FISSION-PRODUCT TRANSPORT MODELLING IN THE ASTEC INTEGRAL CODE: THE STATUS OF THE SOPHAEROS MODULE

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ABSTRACT

Safety assessment of water-cooled nuclear reactors encompasses potential severe accidents where, in particular, the behaviour of radionuclides released into the reactor coolant system is evaluated. The SOPHAEROS code, a module of the ASTEC integral code, models this behaviour. The code modelling is described here along with example calculations taken from the wide variety of validation studies (from highly analytical to integral experiments). Now a robust and relatively mature tool with a reasonable level of accuracy and an acceptable calculation time, SOPHAEROS constitutes a sound basis for completing modelling of the key phenomenology. Short-term improvements include implementing models for aerosol deposition in flow-geometry changes, retention in water volumes, and a more mechanistic model for mechanical resuspension.

Keywords : severe accidents, safety, analysis, fission product, transport, ASTEC, SOPHAEROS.

1. CONTEXT

Safety evaluation of water-cooled nuclear reactors with respect to potential severe accidents must tackle the problem of fission products (FPs), actinides and structural materials released into the reactor coolant system (RCS, or PHTS for the CANDU community). The SOPHAEROS code, developed by IRSN as part of the IRSN-GRS ASTEC integral code [1], models radionuclide transport in the RCS. In the context of increasing international use of this code, the main purpose of the present document is to provide a general description of the SOPHAEROS modelling, illustrate the extensive validation activities, and describe current and future development work.

The principal use of the SOPHAEROS code arises from the following applications:

- IRSN is currently performing a Probabilistic Safety Analysis level 2 for French 900MWe PWRs using ASTEC where SOPHAEROS calculates FP release into the containment;
- SOPHAEROS has been used and validated in the broader European context through the EVITA project [2], part of the European Commission's 5th Framework Programme;
- SOPHAEROS -IST 2.0 (corresponding to SOPHAEROS v2.0 with some generic and CANDU-specific improvements implemented by AECL) is the Canadian Industry Standard Toolset code for analysing FP transport in the PHTS of CANDU reactors [3].

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In addition, it is intended that the ASTEC V1 code be further distributed internationally in the context of the SARNET project submitted to the European Commission for support within the 6th Framework Programme [4]. Within IRSN, beyond the plant assessments mentioned above, the main use of the code arises from the responsibility of performing the bulk of the necessary model validation including application to the tests of the large-scale, integral Phébus FP programme [5].

2. OVERVIEW OF MODELLING

The basic element of SOPHAEROS modelling is the control volume where the RCS must be decomposed into a 1-D sequence of control volumes, each comprising one or several freely-oriented truncated cones. Within each control volume, the vapour and aerosol phenomena modelled (SOPHAEROS v2.1) are summarized in Table 1 where the associated literature source and/or a description for each model is also provided.

In broad terms, an element is determined to be partitioned among its possible chemical species via the use of an independent thermochemical database. SOPHAEROS v2.1 operates with two optional databases, the standard one covering just over 100 chemical species or an extended one covering 65 elements generating 747 compounds (see Table 3). The advantage of the extended database is its relative comprehensiveness where many more species can be included in a given calculation but with the disadvantage that the calculation run time is much increased.

Each chemical species can exist in one of five physical states: vapour; vapour condensed on a wall; vapour sorbed on a wall; aerosol and deposited aerosol. The fraction of a species converted into condensed or deposited states no longer participates in the chemistry where this chemical inactivation is permanent unless revaporization occurs. Aerosol phenomena are handled by discretizing the (arbitrary, freely evolving) size distribution over a user-determined, logarithmic grid of up to 50 classes. Use of a large number of size classes is particularly important in situations where homogeneous nucleation, heterogeneous nucleation, or agglomeration is important.

SOPHAEROS must be provided with thermal-hydraulic conditions, e.g., by the CESAR module via the coupling created in ASTEC v1. In effect, these constitute boundary conditions.

