SOURCE IST 2.0 VALIDATION APPROACH

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ABSTRACT

SOURCE IST 2.0 is a code for calculating the release of fission products from the fuel pellets to the surrounding environment. For most accidents that environment is the Primary Heat Transport System. For other scenarios (such as End-Fitting Failures and Fuel Handling Accidents) it would be the containment atmosphere.

The validation approach being used by the Canadian nuclear industry is founded on the use of:

the Technical Basis Document (which describes controlling phenomena that apply in each phase of a postulated accident),
discipline-specific Validation Matrices (which relate phenomena and ranges of conditions to experimental data sets), and
code-specific Validation Plans (which list the data sets to be simulated and describe their coverage of controlling phenomena and accident conditions).

The controlling phenomena for fission product release from fuel are modelled in the code. For some of these phenomena detailed physical models are employed, but for others assumptions or approximations that lead to limiting consequences are used. This combination of best-estimate and limit-consequence models poses interesting challenges in interpreting validation results.

The nature of SOURCE IST 2.0 as an industry standard tool being developed for multiple platforms has imposed certain requirements on validation activities, *e.g.*, portable test cases, reproducing tests on multiple platforms. This paper describes the approach adopted for SOURCE IST 2.0 in the context of the constraints imposed by the nature of the problem being solved, the nature of the solution methodology selected, and the multi-platform requirements. SOURCE IST 2.0 will be validated using Canadian and international separate effects and in-reactor experimental data sets.

INTRODUCTION

SOURCE IST 2.0 is being developed and validated by Ontario Power Generation Inc., Atomic Energy of Canada Limited, Bruce Power, Hydro-Québec, and New Brunswick Power as

the Industry Standard Tool set code for fission product release from fuel [1]. An Industry Standard Tool is a common code used by all of the partners. An overview of the SOURCE IST 2.0 code and its models is provided in another paper in this conference [2]. The code uses physical models of the phenomena listed as primary phenomena for relevant accidents in the Technical Basis Document and in the Fission Product Release and Transport Validation Matrix to determine the fractions of nuclide inventories that are released during the user-defined scenario. Since the phenomena that govern fission product release from fuel are almost all thermally-driven, it is not practical to perform validation tests on a phenomenon-by-phenomenon basis. For this reason, validation exercises are being performed on a test-by-test basis.

VALIDATION PLAN

The Validation Plan for SOURCE IST 2.0 provides the link between the validation work to be carried out, the Fission Product Release and Transport Validation Matrix, and the Technical Basis Document. The plan identifies the safety concerns related to fission product release and SOURCE IST 2.0. These concerns are:

in-plant dose to plant staff,
dose to in-plant equipment (for environmental qualification), and
dose to the public.

The key input parameters for SOURCE IST 2.0 are:

fuel temperature,
the fuel environment (oxidizing, inert, or reducing), and
fuel burnup.

The fuel type is also important, however, all tests selected have used uranium dioxide fuel. The range of maximum temperatures covered by validation tests is 1373 K to 3030 K. The test environments include: steam, air, argon, argon/2% hydrogen, hydrogen, and steam/hydrogen. The fuel burnup ranged from about 150 MW.h/kgU to 1008 MW.h/kgU. The tests selected included fourteen Canadian tests and four international tests. They can be further broken down as:

6 AECL-Chalk River hot cell tests in steam,
1 CEA Grenoble (France) hot cell test in steam,
3 AECL-Chalk River hot cell tests in air,
3 AECL-Chalk River hot cell tests in inert environments (Ar or Ar/2%H_2),
1 CEA Grenoble hot cell test in hydrogen,
1 Oak Ridge (USA) hot cell test in hydrogen,
2 Canadian in-reactor tests from the Blowdown Test Facility at Chalk River, and
1 International in-reactor test from the PHEBUS test facility in France.

A table in the Validation Plan demonstrates the coverage of primary phenomena for relevant accident classes.

The key output parameters from SOURCE IST 2.0 are the release fractions of radiologically significant radio-nuclides. The release fraction is the fraction of the nuclide inventory that has been released from the fuel. It is anticipated that release fractions from

SOURCE IST 2.0 would normally be used in conjunction with inventories calculated by an isotope generation and depletion code, *e.g.* ORIGEN [3] or ORIGEN-S. Thus, the SOURCE IST 2.0 calculations of inventories *per se* are not key output parameters.

ACCEPTANCE CRITERIA

In formulating acceptance criteria for SOURCE IST 2.0, requirements imposed on the code and experimental uncertainty should be taken into account. A number of criteria were developed based on these inputs.

Bounding Assumptions

Mechanistic models are not available for all of the phenomena modelled by SOURCE IST 2.0. In other cases, modelling of the best state of knowledge is not tractable. In developing SOURCE IST 2.0, design decisions were made so that approximations would result in earlier and/or more complete fission product release. For example, in the absence of knowledge of the chemical speciation and solubility of every fission product in uranium dioxide, the grain boundary sweeping and diffusion models assume that all fission products are swept from the grain by grain boundary movement and that all fission products diffuse from the grains to the grain boundaries. For reasons such as these, calculated results that exceed the experimental observations are deemed to be acceptable.

Required Numerical Accuracy

The required numerical accuracy for the code is stated to be a difference of 0.01 in the release fractions. Thus a difference less than or equal to 0.01 in a release fraction is clearly acceptable.

Relative Tolerance

The differential equation solver [4] and differential-algebraic solver [5] employed in SOURCE IST 2.0 also allow a relative tolerance to be selected. The value used is 10^{-6}. This value is much smaller than the 0.01 numerical accuracy requirement specified for the release fractions in the Software Requirement Specification. Thus, the relative tolerance is not expected to contribute significantly to calculational uncertainty.

