STATUS OF SOPHAEROS FISSION-PRODUCT TRANSPORT CODE VALIDATION

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The IPSN (France) code SOPHAEROS has been selected to simulate FP transport and deposition in the PHTS for CANDU safety and licensing analysis. SOPHAEROS 2.0 was acquired by AECL on behalf of COG and will be validated for heat transport system conditions representative of several CANDU accident scenarios. The validation plan is summarized in this paper. SOPHAEROS 2.0 simulations of fifteen phenomena will be validated using thirty validation data sets. The first sets of data to be used for the validation are BTF-104 and FALCON FAL-ISP. A brief description of these experiments is provided, along with the status of the validation work.

1. INTRODUCTION

Modelling fission product (FP) behaviour in the Primary Heat Transport System (PHTS) during accident scenarios is becoming increasingly important in the assessment of accident consequences. As CANDU® licensing methodologies move from bounding assumptions toward "best estimate plus uncertainty", tools are required to predict the time-dependent distribution of fission products throughout the reactor and containment. Properly accounting for fission product behaviour in the PHTS will help achieve the following objectives: (1) improved estimates of doses to safety equipment in environmental qualification (EQ) analyses, (2) improved estimates of public and operator doses from an improved assessment of less volatile radionuclide behaviour, (3) improved ability to perform best-estimate safety analyses, (4) improved post-accident management plans from a better knowledge of FP location, and (5) less restrictive exclusion area boundary (EAB) designs from better source term estimates, an important consideration for some CANDU markets.

It is also important to recognize that the bounding assumption of neglecting fission-product retention in the PHTS may not always be "conservative"[1]. For example, assuming fission products released from the fuel arrive instantaneously in containment can create high

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concentrations in the containment atmosphere early in an accident sequence. These high fission-product concentrations coincide with a period of high airborne water content (particularly when water sprays are used early in an accident to limit the consequences), resulting in efficient agglomeration and settling that cause a rapid reduction in the amount of airborne fission products. On the other hand, a more protracted release can lead to higher airborne concentrations later in the accident sequence when less steam condensation and aerosol settling are occurring. It is for reasons such as these that the Light Water Reactor (LWR) community has been developing and using fission-product transport (FPT) codes.

Since LWR and CANDU reactors both use uranium oxide fuel, resulting in similar fission product releases under accident conditions, a FPT code developed for LWR applications can be readily adapted to CANDU. The primary differences related to PHTS FPT phenomena are the more complicated piping of the CANDU PHTS, the use of carbon steel for CANDU feeder pipes, the presence of more liquid water in the PHTS during CANDU accident sequences, and the absence of control rod materials in CANDU fuel channels. Nevertheless, these differences can be handled in part by the thermalhydraulic input to the FPT code, and by additions to an LWR FPT code. These additions could be: insertion of CANDU-specific chemical species in the SOPHAEROS chemical databank, vapor deposition correlations for carbon steel, inertial deposition correlations for CANDU-specific geometries and modeling of fission-product transport by water. Therefore, the recommended approach for meeting the need for a CANDU FPT code is to adapt an LWR code.

The IPSN (France) code SOPHAEROS[2] has many features that make it attractive for use in CANDU safety analysis. SOPHAEROS was originally developed to modern SQA standards and has the full suite of associated documentation. SOPHAEROS is undergoing active development. GRS (Germany) is also contributing to SOPHAEROS development, in particular in an area that will improve its ability to model FPT in the presence of water. One feature that is very attractive is the use of modern numerical solution techniques that allow SOPHAEROS to solve complex problems in a reasonable time.

Any computer code used for performing PHTS FP retention calculations for CANDU safety analysis has to be subjected to a rigorous phenomena-based validation against the available experimental data[3]. SOPHAEROS 2.0 was acquired by AECL on behalf of COG and will be validated for heat transport system conditions representative of some phases of CANDU loss-of-coolant accident (LOCA), LOCA with additional loss of emergency core cooling (LOECC), stagnation feeder break (SFB), feeder off-stagnation break (FOSB), flow blockage (FB), and fuel handling (FH) accident scenarios. Up to 30 validation exercises will be performed. Canadian and international experimental data will be used, progressing from single-effect experiments through to integrated-effect in-reactor experiments. This paper describes the plan and status of validation of SOPHAEROS 2.0 for application to CANDU safety and licensing analysis.