The mass-balance equations resulting from the above intra-volume phenomena combined with inter-volume transport produce a nonlinear system solved numerically by a Newton-Raphson method. This implicit method allows the coupling between condensation/evaporation on/from aerosols, agglomeration and fall-back to be handled correctly while leading to satisfactory code run times.

To illustrate how the code deals with the diverse phenomenology involved in the transport process outlined above, we take the aerosol state (state 2 in SOPHAEROS, hence suffix 2 below) entailing the following mass-conservation equation for a given aerosol size class *i*:

$$\frac{dm_{2,i}}{dt} = s_{2,i} + (\tau_{f,i}^{up} m_{2,i}^{up} - \tau_{f,i} m_{2,i}) + \dot{m}_{agg,i} + \dot{m}_{cond,i} - \tau_{d,i} m_{2,i} + \tau_{r,i} m_{4,i} + \delta_{1,i} \sum_{n=1}^{vapours} J_n$$

where, taking each right-hand-side term successively,

s is an aerosol source rate,

the τ_f terms are flow-dependent transport rates into and out of the volume (including the effect of aerosol fall back/forward),

$\dot{m}_{agg,i}$ is a compound term representing particle agglomeration into and out of size class i

$\dot{m}_{cond,i}$ is a compound term representing heterogeneous nucleation onto smaller particles bringing mass into size class i and evaporation from class i particles taking mass out,

τ_r is the mechanical resuspension rate of class i deposited aerosols (state 4, hence suffix 4),

J_n is the mass rate of formation of aerosols due to homogeneous nucleation of vapour species n where the Dirac delta is zero except for i=1, i.e., vapours are seeded into the smallest size class only.

3. VALIDATION

A wide variety of data sources is employed for validation. Table 2 shows the currently-used experiments where a full reassessment of the experimental database is underway (i.e., cases will be added while some may be abandoned). The following experiments are shown here to illustrate the diversity of cases studied: TUBA TT28, an analytical, thermophoresis test [24]; STORM test SR11 (ISP-40), an aerosol deposition and resuspension test [25]; Falcon test Fal-18, a small-scale, semi-integral test [26]; and Phébus FPT1, a large-scale, in-pile, integral test [5].

The TT28 test comprised a dilute CsI aerosol in a turbulent flow (average Re≈5700) at 367°C entering a simulant steam-generator tube (∅=1.81cm) held at 73°C. The aerosol is subject to a thermophoretic force and the deposition that results is shown in Figure 1. SOPHAEROS is seen to be in excellent agreement with the data (where these entail a ±10% error).

In test SR-11, the deposition and resuspension of a SnO_2 aerosol was studied. The resuspension phase comprised six steps characterized by zero flow followed by sudden increase to steady-flow conditions; the Reynolds number grew from 22000 during deposition to 153000 in the last step. Figure 2 shows the evolution of the deposit where good agreement is obtained with SOPHAEROS except for the last step. What is not apparent from Figure 2 is that the rapidity of the resuspension event is not reproduced by the model, i.e. there is problem with the rate.

The comparisons with the Fal-18 (Figures 3 and 4) and FPT1 (Figures 5 and 6) tests highlight the critical role of chemistry in determining deposition profiles and overall retentions. From a purely transport point of view, the tests involved injection of a complex vapour source, that of FPT1 including a full inventory of FPs, into progressively cooler conditions. The vapours react, nucleate, condense on walls and the aerosols formed agglomerate and deposit (mainly due to thermophoresis here). The iodine results for Fal-18, Figure 3, are correctly reproduced where it is apparent that a single dominant species condenses followed by mixed deposition (vapour and aerosol). The caesium result is less satisfactory where a number of species are involved and SOPHAEROS may well not correctly replicate their relative concentrations. For FPT1, deposition occurred in two zones of strong cooling where SOPHAEROS has some difficulty reproducing the first of these due, essentially, to entrance effects that enhanced mass transfer. Overall agreement is good once this is corrected as seen in the results of sensitivity calculations of Figures 5 and 6 where treatment of mass transfer has been improved by taking account of the hydrodynamically and thermally developing laminar flow and the non-simple geometery.

