptions covering background material not included here.

### 2.1 Modelling of release from solid fuel

All radioelements are classified by behaviour as either volatile (e.g. fission gases, *I*, *Cs*, *Br*, etc.), semi-volatile (*Sr*, *Ba*, *Ru*, *La*, *Ce*, *Y*, *Eu* and *Mo*) or non-volatile (actinides, *Zr*, *Tc*, etc.). Release of volatile elements is modelled as atomic diffusion within the fuel grains whereas semi-volatile FP release is governed by evaporation-driven mass transfer involving simplified consideration of their chemical forms. The non-volatile category is considered as being released only as the uranium fuel itself volatilizes. Two fuel configurations are dealt with using this approach: intact fuel and fuel debris where the difference in geometry is accounted for in the calculation of oxidation of the uranium, vital in determining diffusion rates for the volatile class.

Concerning the volatile class of elements, where the fuel rod is intact and the Zircaloy clad is not fully oxidized, the trapping of certain FPs, viz. *Te*, *Se* and *Sb*, by the Zircaloy is modelled. This leads to reduced release for these three FPs until the clad is fully oxidized.

We note that the above models have been developed for uranium fuel and their applicability in relation to mixed-oxide (MOX) fuel must be evaluated. Limited results from the IPSN programme VERCORS,

namely tests RT2 and RT7, show release from the MOX fuel used in France to behave differently from uranium fuel where preliminary interpretation would indicate a dependence on the *Pu* enrichment and/or the linear power to which the MOX has been subjected. It seems clear that the current uranium models will require, as a minimum, adjustment.

## 2.2 Modelling of release from liquefied fuel

Two distinct situations arise in which liquefied fuel forms. The first is due to interaction of Zircaloy clad with the uranium of the pellets leading to liquid eutectic formation and relocation (“candling”) of the liquid fraction in conjunction with, potentially, solid fuel fragments from the disintegrating pellets. It is usual at this stage of fuel degradation that most of the volatile FP inventory has been released and that liquefaction leads to release of virtually the whole of the remaining volatile inventory except, perhaps, for a non-negligible fraction of the caesium. It is also thought that the relocation event is rapid. Hence, in ELSA v2.0, candling is approximated by full release of the remaining volatile FPs to the gas phase while all other radioelements remain with the relocating fuel.

The second situation involves a more complex liquid phase, in fact an entirely general one covering a mixture of all possible elements in the core. This configuration, called a molten pool, is dealt with by assuming thermochemical equilibrium of the pool at the liquid-gas interface followed by mass-transfer-limited evaporation [5]. Within the liquid phase only diffusion is considered. Mixed configurations of solid debris and a liquid phase are dealt with in the same way, release only occurring at the liquid-gas interface.

It should be noted that release of all elements in the molten pool are modelled in this way, be they fission products, actinides or of structural origin (e.g. *Sn*, *Fe*, *Ni*, etc.)

## 2.3 Modelling of releases other than radioelements

Silver-indium-cadmium control rods release significant quantities of their constituent metals to the gas phase during degradation where all three metals can react with iodine. Reasonable quantification of their release is therefore important. Improvement of this modelling in ASTEC V0 has been identified [6] and incorporated into ELSA v2.0 for ASTEC V1. Two control-rod rupturing possibilities are considered by the model (as determined by the core degradation code): early bursting due to interaction of the steel sheath with the Zircaloy guide tube or rupture due to melting of the steel sheath. In the first case, if the bulk atmosphere is reducing, only a fraction (10%) of the *Cd* vapour in the control rod is released the remainder being released when the sheath melts; otherwise all *Cd* vapour is released instantaneously. Following rupture due to sheath melting, all *Cd* vapour is released and the evaporation rate of *Ag*, *In* and *Cd* from the molten alloy is modelled by temperature-dependent correlations. This is probably adequate for *Cd* and *Ag* which are relatively insensitive to the bulk gas composition, but *In* volatility is affected by the oxygen potential of the atmosphere and improvement with respect to hydrogen-rich atmospheres may be required.

Releases arising from control rods containing boron carbide are not yet modelled in ELSA. Reaction of  $B_4C$  with a hydrogen/steam atmosphere produces methane (lower temperatures) and carbon monoxide and dioxide (higher temperatures) along with volatile boric acid(s) and boric oxide. The relevant literature has been surveyed [7] and, independently of ELSA, a preliminary model of the  $B_4C$  oxidation rate has been implemented in the IPSN core-degradation code ICARE2 [8]. However, further experimental data are now required before significant progress can be made and these will be forthcoming when the IPSN experimental programme MADRAGUE [9] commences.