2. SOPHAEROS VALIDATION

The validation of SOPHAEROS will be performed using the following five-step phenomena-based methodology:

1) review of postulated accidents in the design basis and their associated physical phenomena,
2) assembly of validation matrices that relate postulated accidents to physical phenomena and data sets,
3) preparation of the validation plan,
4) performance of the validation exercises, and
5) preparation of validation reports and validation manuals that document the results of the validation exercises.

This section provides a summary of the steps to be taken to validate SOPHAEROS 2.0 for its required applications.

2.1 Required Applications

SOPHAEROS 2.0 will be validated for the following CANDU design-basis accidents: large break LOCA, LOCA/LOECC, SFB, FOSB, FB and FH accidents. It will not be validated for accident phases or scenarios in which the primary heat transport system remains almost completely full of liquid water, because the current version of the code does not have the capability of simulating fission-product transport in flows of liquid water. The ranges of conditions of interest (pressure, temperatures, flow rate, gas composition, condensation of steam onto walls, fission product and structural material concentrations) for SOPHAEROS validation are the conditions found in CANDU accidents.

The key output parameters upon which SOPHAEROS will be validated are:

- fractional retention of each fission product or simulant in the experimental apparatus between the point of release of fission products into the system and the "break location"[(a)],
- fraction of iodine in vapour phases other than CsI at conditions similar to the "break location", and
- agreement between observed and calculated deposition patterns for each fission product element.

(a) The term "break location" is defined to mean "the location in an experimental apparatus where the conditions are closest to those that would be expected in a CANDU accident scenario at the HTS break". The "break location" for each test will be subject to interpretation depending on the nature of the experimental apparatus.

2.2 Application and Validation Data Set Phenomena

The fission-product release and transport (FPR&T) validation matrix identified 24 FPT phenomena. SOPHAEROS will not be validated for some of these phenomena, either because they are not included in version 2.0 of the code (e.g., they involve liquid water), or because they have not been assigned as primary phenomena for any phase of any CANDU accident scenario.

Fifteen primary phenomena remain for SOPHAEROS 2.0 validation. Thirty test data sets from 15 experiments will be used for the validation of these phenomena. Table 1 lists the importance of the validation phenomena (P-primary and S-secondary) in each of the validation data sets (grouped by experiment type). The table shows that each phenomenon is of primary importance in at least one of the data sets. Indeed, most phenomena are of primary importance in several data sets. However, data sets which cover the same phenomena often do so over different ranges of conditions, so they are not redundant. Each of these data sets will be the subject of a separate validation exercise.

2.3 Validation Exercises

Each validation exercise will be performed according to the following guidelines:

1) Review the data set(s) and the associated experiment. If necessary, qualify the data set(s) by assigning uncertainties to the parameters related to code input and output. Extract the information required to simulate the experiment, including the geometry, operating conditions, key measured parameters, and the uncertainty in each of these values.
2) Prepare the SOPHAEROS input file(s) required to simulate each test case.
3) Run SOPHAEROS 2.0 using the input file(s) and determine the key parameters from values in the SOPHAEROS output file(s).
4) Perform an uncertainty assessment and sensitivity analysis[4].
5) Compare the predicted and measured key parameters, determine the differences and identify any systematic bias.
6) Document the exercise and summarize the results in a validation exercise report.

2.4 Acceptance Criteria

Defining acceptance criteria for simulations of experimental results and deposition under accident conditions in objective, numerical terms is difficult. Clearly, a "base-line" simulation (i.e., one with no changes in the boundary conditions from the best published or calculated estimates) that agrees with an experiment within the uncertainty of the measurements of the key parameters must be described as having "excellent" agreement. The agreement between simulated and experimental deposition data should also be described as "excellent" if they agree within the key parameter uncertainties derived using the uncertainties in experimental boundary conditions.

The agreement between simulated and experimental deposition data will be described as "acceptable" if the simulated data show the same general behaviour as the observed data. The same agreement will be described as "unacceptable" if the calculation does not show the same phenomena as observed in the experiment, or if the location of deposition is grossly shifted.

Criteria must also be placed on the acceptability of the SOPHAEROS 2.0 code for use in safety analysis. In order to credit deposition of a particular fission product in the safety analysis of a particular accident scenario, the code must be able to describe the total deposition of the fission product to the "break location". This must be done within the bounds of:

- the uncertainty related to the accident scenario boundary conditions,
- the experimental errors in those data sets with boundary conditions closely related to the accident conditions, and
- a limited amount of additional code-related model uncertainty (20% of observed deposition for validation against experimental data).