4. FUTURE IMPROVEMENTS

Future work is determined essentially on the basis of applications requirements and the feedback from validation activities. Hence, in the short term, this work will include implementing models for inertial aerosol deposition in flow contractions [27,28] and more complex geometries (e.g. steam generator secondary side as part of the ARTIST project, [29]) as well as retention by water volumes that arise in the RCS [30]. A more mechanistic model for mechanical resuspension will also be implemented [31].

Longer term objectives include verification of the thermochemical data and completion of the species considered. The first stage of this work has been to compare the list of species used by SOPHAEROS (originating mainly from the SGTE database [32]) with species included in other database collections, namely FACT [33] and THERMODATA [34]. Figure 7 illustrates the results of this comparison. The next step is to prioritize the 65 elements in terms of importance and then begin the process of data verification. Also longer term, development of physical models may address gas-phase chemical kinetics; this has arisen from feedback from Phébus studies and has led IRSN to prepare the CHIP experiments in order to study gas chemistry.

In the context of improving accident-analysis capabilities, the study of cold-leg break sequences requires that steam condensation onto aerosols be examined while development of the ability to deal with a distributed source is needed for study of transport within the core.

5. CONCLUSIONS

The modelling and validation work performed by IRSN in the development of the SOPHAEROS code has been described. It is seen that fairly comprehensive treatment of the phenomenology arising in severe accidents is allowed. The performance of extensive validation studies has shown that the code can provide very satisfactory results in simplified and involved situations. This work has, in part, allowed identification of a number of areas for improvement, i.e., either enhancement of existing models or additional models for completion of coverage of the important phenomena.

In conclusion, SOPHAEROS, now a robust and relatively mature tool, provides a sound basis for completing modelling of the relevant phenomenology and comprises a suitable tool for prediction of FP transport with a reasonable level of accuracy and an acceptable calculation time.

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Table 1: phenomena modelled in SOPHAEROS V2.1

	Mechanism		Literature source and/or brief description
Vapour Phenomena	vapour-phase chemistry		Equilibrium; standard database or extended database (100 or 800 species).
	homogeneous nucleation		[6] for condensation rate.
	heterogeneous nucleation (reversible)		Brownian-diffusion-limited mass transfer onto a sphere, inclusion of Mason effect [7].
	sorption on metal-alloy surfaces		Empirical velocities as a function of temperature.
	condensation on surfaces (reversible)		Chilton-Colburn analogy [8]; laminar, Nu=3.66 (cylinder); turbulent [9]
Aerosol Phenomena	sedimentation		Stokes' velocity with Cunningham correction.
	turbulent (eddy) impaction		[10]
	diffusion	laminar (Brownian) turbulent	[11] laminar; [12] turbulent.
	thermophoresis		[13]
	diffusiophoresis		Based on Stefan velocity [17]: [14] for free molecular regime; option of [15,16] for slip flow.
	bend impaction		Hybrid model based on [18] for laminar flow, [19] for turbulence; option of centrifugal model.
	agglomeration	Brownian, gravitational, turbulent	[20] continuum regime, [12] free molecular regime; [21] gravitational; [22] turbulent.
	mechanical resuspension		Semi-empirical resultant-force model devised for ECART, retuned by GRS [23]
	inter-volume aerosol fall-back/forward		Sedimentation velocity superimposed on vertical component of mean flow velocity.