Currently, releases of other structural elements, viz. *Sn*, *Fe*, *Cr*, *Ni*, etc., are only calculated for the molten pool configuration in ELSA. This is not satisfactory in the case of tin where high release of this

metal, as an oxide, will occur as the Zircaloy clad is oxidized. This may be important since *Sn* will be a significant contribution to release in terms of mass in the early stages of degradation where, otherwise, *Cd* and the volatile fission products will dominate release.

## 2.4 Validation status and further needs

The different validation studies which have been performed for FP release are summarized in Table 1 and an example calculation for volatile FP release from intact fuel (taken from [10]) is shown in Figure 1. This example shows, in particular, the release rate at intermediate temperatures not being adequately captured though the comparison is otherwise reasonable.

Table 1 shows studies that refer to versions of ELSA preceding v2.0 since v2.0 is too recent to have been the subject of rigorous validation. That said, the conclusions are generally valid for v2.0 since (i) modelling for the solid fuel configuration has not changed except to remove molybdenum from the non-volatile class and add it to the semi-volatile class (hence comments referring to incompleteness in the fifth column of Table 1 are now redundant) and (ii) validation of preliminary models refers to the molten-pool approach which has been tested on data from a E.U. 4<sup>th</sup> Framework project as well as on the large-scale test, Phebus FPT0.

As far as needs are concerned, further validation of the molten pool model is required. Whilst some validation possibilities exist (e.g. the SASCHA experiments), it is likely that molten-pool validation will remain somewhat inadequate until experimental data is produced by the 5<sup>th</sup> Framework project “Late-phase Phenomena” (LPP), in which IPSN participates. Further validation of the solid fuel models is required for very high and low burn-up fuel as well as fragmented fuel, e.g. on VERCORS RT and HT results as well as experiments performed by Atomic Energy of Canada Limited (AECL). Phebus applications must also continue with the aim of checking the global performance of the code.

In terms of modelling, additional efforts are required for MOX fuel, boron-carbide-containing control rods (as a function of data arising from the MADRAGUE programme) as well as for tin release during Zircaloy oxidation. Improvement of modelling is required for (i) solid fuel regarding the release of volatile FPs at intermediate temperatures (significant underestimation) ; (ii) release of volatile FPs from low burn-up fuel ; (iii) oxidation and volatilization of uranium fuel where the steam-uranium surface reaction can be the limiting phenomenon except at very high temperatures and (iv) include probable trapping effects of *Ba* on Zircaloy. It should be mentioned that the first three of these improvements might well be helped by the physical insight gained from work in progress validating the mechanistic release code MFPR [11].

## 3. FISSION PRODUCT TRANSPORT IN THE REACTOR COOLANT SYSTEM

Following release from the core, analysis of the source term to the containment (or directly to the environment for containment bypass sequences) requires evaluation of the transport of radionuclides in the RCS. Retention in the RCS is highly sequence-dependent: for volatile FPs, retention can be negligible in a hot-leg break since these FPs reach the breach as vapours; for a cold-leg sequence with the secondary side operational, retention is virtually 100% due to aerosol formation and thermo-diffusiophoretic deposition in the steam generator. Like release, transport also involves complex processes which can lead to a significant calculational burden. However, simplification here leads rapidly, for some phenomena, to loss of credible predictions. Hence, in the SOPHAEROS code used in ASTEC for transport in the RCS, some areas retain relatively complex models and a significant effort has been made with respect to efficient numerical techniques.

### 3.1 Modelling of FP transport

SOPHAEROS models equilibrium vapour-phase chemistry, chemisorption of vapours, homogeneous and heterogeneous nucleation, aerosol agglomeration, the main aerosol deposition mechanisms as well as thermal and mechanical remobilization of deposits. Documentation of the models in SOPHAEROS v2.0 rev.2 is given in [12] corresponding to the version implemented in ASTEC V0.3. Work very near completion on models for SOPHAEROS v2.1, to be implemented in ASTEC V1, adds a model for aerosol trapping in a water pool (known as pool scrubbing) [13] as well as a comprehensive thermochemical database for vapour-phase chemistry [14]. Only these latest additions are described here as description of the other models cannot be tackled adequately here while the reader is referred to [15] for a summary of the development and validation status of the preceding version of the code, v2.0.

The transport of a FP in the RCS and its subsequent behaviour are sensitive to chemical reactions occurring in the RCS. One persistent uncertainty in such analyses concerns the ability to treat a full range of chemical reactions whilst modelling the dynamics of other phenomena such as aerosol formation and deposition. Hence it was decided to improve vapour-phase chemistry modelling by abandoning the somewhat *ad hoc* scheme used previously and applying a rigorous approach. SOPHAEROS version 2.0 deals with 32 elements of which 23 can participate in vapour-phase reactions where 84 compound species are catered for. Most of the data for this version were determined with the GEMINI1 database [16]. The new thermodynamic database [14] for use with SOPHAEROS v2.1 involved a systematic assessment of significant species in accident conditions. Starting from the identification of 65 elements as being required for full analyses, thousands of thermodynamic equilibrium calculations were performed on subsets of these elements using thermodynamic data from the Scientific Group Thermodata Europe database supplemented by species from the NUCLMAT database (AEA Technology) covering over 5000 chemical species. After elimination of insignificant species, the new FP transport database comprises nearly 800 vapour species. This forms the basis of the new database and Phebus-FP applications using it with a preliminary version of SOPHAEROS v2.1 are starting.