Results for fission products which may be co-deposited (for example, cesium and iodine) should also be inspected carefully if one of them proves to be outside the chosen criterion. The agreement of calculation results with deposition data should be "excellent" or "acceptable". If an experimental boundary condition to which the deposition results are very sensitive was neither controlled nor measured, the data set may have to be rejected from the list of validation exercises.

3. STATUS

As stated above, a total of 30 data sets will be used to validate SOPHAEROS. The first sets of data to be used for the validation of SOPHAEROS, and for which the analysis has begun, are from the BTF-104 and FALCON FAL-ISP experiments.

3.1 BTF-104 Experiment

The objective of the Blowdown Test Facility (BTF) experimental program is to obtain fission product release and transport, and fuel behavior data from in-reactor, all-effects tests under representative accident conditions for benchmarking computer codes used in CANDU safety and licensing analysis. The primary objective of the BTF-104 experiment was to determine the timing, amount and transport characteristics of fission products released from a previously irradiated CANDU-sized fuel element subjected to a high-temperature transient representative of a LOCA with additional LOECC. This experiment was performed in 1993 September in the National Research Universal (NRU) reactor at the Chalk River Laboratories of AECL[5,6]. It was determined that this set of data allows validation on the fractional retention of iodine, cesium and tellurium.

The SOPHAEROS input file for BTF-104 was written based on an earlier VICTORIA idealization[6].

Figure 1 shows a preliminary comparison between calculated and experimental data. A preliminary evaluation of the uncertainties on the experimental data was also made, and they are shown on the figure. For this first comparison, diffusiophoresis has not been modelled, in part because we do not have the requisite thermalhydraulic input data. As a result, the SOPHAEROS simulation underestimated the fractional retentions for I, Cs and Te. The measured depositions of I, Cs and Te were between 80 and 100% and the calculated depositions were approximately 50%. An additional complication is that the blowdown filter in the BTF facility is an effective trap for fission products that is very difficult to model. Additional work is underway to better quantify the experimental uncertainties and to perform the necessary sensitivity analyses to establish the overall modelling uncertainty. With the additional work, we expect that the agreement will be acceptable.

3.2 FALCON Experiment

FALCON[7] is a small-scale facility designed to study the transport and deposition of fission products through a complex pathway that simulates conditions in an LWR severe accident when overheating of the fuel occurs. The Falcon facility was built at Winfrith in the UK. Falcon consists of a high-temperature region to simulate an over-heating core, pipework simulating the upper plenum and hot-leg structures and a containment vessel. An extensive test program led up to the execution of the Falcon International Standard Problem experiments 1 and 2 (FAL ISP-1 and FAL ISP-2, respectively). The purpose of these experiments was to test and assess different models used for fission-product transport and deposition behaviour within the primary circuit and containment. The FALCON FAL ISP tests provided data on (1) the release of fission products and aerosols from simulant fuel and reactor components (control rods) and (2) the subsequent transport and behavior of these aerosols in a simulated PHTS. These tests were performed in a steam/helium environment. The FAL ISP-1 test had a relatively high particle concentration while the FAL ISP-2 test had a lower particle concentration.

An input file for FALCON FAL ISP-1 has been created and preliminary sensitivity studies are underway. Here we present the results of two runs that demonstrate the importance of sensitivity studies. The FALCON facility contained silica components that released Si during the experiments. For the first run, the silicon release was set to zero, and for the second a release rate was chosen that bounded the observed experimental behaviour. (Note that in addition to silicon, boron (an additive to LWR coolant) was also present in the experiments; both these elements lead to the formation of species not typically seen in CANDU accidents). The calculated fractional retention data are shown in Figure 2, with the experimental data. Calculated depositions for Ag, In and U were in reasonable agreement with the experimental results for both runs and Si had a negligible influence on their fractional retentions. The addition of silicon lowered the fractional retention of Cs and B. This can be explained by the fact that when Si is added, less $CsBO_2$ and CsOH were formed, and Cs-Si compounds were present in important quantities. The Cs-Si compounds did not deposit as much as $CsBO_2$ and CsOH did, which explains the lower retention of Cs. More gaseous B compounds (HBO_2 and BO_2) were also formed, which also leads to a lower retention of B.

Based on the results of two sensitivity runs, the fractional retention of Cs and B is influenced by the presence of Si, and their calculated retention values bracket the observed retention values. The deposition behaviour of other elements was not affected by variations in Si, but they can be influenced by other experimental uncertainties, including the release rates of other elements or thermalhydraulic conditions. A complete sensitivity study is required to establish whether or not SOPHAEROS predictions are within the expected range of values that can result from the uncertainties in experimental boundary conditions.