Table 2: current validation matrix

Test Type	Project	Character	Tests Used	Main Phenomena
aerosol phenomena	LACE *consortium*	aerosol, large-scale, semi-analytical	**1** LA3B	•eddy impaction •90°-bend impaction
	TUBA-T *IRSN*	aerosol, SGT-scale, single-effect	**9** TT14,22,24-31	•thermophoresis
	TUBA-D *IRSN*	aerosol, SGT-scale, analytical	**12** TD01-TD12	•diffusiophoresis •thermophoresis
	TRANSAT *IRSN*	aerosol, large-scale, semi-analytical	**7** TR1, 2, 4-8	•eddy impaction •90°-bend impaction •settling
	DEPAT *IRSN*	aerosol, large-scale, analytical	**6** DEPAT01-03 DEPM01-03	•eddy impaction
	ADPFF *AEA Tech.*	aerosol, full-scale, analytical	**15** WT10-23, 25	•eddy impaction •90°-bend impaction •settling
	STORM *CEC-ENEL*	aerosol, large-scale, semi-analytical	SD 04, ISP 40 SR (in progress)	•thermophoresis •eddy impaction •mechanical resuspension
vapour & mixed phenomena	DEVAP *IRSN-CEA*	vapour, small-scale, analytical	**7** 8,13-15, 17, 18, 20	•chemisorption •condensation
	AERODEVAP *IRSN-CEA*	aerosol/vapour small-scale, semi-analytical	**3** 01, 02, 04	•heterogeneous nucleation •condensation •vapour-aerosol interaction
	Falcon *AEA Tech.*	simulant fuel, small-scale, semi-analytical	**4** Fal-17, 18, 19, 20	•vapour chemistry •condensation •vapour-aerosol interaction
	REVAP-ASSESS *4thFramework*	vapour, small-scale, analytical	**3** 2 VTT tests, Fal-25	•revaporization
integral	VERCORS HT *IRSN-EDF-CEA*	irradiated fuel, small-scale, integral	**3** HT1, 2, 3 (in progress)	•full range
	HCE *COG*	irradiated fuel, small-scale, integral	**1** 3 (in progress)	•full range
	BTF *COG*	irradiated fuel, in-pile, integral	**1** 104 (in progress)	•full range
	PHEBUS-PF *IRSN-CEC-EDF*	irradiated fuel, in-pile, integral	**3** FPT0, 1, 2, 4 (in progress)	•full range

Table 3: Periodic Table showing the elements and the number of associated compound species included the ASTEC/SOPHAEROS database. Shaded elements are not in the database.

1 IA 1A	2 IIA 2A	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8 VIII	9 VIII	10 VIII	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 VIIIA 8A
H 160																	He 0
Li 17	Be 16											B 40	C 29	N 17	O 259	F	Ne
Na	Mg											Al 35	Si 41	P 27	S 64	Cl 114	Ar
K	Ca	Sc --	Ti 19	V 7	Cr 24	Mn 16	Fe 13	Co 8	Ni 10	Cu 20	Zn 10	Ga 24	Ge 15	As 33	Se 34	Br 81	Kr 0
Rb 15	Sr 15	Y 4	Zr 22	Nb 6	Mo 22	Tc 1	Ru 8	Rh 3	Pd 1	Ag 15	Cd 11	In 23	Sn 18	Sb 23	Te 41	I 92	Xe 0
Cs 29	Ba 18	*La-Lu*	Hf 11	Ta	W 11	Re 6	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	*Ac-Lr*	Rf	Db	Sg	Bh	Hs	Mt									

La 7	Ce 8	Pr 3	Nd 7	Pm 1	Sm 1	Eu 9	Gd 4	Tb --	Dy --	Ho --	Er --	Tm --	Yb --	Lu --
Ac	Th 8	Pa 0	U 16	Np 0	Pu 0	Am 0	Cm 0	Bk --	Cf --	Es --	Fm --	Md --	No --	Lr --