Pool scrubbing is a term used to describe aerosol and soluble-gas removal (or decontamination) from gas/steam mixtures passing through water pools. Originally, pool scrubbing models were developed for evaluating retention in boiling-water reactor pressure-suppression systems. In a PWR, the phenomenon can occur in the RCS and in the containment. For ASTEC, starting with the SPARC-90 code, the available modelling was reviewed and the code improved notably by standardizing thermal-hydraulic formulae and refining models that cover a vast range of pool scrubbing boundary conditions [17]. Semi-empirical models describe fluid injection, bubble formation at the injection orifice, and bubble formation in the bubble-rise zone in the improved code, SPARC-B/98. Aerosol retention is modelled as deposition on the bubble-water interface due to the usual deposition mechanisms including the effect of relative motion between bubble and contained aerosol. The code also allows for entrainment in the flow of FP-containing water droplets formed at the pool surface. SPARC-B/98 is used by ASTEC both for pool scrubbing in the containment system (where it is coupled to the containment thermal hydraulic and aerosol module CPA) as well as in the RCS, coupled to SOPHAEROS. The coupled code SOPHAEROS(v2.0rev.1)-SPARC-B/98 has been thoroughly tested leading to further improvement of many models as well as the code performance [18]. The module has been validated on POSEIDON, CIEMAT, and EPRI 3 experiments [17] for insoluble aerosols where, usually, underestimation of decontamination was seen. For soluble aerosols, the improved SPARC-B/98 results in plausible decontamination factors but validation is not possible due to lack of data.

### **3.2 Validation status and further needs**

The different validation studies which have been performed with SOPHAEROS (pool scrubbing aside)

are summarized in Table 2 while an example calculation on the STORM experiment SR11 for thermophoretic and turbulent deposition followed by mechanical resuspension of aerosols is shown in Figure 2 (from [15]). In the example it is seen that results are good for both deposition and resuspension phases of the experiment but what is not shown is that the resuspension rate is poorly reproduced.

In terms of existing models, further validation needs primarily concern aerosol deposition in bends, for which available data is unreliable, and identification of chemical species. Pursuit of applications on integral tests, such as Phebus FP and VERCORS HT, will be very important in checking the global performance of the code. Further to this, it will be necessary to compare the results of SOPHAEROS v2.1 with results of IPSN's CHIP programme investigating vapour-phase equilibria and reaction kinetics in primary circuit conditions, thus testing the chemical equilibrium approach.

As far as modelling is concerned, a number of areas need to be addressed: improvement of the mechanical resuspension model dynamics; the ability to address a closed-loop geometry where there is partial release from a breach with the remaining flow returning through the primary circuit into the vessel; steam condensation onto aerosol particles which, certainly for cold-leg and bypass sequences, could significantly reduce the early release from the RCS (or directly to the environment in the case of containment bypass); chemical interaction between the gas flow and deposits, especially a hydrogen-rich deposition phase followed by a more oxidizing flow which might remobilize deposited iodine; and aerosol deposition in singularities (simple contractions, expansions) and more complex geometries such as steam generator components (for which there is little or no published data).

#### **4. FISSION PRODUCT BEHAVIOUR IN THE REACTOR CONTAINMENT BUILDING**

Once in the containment building, significant quantities of fission products are not predicted to remain in the vapour phase except for noble gases and some small fraction of the iodine (and, possibly, some of the ruthenium in the case of air ingress into the reactor vessel). Furthermore, for all except iodine, FPs remain in condensed form, i.e. as aerosols, depositing on surfaces and, to some extent, collecting in the sump. Hence, beyond accounting for aerosol processes as a function of thermal hydraulic conditions (calculated by the CPA module in ASTEC), only the behaviour of iodine is modelled in detail. Further to this picture, however, we must add the possibility of an unrecovered core-melt accident leading to melt-through of the vessel and interaction of the molten corium with the concrete basemat. Release of radionuclides to the containment atmosphere during the late phase of a severe accident is likely to be dominated by phenomena associated with molten corium concrete interaction (MCCI). This situation, also known as an ex-vessel molten pool, would produce releases which are still a significant uncertainty in accident analyses.

Iodine behaviour is modelled by the IODE code which generally applies semi-empirical approaches based on a significant database of experimental results. IODE v5.0 is implemented in ASTEC V0.3 whereas IODE v5.1 is being prepared for ASTEC V1. Releases from ex-vessel molten pools are not currently dealt with by ASTEC though, as described below, very preliminary preparatory work has started.