4. SUMMARY

SOPHAEROS 2.0 has been acquired by AECL on behalf of COG and will be validated for fission-product retention calculations under heat transport system conditions representative of several CANDU accident scenarios. The validation process comprises five steps, including the preparation of the validation plan, performance of the validation exercises and the preparation of the validation reports.

The validation plan describes the required applications, the application and validation data set phenomena, the validation exercises and the acceptance criteria. The first validation exercises will use the BTF-104 and FALCON FAL ISP data sets. The preliminary work on the validation exercises demonstrates the importance of complete sensitivity studies to the proper assessment of agreement between experiment and simulation. In the BTF-104 experiment, uncertainties in modelling diffusiophoretic aerosol deposition and in modelling the effects of the blowdown filter must be accounted for. For the FALCON FAL ISP-1 experiment, preliminary runs have shown that uncertainties in silicon release rates can bracket the observed deposition behaviour of Cs and B. Further runs are required to assess the effects of experimental uncertainties in the release rates of other elements, and in thermalhydraulic conditions, on predicted retentions.

5. ACKNOWLEDGMENTS

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6. REFERENCES

1. MALINAUSKAS A.P., "Phenomena Occurring in the Reactor Coolant System During Severe Core Damage Accidents," in Fission Product Transport Processes in Reactor

Accidents, ROGERS J.T. (Ed.), Hemisphere Publishing Corporation, New York, 1990.

2. MISSIRLIAN M. and LAJTHA G., "Validation of SOPHAEROS V1.3 Code Based on Falcon Experiments," Proc. 18th Canadian Nuclear Society Conference, Toronto, Ontario, 1997 June 8-11.

3. MOECK E.O., LUXAT J.C., PETRILLI M.A. and THOMPSON P.D., "Status of Validation Matrices for CANDU® Power Plants," Proc. 18th Canadian Nuclear Society Conference, Toronto, Ontario, 1997 June 8-11.

4. SILLS H.E., DUFFEY R.B. and ANDRES T.H., "MAPLE Research Reactor Safety Margins Uncertainty Assessment Methodology," Proc. 20th Annual Conference of the Canadian Nuclear Society, Montréal, Québec, Canada, 1999 May 30 - June 2.

5. DICKSON L.W., ELDER P.H., DEVAAL J.W., IRISH J.D. and YAMAZAKI A.R., "Preliminary Results of the BTF-104 Experiment: an In-Reactor Test of Fuel Behavior and Fission-Product Release and Transport Under LOCA/LOECC Conditions," Proc. 1995 Canadian Nuclear Society Annual Conference, Saskatoon, Saskatchewan, Canada, 1995 June 4-7.

6. DICKSON L.W., DEVAAL J.W., IRISH J.D., ELDER P.H., JONCKHEERE M.G. and YAMAZAKI A.R., "The BTF-104 Experiment: an In-Reactor Test of Fuel Behaviour, and Fission-Product Release and Transport under LOCA/LOECC Conditions," Proc. 4th International Conference on CANDU Fuel, Pembroke, Ontario, Canada, 1995 October 1-4.

7. WILLIAMS D.A, "OECD International Standard Problem Number 34; Falcon Code Comparison Report," AEA RS 3394, 1994 December.

Table I: Validation Phenomena Covered by Each Experiment

	Validation Experiment												
Fission-Product Transport Phenomenon	BTF-104, BTF-105B	PHEBUS (FPT0,1)	TUBA-D	HCE3, HCE4	Marviken	Mulpuru 2	Mulpuru 4	ORNL VI, CEA VERCORS	CEA DEVAP	FALCON FAL ISP	LACE LA LA3B	Johnson	STORM ISP
Vapor Deposition and Revaporization	P	P		P	P			P	P	P	S	P	
Vapor/Structure Interaction	P	P		P	P			P	P	P		P	
Aerosol Nucleation	P	P		P	P	P	P	S	P	P	S	P	
Gravitational Agglomeration in PHTS	S	P	S	S	P			S		S	S	S	
Brownian Motion (Diffusional) Agglomeration in PHTS	S	P	S	P	S			P		P	S	P	
Turbulent Agglomeration	P	S	S		P						P	S	S
Aerosol Growth/Revaporization	P	P		P	P		P	P		P	S	P	
Thermophoretic Deposition in PHTS	P	P	P	P	P	P	P	P		P	P	P	P
Diffusiophoretic Deposition	S		P		P								
Gravitational Deposition	S	P		S	P			S		P	S	S	
Turbulent Deposition in PHTS	P	S	P		P	P					P	S	P
Laminar Deposition		P	S	P			P	P		P	S	P	S
Inertial Deposition	P	P			P			S		S	P	S	
Aerosol Resuspension	S	S	S		P						P	S	P
Chemical Speciation	P	P		P	P	S		P	P	P	P	P	

