VALIDATION OF SOPHAEROS V1.3 CODE BASED ON FALCON EXPERIMENTS

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SUMMARY

A key problem in source term evaluation in nuclear reactor severe accidents is determination of the transport behaviour of fission products (f.p.) released from the degrading core. The SOPHAEROS computer code is being developed aiming at predicting in a mechanistic way f.p. transport in LWR circuits. In the first version of the code (1), released in 1994, the main aerosol (coagulation and numerous deposition mechanisms) and fission product vapour (condensation, evaporation and sorption) phenomena were modelled for 12 fission product species. The large number of mass balance equations with non-linear terms were solved using an efficient implicit numerical method.

In the version of the code used in this study, version 1.3 (2), progress has been mainly made with the introduction of vapour-phase chemistry. The basis of the chemical modelling is the calculation of thermodynamic chemical equilibrium of vapour-phase species from elements in the vapour-phase.

Before adding the chemistry module different approaches were considered to determine the fastest numerically robust method. A transient approach based on the deviation from equilibrium was chosen for solution of the equations with 'ideal kinetics'. This means that an artificial mathematical transient is applied to reach the real steady state (equilibrium). The 'kinetics' associated with equilibrium are directly related to the deviation from equilibrium.

The thermodynamic equilibrium assumption means that chemical speciation changes with temperature, carrier gas composition, and the concentrations of vapours. The number of species considered in the calculation can be easily increased or modified by adding data for the new species (name, molar mass, stoechiometric coefficients, equilibrium constant, etc) to the data bank. The default data bank comprises 30 elements and the compound species from these elements.

The SOPHAEROS code has in the past been validated on analytical experiments such as DEVAP, LACE, TRANSAT, TUBA as well as on integral tests of the PHEBUS FP program. In this paper, an example of validation for the fission product vapour transport (chemistry and condensation/evaporation) models is shown. Some tests of the Falcon (3) thermal gradient tube experiments (FAL-17, FAL-18, ISP-1, etc) are used.

The results of the SOPHAEROS 1.3 calculations are compared with the results of the VICTORIA code (4) and the measured data, see Table 1. The input data of the two codes were determined in the same way. It is seen that SOPHAEROS can predict the dominant chemical species and the element retention factors in the silica pipe quite well.

These applications of the SOPHAEROS code to the Falcon experiments, along with others which are not presented here, indicate that the numerical scheme of the code is robust, and no convergence problems are encountered. The calculation is also very fast being 3 times longer on a Sun SPARC 5 workstation than real time and typically about 10 times faster than an identical calculation with the VICTORIA code.

The study demonstrates that the SOPHAEROS 1.3 code is a suitable tool for prediction of vapour chemistry and f.p. transport with a reasonable level of accuracy.

Furthermore, the flexibility of the code « material databank » allows improvement of understanding of fission product transport and deposition in the circuit.

Table 1

Comparison of retention the results for the calculations and measured values

	Cs	I	Mo	Ba	Cd	In	Ag	Te	B	Si
FAL-17 **Experiment**	45%	20%	65%	56%	57%	72%	76%	-	24%	22%
SOPHAEROS	64%	26%	62%	76%	41%	61%	57%	-	19%	19%
VICTORIA	28%	24%	27%	34%	18%	30%	27%	-	32%	-
FAL-18 **Experiment**	55%	75%	-	-	31%	57%	57%	21%		-
SOPHAEROS	47%	29%	-	-	31%	58%	31%	58%		-
VICTORIA	18%	30%	-	-	18%	30%	28%	29%		-

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NUREG/CR-5545 SAND90-0756 Rev.1 December 1992