##### **4.1 Modelling of iodine behaviour**

IODE v5.0 takes account of 15 physico-chemical phenomena. These include: adsorption/desorption of iodine on painted or stainless steel surfaces in the gas phase; aqueous-phase chemistry ( $I_2/I^-/HOI/IO_3^-/OI^-/H^+/AgI$  plus the effect of radiation on the  $I^-/I_2$  and  $IO_3^-/I_2$  equilibria); gas-phase chemistry ( $I_2/O_3$  and  $I_2$ /organic vapour); simple, empirical modelling of organic iodide formation and destruction (hydrolysis and radiolysis) in the liquid phase; and mass transfer between the sump and gas phase

[19].

The most recent development of the code has been to generalize its application when functioning in the environment of the ASTEC code. IODE v5.0 is a multicompartment version of v4.2 (without other modelling changes) allowing ASTEC V0.3 to take into account any significant heterogeneity in iodine concentration over the containment atmosphere.

#### **4.2 Modelling of ex-vessel FP release**

Though ex-vessel molten pool releases are not currently dealt with by ASTEC, very preliminary ideas on the required modelling exist [20]. Furthermore, the ELSA database required for in-vessel molten pools [5] already includes the additional elements and compounds arising from molten core concrete interaction since the in-vessel and ex-vessel models have a common feature in applying equilibrium chemistry. A simple model can be envisaged taking account of the main phenomena for which reliable modelling can be described. It is likely that a number of simplifying assumptions are possible allowing an approach based on the thermodynamic equilibrium of a well-defined, isobaric system. One particular uncertainty which should be mentioned concerns the mechanical generation of aerosols at the surface of the pool due to bursting bubbles, especially fragments of the film. Current models are based on experiments with water (c.f. pool scrubbing) and their validity with respect to magma remains uncertain.

The input required from other computer codes, i.e. core degradation, MCCI and, possibly, containment thermal hydraulics, constitutes boundary conditions for such a model functioning in the environment of ASTEC. Hence, progress on modelling for ex-vessel molten pools will evolve as a function of the models in these other areas.

#### **4.3 Validation status and further needs**

Wide-ranging validation of the IODE v4.2 has very recently been performed [21,22] while the models themselves have also been thoroughly reviewed [23]. An example of IODE results is given in Figure 3 where satisfactory comparison is seen in relation to one of the tests of the ACE/RTF series (performed by AECL). The conclusions which follow are based on the two recent reviews. In terms of validating IODE v5.1, it will be important to return, in particular, to the medium-scale CAÏMAN experiments which are a rich source of data on iodine behaviour in irradiated conditions including tests with and without painted coupons. Pursuit of applications regarding the Phebus tests will also be important to check the global performance of the code. It is also necessary to mention longer term validation based on IPSN's EPICUR programme which will focus on investigating radiolysis effects at high dose rates with respect to iodide solution, silver iodide, air, paints and cables.

As far as the current modelling is concerned, improvements have been defined with respect to radiolytic oxidation of  $I^-$  [24] and work is in progress on formation of organic iodides due to paints, in both gas and liquid phases and on checking mass transfer at the liquid-gas interface. The aqueous-phase formation of organic iodides due to paints is a particularly important improvement for which new modelling based on the wash-out of organic solvents/additives from the paints has been proposed [25]. It is intended to include the above improvements in IODE v5.1 for ASTEC V1. In terms of new models in the longer term, radiolytic destruction of organic iodine in the gas phase and inclusion of the effects of air radiolysis on gas-phase iodine chemistry must be added. Subsequently, radiolytic destruction of iodates, currently an empirical model, must be improved as must adsorption of iodine on painted surfaces where the effect of temperature and the potential saturation of the surface must be taken into account. This latter aspect requires further experimental data, notably from the EPICUR programme.

## 5. CONCLUSIONS

The modelling of the FP modules of the ASTEC code has been described. It is seen that even with a significant amount of necessary simplification, a wide variety of phenomena need to be modelled in some detail for adequate prediction of FP behaviour. These models, generally semi-empirical or more mechanistic in nature, aim to provide reliable results for reactor analyses as well as, where possible, an adequate degree of physical insight into the important processes for interpreting experiments (underpinning confidence in the models). A number of significant improvements to these codes have been outlined above aiming to extend the modelling range to all the important phenomena occurring in severe accident conditions.

Continued validation of the codes, especially given the significant developments which have been recently or will shortly be implemented, is crucial to ensuring an adequate level of confidence in the codes. The most noteworthy sources of experimental results can be summarized as follows: release data from VERCORS, Phebus FP, the 5<sup>th</sup> Framework LPP molten pool tests and certain AECL tests ; transport data from CHIP, Phebus FP and the VERCORS HT tests; iodine data from CAÏMAN, EPICUR, Phebus FP as well as the 5<sup>th</sup> Framework ICHEMM project.