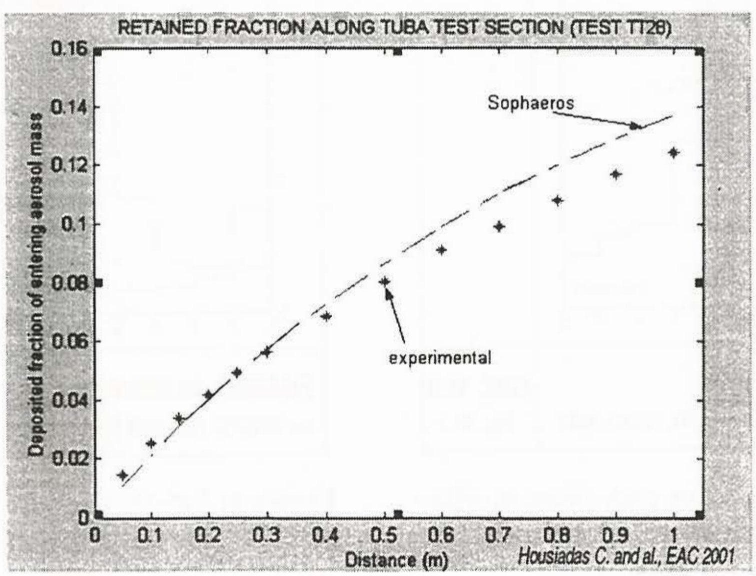

Figure 1: TUBA TT28, aerosol deposition profile, SOPHAEROS/data comparison

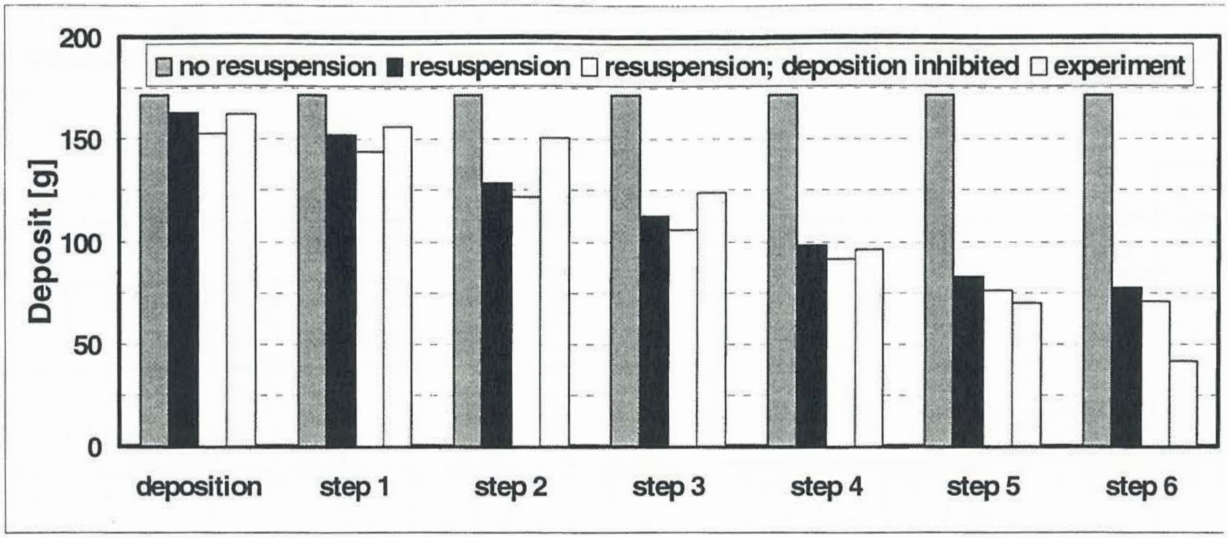

Figure 2: ISP-40 (STORM SR11), the deposition and the 6 resuspension steps, SOPHAEROS/data comparison with options of no resuspension, normal resuspension (base case) and inhibition of deposition (option now abandoned)