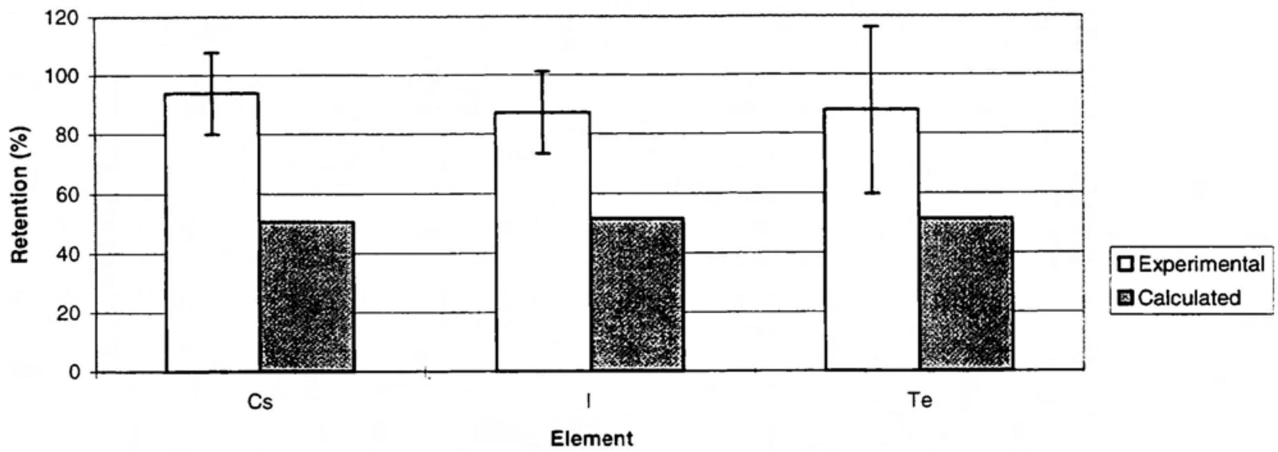

Figure 1: Comparison Between Experimental and Calculated Retentions for the BTF-104 Experiment

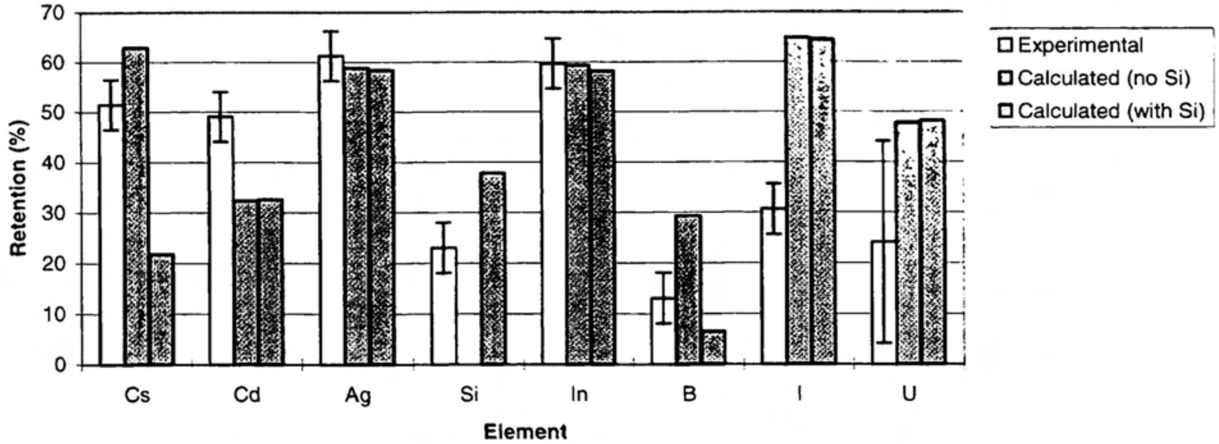

Figure 2: Comparison Between Experimental and Calculated Retentions of Elements in FALCON FAL ISP-1