Absolute Tolerance

The use of purely relative error control in the numerical solvers can lead to situations in which great computational effort is expended to get accurate results for insignificantly small numbers. The absolute tolerance (ATOL) specified for the solvers allows the programmer to select a value for each variable that is a level at which the answer is deemed to be negligibly small. When the error estimate for a variable is smaller than this value, the result is accepted. Since SOURCE IST 2.0 allows the analyst to determine the mass of initial uranium in the basis

unit, the developers could not select one absolute tolerance that would be appropriate for all cases. A more appropriate choice is to take the absolute tolerance to be related to the initial mass of uranium present. The choice of absolute tolerance for nuclide inventories (in atoms) is 10^{12} times the initial mass of uranium (in kilograms). This corresponds to a mole fraction of about 4×10^{-13} for each fission product or actinide.

The impact of absolute tolerance on SOURCE IST 2.0 results shows up in a number of places. Very short-lived progeny of long-lived parents may exist in a very small mole fraction. In some cases, the short-lived progeny may be the nuclide that emitted the gamma radiation that was counted in the experiment. In these cases, comparison of the calculated parent release fraction to the experimental release fraction for the short-lived progeny is more appropriate.

Also for validation cases with shutdown and decay times that are large relative to the half-life of a fission product (and where appropriate, of its controlling longer-lived parent), the inventory of a fission product may be vanishingly small. The numerical results in this case may be smaller than the error tolerance. In this case, it is unlikely that enough activity from the nuclide is present to be counted in the gamma spectroscopy, so validation comparisons to experiments would not be possible.

Accountings for uncertainties due to absolute tolerance suggest that the calculated release fraction is in fact bounded by values perturbed due to absolute tolerance. The release fraction is given by:

$$\textit{Release Fraction} = \frac{\textit{Atoms Released}}{\textit{Total Inventory}}$$

However, if the atoms released and the total inventory are both perturbed by 2 ATOL then minimum and maximum limits on the release fraction become:

$$\textit{Release Fraction}_{min} = \frac{\textit{Atoms Released} - 2\,\textit{ATOL}}{\textit{Total Inventory} + 2\,\textit{ATOL}}$$

and

$$\textit{Release Fraction}_{max} = \frac{\textit{Atoms Released} + 2\,\textit{ATOL}}{\textit{Total Inventory} - 2\,\textit{ATOL}}$$

Experimental Uncertainty

Experimental uncertainties in release fractions also provide a source of difference between experimental observations and calculated results. When experimental uncertainties in release fractions are available, agreement will be deemed to be acceptable if the calculated results are within 2σ of the experimental results.

MEASURES OF AGREEMENT

Providing measures of accuracy for a code is part of the validation process. Two simple statistical measures [6] have been adopted for SOURCE IST 2.0. These are the mean difference and the root mean square difference between the calculated and experimental values of a release fraction. The sign convention adopted for the difference is intuitive in that a negative difference implies that the code calculation was smaller than the experimental value. The measures are defined mathematically as follows:

$$Difference = Code\ Calculation - Experimental\ Value$$

$$MeanDifference = \frac{\sum_{i=1}^{n} Difference_i}{n}$$

$$RootMeanSquareDifference = \sqrt{\frac{\sum_{i=1}^{n} \left(Difference_i^2 \right)}{n}}$$

The sums are calculated for each nuclide for which pairs of calculated and experimental values are available.

COMPUTER PLATFORM ISSUES

To date all SOURCE IST 2.0 validation exercises have been performed using executables created with Digital (COMPAQ) Visual Fortran and run on Intel-based desktop computers using Windows operating systems. At the start of SOURCE IST 2.0 development, each partner selected a target platform on which to run the code. The intention is to repeat the base cases of each validation exercise on each to determine whether platform-related issues have any effect on results. Some of the development of the code has been undertaken on other platforms employed by the IST partners and platform dependencies have been identified and managed.

Language Standards

SOURCE IST 2.0 is written in Fortran-77 [7] with a limited number of Fortran-90 [8] extensions. The extensions were selected based on wide support by compiler vendors and the belief that selected extensions would allow a better quality of Fortran code to be written. The intent is to allow SOURCE IST 2.0 to run on platforms selected by the industry partners, to isolate platform dependencies, and to allow the code to be patched where necessary for each platform. For example, the record length for unformatted files is stated in bytes for COMPAQ

Visual Fortran running on Intel-based desktop computers and for xlf on the IBM RS/6000, but is specified in four-byte words for Lahey-Fujitsu Fortran running on the same Intel-based desktops. Since this value is platform-dependent, it has been isolated as a parameter for the code. The value of the parameter can be altered prior to compiling for a different platform. A naming convention has been established which allows code versions for different platforms to be identified.

Numerical Floating-Point Issues

All of the hardware selected provides support for the Binary Floating Point Standard (IEEE-754-1985) [9]. For this reason numerical results should be in good agreement across platforms. The software support of this standard by each compiler vendor is generally very good. In fact, SOURCE IST 2.0 development led directly to improved support by one vendor.

CONCLUSIONS

1. Industry cooperation with development and qualification of SOURCE IST 2.0 has been invaluable.

2. SOURCE IST 2.0 is being validated against 18 experiments covering a range of experimental conditions for key input parameters.

3. Simple statistical measures can be used to quantify the differences between experimental observations and code calculations.

4. Cross-platform development of SOURCE IST 2.0 has allowed some platform dependencies to be identified and addressed during development. Cross-platform validation is planned to identify whether there are more issues on any of the other platforms selected by the IST partners.

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