The latest versions of ELSA, SOPHAEROS and IODE will, in 2001, be integrated into ASTEC V1 due to appear in early 2002.

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Table 1: summary of validation studies for ELSA v1.1 and preliminary v2.0 models,

- (i) solid fuel (6 programmes)
- (ii) liquefied fuel (one programme)
- (iii) integral tests (3 programmes)

PROJECT	TEST TYPE	TESTS USED	volatile FPs	semi/low-volatiles	non-volatiles and actinides
<b>AECL/CRL COG</b>	small-scale, clad & unclad, analytical, T ≤ 2350K	7 tests: MCE1, HCE2..	conclusive: global release & rate OK but burn-up < 22GWd/t except HCE2-LM2	inconclusive: analysis/data incomplete	conclusive: tuned for T ≤ 2270K/air; T ≤ 1923K/H <sub>2</sub> O
<b>HI-VI NRC-ORNL</b>	small-scale, clad, analytical, HI, T ≤ 2275K; VI, T ≤ 2720K	HI, all 6 VI, all 7	conclusive: OK but rate underestimated T < 2000K	conclusive: within a factor of 3; pO <sub>2</sub> effect on Ba, Ru, Mo ignored; class incomplete - Mo	<i>not applicable</i>
<b>FPRMP 4<sup>th</sup> Framework</b>	small-scale, P=0.1MPa, T ≤ 2070K	6 urania disk tests	<i>not applicable</i>	<i>not applicable</i>	conclusive: model adequate but surface reaction model better
<b>HEVA IPSN-EDF-CEA</b>	small-scale, clad, analytical, P=0.1MPa, T ≤ 2370K	1 to 6, 8	conclusive: global release OK	conclusive: OK within a factor of 2; class incomplete, e.g. Mo	<i>not applicable</i>
<b>VERCORS IPSN-EDF-CEA</b>	small-scale, clad, analytical, P=0.1MPa, T ≤ 2570K	1 to 5 (6)	conclusive: OK but rate underestimated T < 2000K	conclusive: within a factor of 2; pO <sub>2</sub> effect on Ba, Ru, Mo ignored; class incomplete - Mo	<i>not applicable</i>
<b>VERCORS RT,HT IPSN-EDF-CEA</b>	small-scale, clad & unclad, analytical, P=0.1MPa, T ≤ 3000K	HT1	conclusive: OK but rate underestimated T < 2000K	conclusive: OK within a factor of 2; class incomplete, e.g. Mo	too early (RT series)
<b>FPRMP 4<sup>th</sup> Framework</b>	small/medium scale, simulant fuel, P=0.1MPa, T ≤ 2070K	metallic/ceramic molten pool tests	<i>not applicable</i>	semi-conclusive: model credible but large experimental uncertainty	semi-conclusive: model credible but large experimental uncertainty
<b>ACRR NRC-SNL</b>	large-scale, in-pile, P ≤ 1.9MPa, T ≤ 2500K	ST-1, ST-2		semi-conclusive: OK but releases low	<i>not applicable</i>
<b>PBF-SFD NRC-INEL</b>	large-scale, in-pile, P=6.9MPa, T ≤ 2800K	ST, 1-1, 1-3, 1-4	conclusive: OK if burn-up accounted for	semi-conclusive: OK but releases < 1%	<i>not applicable</i>
<b>PHEBUS FP IPSN-CEC-EDF</b>	large-scale, in-pile, P=0.22MPa, T ≤ 2900K	FPT0, 1, 4 - in progress	conclusive: reasonable if burn-up accounted for.	preliminary conclusion: adequate except for Ba – Zrly trapping?	too early (FPT4)

Table 2: summary of validation studies for SOPHAEROS v2.0,

- (i) aerosol phenomena (7 programmes)  
(ii) vapour and vapour/aerosol phenomena (3 programmes)  
(iii) integral phenomena (6 programmes)