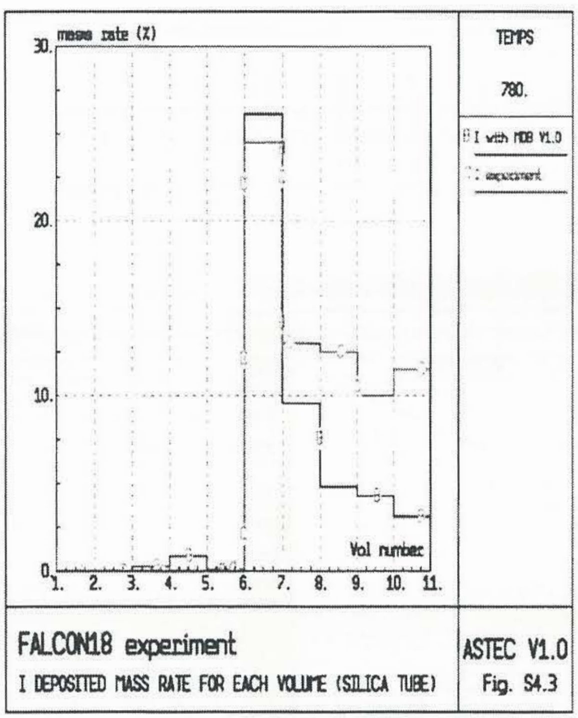

Figure 3: Fal-18, iodine deposition profile, SOPHAEROS/data comparison

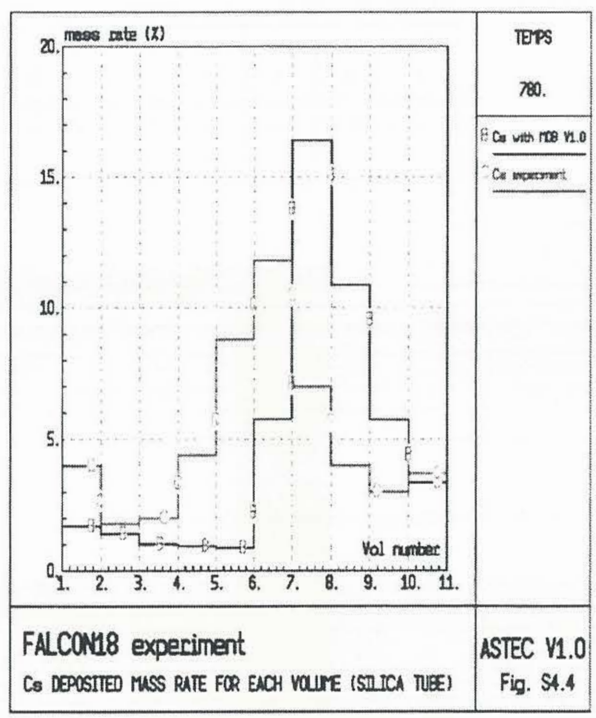

Figure 4: Fal-18, caesium deposition profile, SOPHAEROS/data comparison

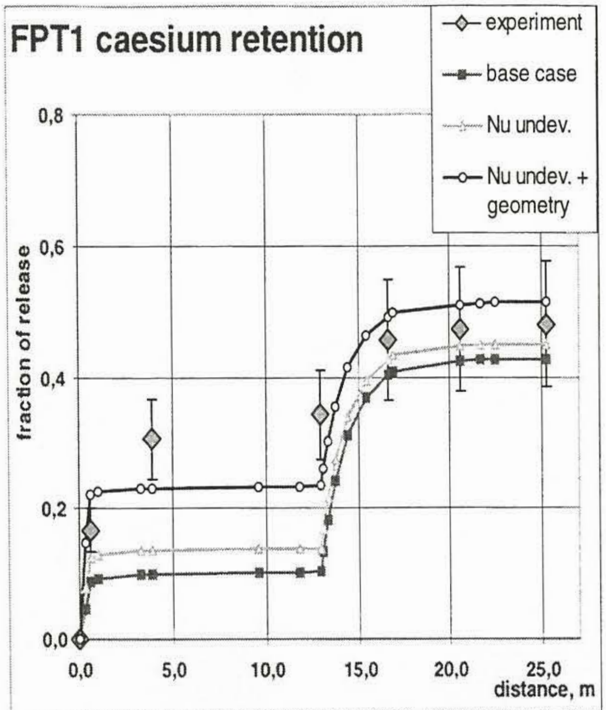

Figure 5: FPT1, caesium deposition profile, SOPHAEROS/data comparison exploring better modelling of mass transfer in the entrance zone.