PROJECT	TEST TYPE	TESTS USED	MAIN PHENOMENA	CONCLUSION
<b>LACE consortium</b>	aerosol, large-scale, semi-analytical	1 LACE3B	•eddy impaction •90°bend impaction	semi-conclusive: global retention under-predicted (esp. bends) but unquantified resuspension
<b>TUBA-T IPSN</b>	aerosol, SGT-scale, single-effect	9 TT14,22,24-31	•thermophoresis	conclusive: laminar flow OK; semi-conclusive for turbulent flow (too few tests)
<b>TUBA-D IPSN</b>	aerosol, SGT-scale, analytical	12 TD01-TD12	•diffusiophoresis •thermo-diffusiophoresis	conclusive: aerosol model OK but sensitive to steam condensation model
<b>TRANSAT IPSN</b>	aerosol, large-scale, semi-analytical	7 TR1, 2, 4-8	•eddy impaction •90°bend impaction •settling	inconclusive : deposition over-predicted but unquantified rebound
<b>ADPFF AEA-T</b>	aerosol, full-scale, analytical	15 WT10-23, 25	•eddy impaction •90°bend impaction •settling	inconclusive : some good agreement but injected mass uncertain
<b>DEPAT IPSN</b>	aerosol, large-scale, analytical	7 DEPAT01-04 DEPM 01-03	•eddy impaction	semi-conclusive: net deposit overestimated, rebound confirmed
<b>STORM CEC-ENEL</b>	aerosol, large-scale, semi-analytical	SD 04, ISP40 SR (in progress)	•thermophoresis •eddy impaction •mechanical resuspension	conclusive: turbulent+thermophoretic deposition slightly over-predicted; integral resuspension OK ; resuspension rate model requires improvement
<b>DEVAP IPSN-DRN</b>	vapour, small-scale, analytical	7 8,13-15, 17, 18, 20	•chemisorption •condensation	chemisorption correlations (CsI,CsOH,Te) tuned on data
<b>AERODEVAP IPSN-DRN</b>	aerosol/vapour, small-scale, semi-analytical	3 01, 02, 04	•heterogeneous nucleation •condensation •vapour-aerosol interaction	inconclusive: interpretation could be re-examined with new chemistry
<b>REVAP-ASSESS 4<sup>th</sup> Framework</b>	vapour, small-scale, analytical	3 2 VTT tests, Fal-25	•revaporization	conclusive: tend to over-predict rate
<b>FALCON AEA-T</b>	simulant fuel, small-scale, semi-analytical	3 FAL17, 18, ISP	•vapour chemistry •condensation •vapour-aerosol interaction	semi-conclusive: deposits for many elements OK but very sensitive to chemistry (no species data)
<b>VERCORS IPSN-EDF</b>	irradiated fuel, small-scale, integral	2 4, 5	•full range	inconclusive: temperature (cold spot) and source (e.g. Sn) data insufficient
<b>VERCORS HT IPSN-EDF</b>	irradiated fuel, small-scale, integral	1 HT1 (planned)	•full range	too early
<b>HCE COG</b>	irradiated fuel, small-scale, integral	1 3 (in progress)	•full range	Cs, I retentions OK; speciation credible except Te,Sb; chemisorption of I <sub>2</sub> & HI on steel, Ba on ZrO <sub>2</sub> ? deposit chemistry?
<b>BTF COG</b>	irradiated fuel, in-pile, integral	1 104 (in progress)	•full range	global retentions OK
<b>PHEBUS-PF PSN-CEC-EDF</b>	irradiated fuel, in-pile, integral	3 FPT0, 1, 4 (in progress)	• full range	preliminary conclusion: global retentions reasonable but very sensitive to source (complex); deposits remobilize.

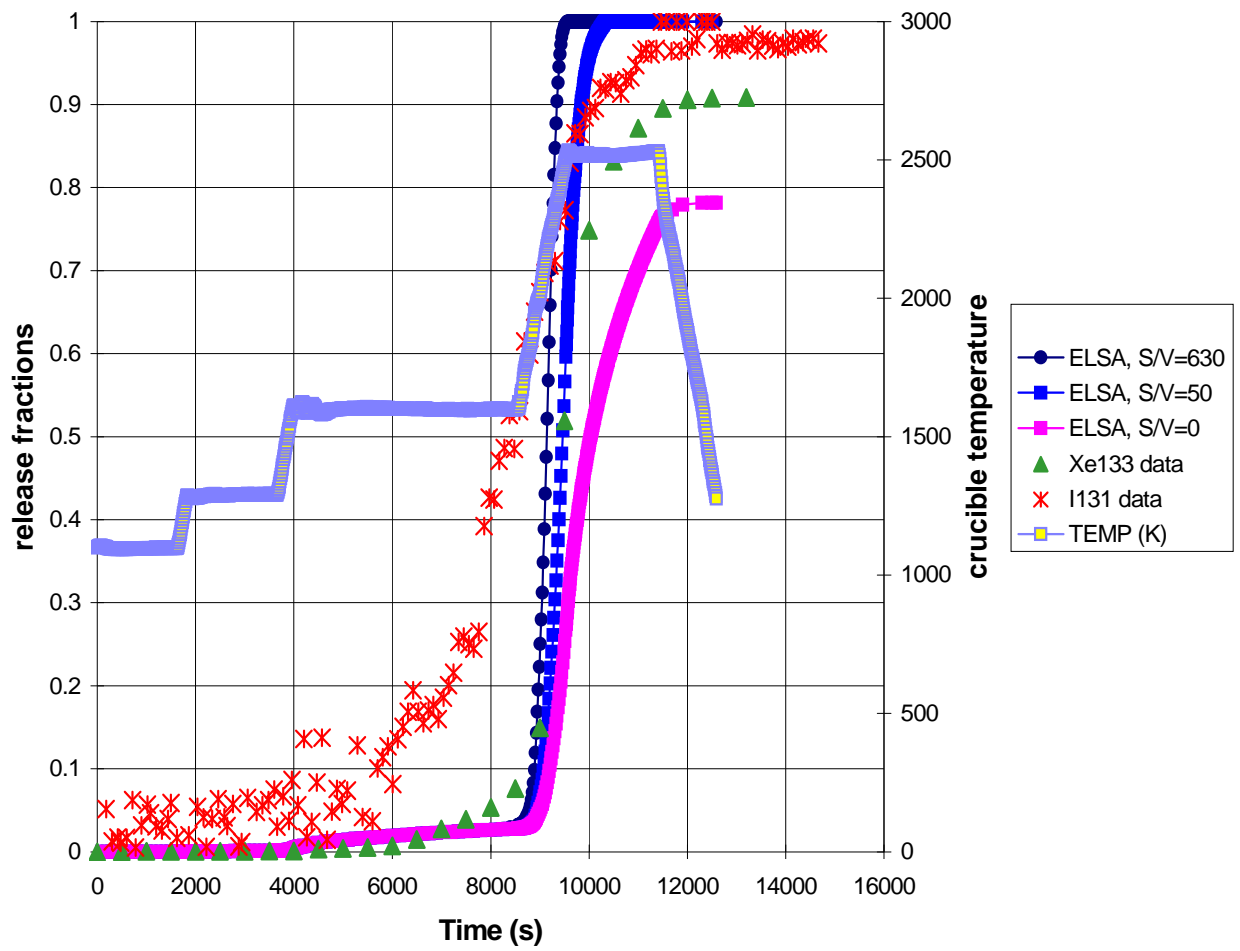


Figure 1: volatile FP release as calculated by ELSA (3 different fuel oxidation rates) for VERCORS 5 (after reference [10]).

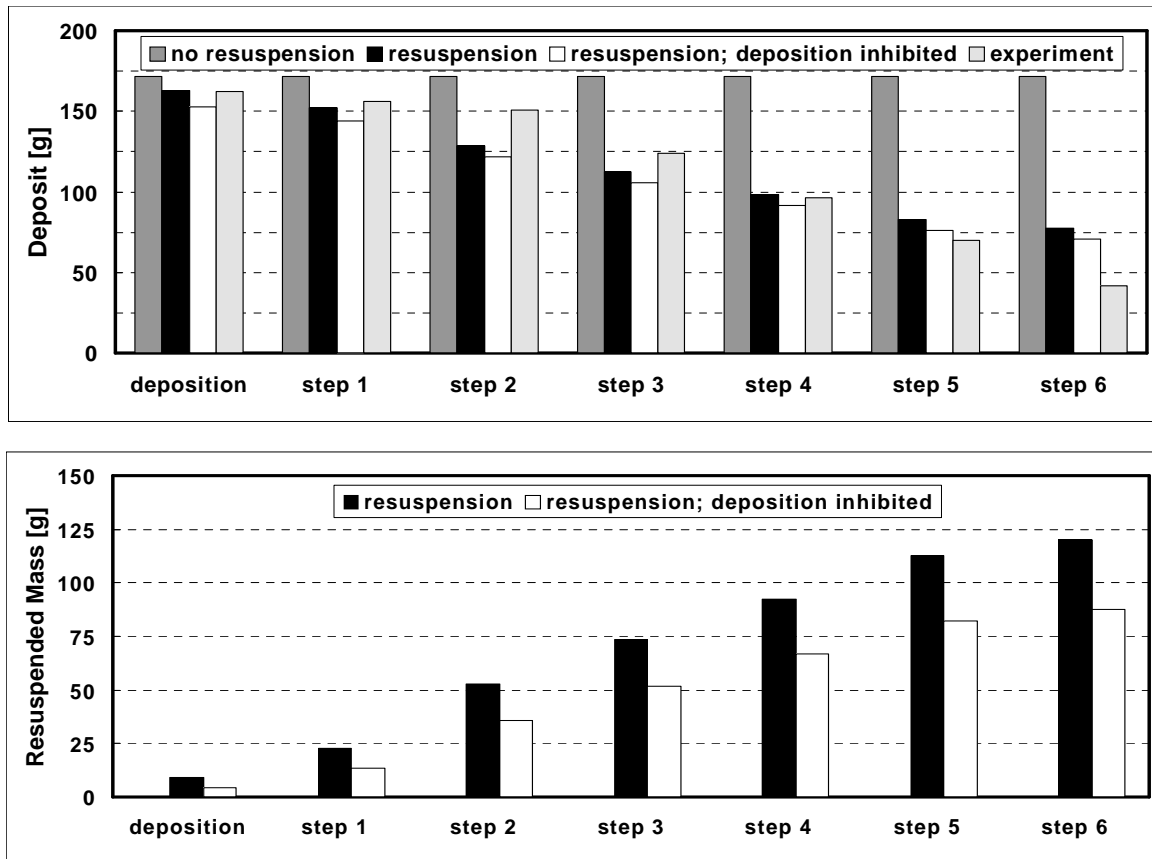


Figure 2: comparison of SOPHAEROS v2.0 with STORM test SR-11 (ISP-40)