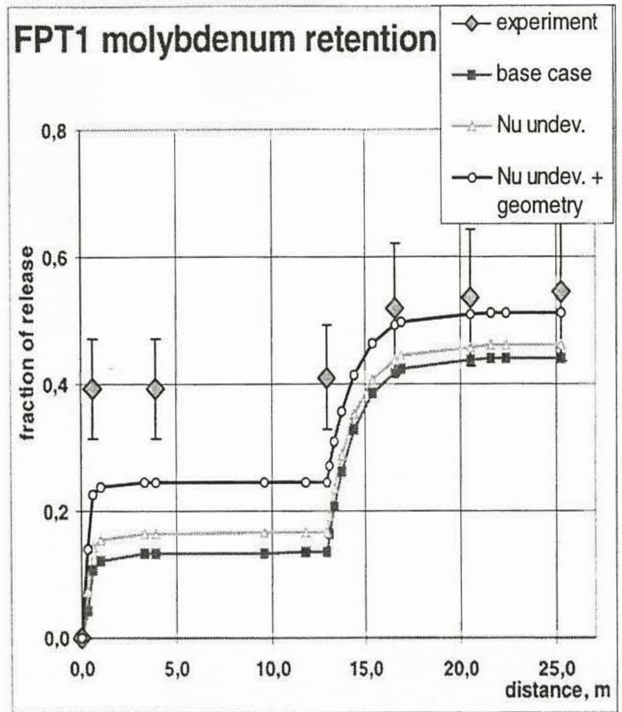

Figure 6: FPT1, molybdenum deposition profile, SOPHAEROS/data comparison exploring better modelling of mass transfer in the entrance zone.

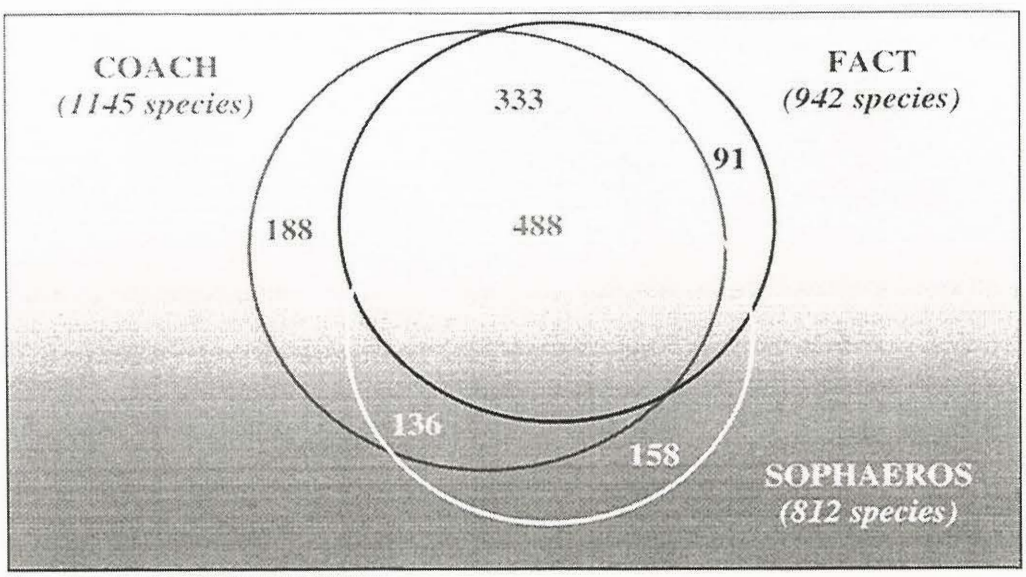

Figure 7. Venn diagram showing the distribution of species within the SOPHAEROS, FACT v2.1 [31] and COACH [32] databases.