- deposited mass after deposition phase and remaining after each resuspension step,
- resuspended mass during deposition phase and during each resuspension step.

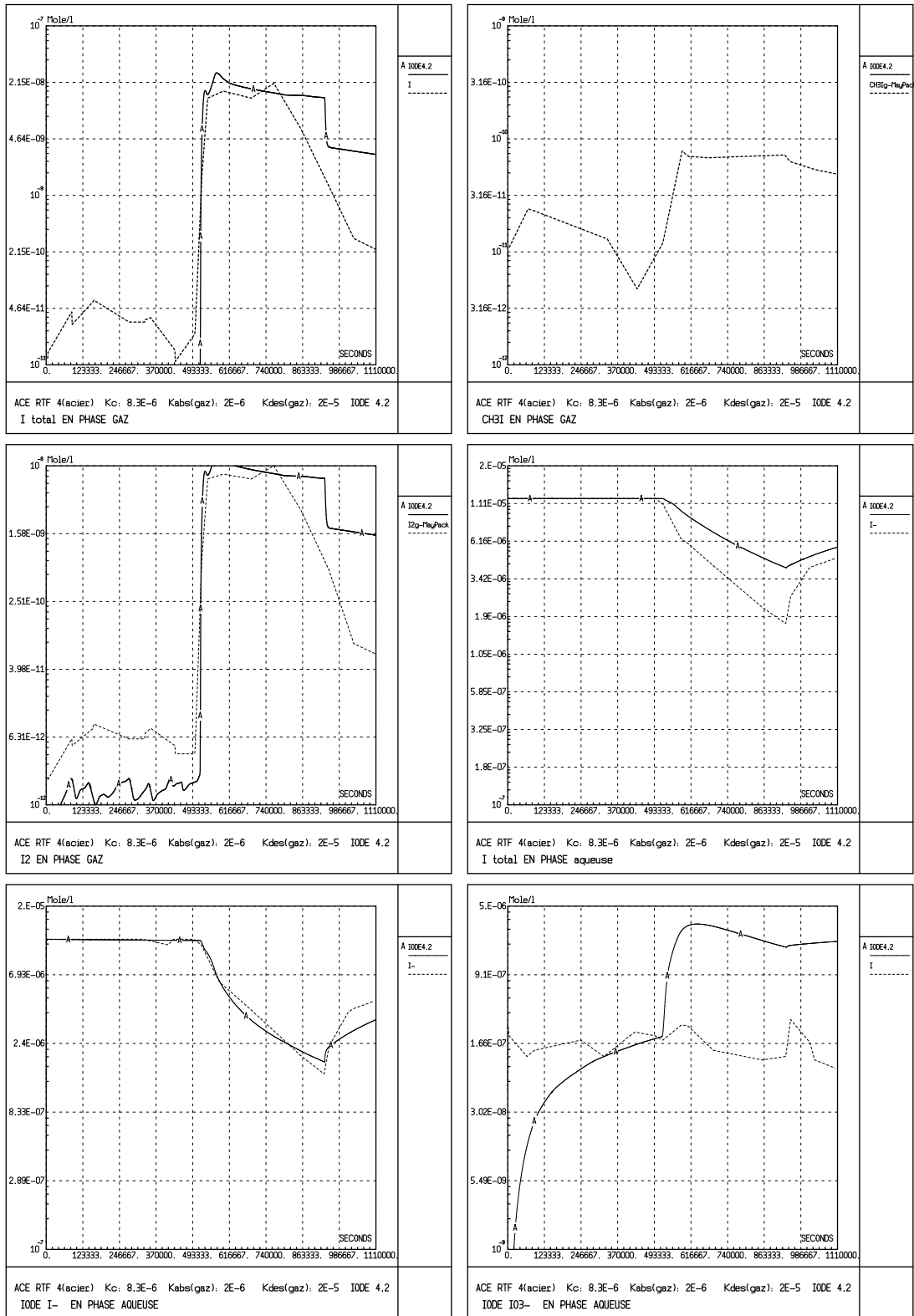


Figure 3: comparison of IODE with ACE/RTF 4 experiments