SIMULATION CODES AND THE IMPACT OF VALIDATION/UNCERTAINTY REQUIREMENTS

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ABSTRACT

Several of the OECD/CSNI members have adapted a proposed methodology for code validation and uncertainty assessment. Although the validation process adapted by members has a high degree of commonality, the uncertainty assessment processes selected are more variable, ranging from subjective to formal. This paper describes the validation and uncertainty assessment process, the sources of uncertainty, methods of reducing uncertainty, and methods of assessing uncertainty.

Examples are presented from the Ontario Hydro application of the validation methodology and uncertainty assessment to the system thermal hydraulics discipline and the TUF (1) system thermal hydraulics code.

1. INTRODUCTION

The OECD/CSNI validation methodology can be broken into five stages, each associated with one of a structured set of documents, as shown in Figure 1. The first two stages, the Technical Basis Document and the Validation Matrix, are generic documents for a specific discipline without reference to any specific simulation code. The remaining stages, the Validation Plan, the Validation Exercises and the Validation Manual, are concerned with a specific code version. The purpose of the validation process is to:

1) develop a consistent basis for validation within the various disciplines associated with safety analyses;

2) clarify the phenomena and inter-relationships with other phenomena, with specific accident scenarios and with safety concerns;

3) cross reference these phenomena to qualified data sets; and

4) document the comparison to these data sets and the uncertainty in the comparison.

The foundation for uncertainty assessment is laid with the Technical Basis Document and is finalized in the Validation Exercises and Validation Manual.

2. VALIDATION PROCESS DOCUMENTS

Technical Basis Document

The primary purpose of the Technical Basis Document is to relate key safety concerns (*e.g.*, fuel channel integrity) with phenomena[1] and provide an overview of the technical basis for accident analyses performed to quantify the consequences of events in an accident scenario (*e.g.*, large break LOCA).

The process begins by listing **all** phenomena associated with the discipline in question. The key parameters by which each phenomenon would be identified should also be developed at this point. The key parameters become the focus of the uncertainty analysis.

The Technical Basis Document also identifies the accident scenarios and the phases of those accidents which are to be validated. For each phase of an accident scenario, the appropriate governing and secondary phenomena should be identified.

The process of creating a Technical Basis Document provides, for each accident scenario, a justified and rational set of governing phenomena and key parameters which address key safety concerns. Table 1 provides an example of a cross-reference table of phenomena and accident scenarios.

2.1 Validation Matrix

The purpose of the validation matrix is to relate important phenomena to data sets in which the phenomena are known (or expected) to occur. The data sets can be from operational experience, analytic solutions, single effect tests, integral tests and/or cross-code comparisons with other validated codes. The data sets themselves must be validated, qualified and their sources of error/uncertainty identified. Data sets which have been used for model building should not be used for model validation.

The key matrices in this document cross-reference the phenomena (rows) with data sets (columns) which provide validation of the selected phenomena for each accident scenario. The number of filled cells in the matrix, particular in the same column, provides a convenient summary of the ability to validate codes in the selected discipline. Table 2 provides an example of a cross-reference matrix of phenomena and data sets.

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[1] Although several definitions can be found, a useful way of selecting phenomena is to assume they are the cause of a change of state. Phenomena are not properties of materials nor quantities used to characterize a process (*e.g.*, thermal conductivity).

A summary description of the phenomena and the test facilities would complete this document. A suggested phenomenon summary would include:

1) a technical background indicating the manner in which the phenomena influence behaviour during accident scenarios;

2) a summary of the state of knowledge and uncertainties in qualifying the phenomenon;

3) a brief summary of the potential impact of uncertainties in the phenomenon on expected behaviour during accidents;

4) a listing of related phenomena; and

5) key references to papers or reports that describe or quantify the phenomenon.

2.2 Validation Plan

The Validation Plan is a specification document for a particular code version. This document details what will be done to demonstrate that the code version accurately represents the governing phenomena for selected accident scenarios. The plan also identifies the intended application(s) for which the code version is being validated.

The criteria for the selection of sub-matrices from the validation matrix should be identified. The selection criteria should be based on the key parameters and governing phenomena for the code application(s) being validated. Important interactions between phenomena should be addressed through integral experiments or by selecting tests having multiple (and over-lapping) phenomena represented.

The method by which uncertainties will be assessed should also be addressed in the plan document.

2.3 Validation Exercises

The Validation Exercises reference the governing phenomena to be assessed and the data set, or related data sets, to be used for validation. The quality, errors and uncertainties associated with the data sets should be discussed. The test apparatus and procedure associated with the data sets should be described.

If code modifications are required to match test conditions, the impact of those modifications on the validation must be addressed.

On completion of the simulations and comparisons, the sensitivity of key output parameters to key input parameters, and the accuracy and uncertainty of the comparisons should be qualified.

2.4 Validation Manual

The Validation Manual is a summary document based on the Validation Plan and Validation Exercises illustrating how the technical basis for validation has been satisfied. The document also summarizes the accuracy and uncertainty associated with code predictions for intended applications.

3. EXPERIMENTAL UNCERTAINTY AND QUANTIFICATION OF PHYSICAL PHENOMENA

There are several issues to be addressed when comparing simulation predictions to data sets. These issues include:

1) ascertaining the portion of the uncertainty in a code-to-data comparison that is attributable to the code;

2) choosing the appropriate form of data reduction to reduce uncertainty;

3) evaluating the effect of sensor characteristics and response on data values (*e.g.*, eliminate sensor variable response by time series analysis);

4) identifying inherent large scatter data (*e.g.*, waterhammer; a stochastic process) and designing methods of treating it;

5) minimizing the impact of uncertainties with respect to margins to the limit of the operating envelope; and

6) selecting a tractable uncertainty analysis methodology.

The validation documentation identifies and ranks the governing phenomena, key parameters and supporting data sets. Uncertainties in the process must be explicitly recognized either as probabilistic, through sensitivity/parametric analysis, expert judgement, use of conservative assumptions, *etc.*

Some phenomena cannot be measured directly either due to their nature, a hostile test environment (*e.g.*, BTF), and/or measurement difficulties (*e.g.*, quality meter, two-phase flows).

Figure 2 illustrates the components of uncertainty whether from experimental or modelled behaviour. On the experimental side, gain, systematic error (bias) and random variation exist. On the modelling side, a "user" effect[2], time/space resolution approximations, uncertainty in initial and boundary conditions, and sub-model uncertainties and bias exist. The measurement

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[2] The user effect is related to the range of answers possible when different users create the "same" simulation.

error can be systematic or due to impact of the sampling rate of digital data, sensor drift (*e.g.*, aging, transmutation), sensor dead time, data "smoothing"/filtering, environmental uncertainties, and noise.

The simulation bias determined from the validation exercise is the error or accuracy of our simulation. Uncertainty is not error, it is just uncertainty. Uncertainty in key parameters can be assessed either by formal statistical means or, where formal methods are not available, as the high/low range based on expert judgement/consensus.

4. UNCERTAINTY METHODOLOGY

A number of methods of assessing uncertainty in simulation codes have been, or are being, developed. For our large simulation codes, only a few of the methods are practical. The method adopted should account for changing sensitivities during the course of the simulation and cross-correlation between parameters.

In some applications, a simple root mean square (RMS) approach is used to combine uncertainties. This method assigns all uncertainties equal importance, implies that each uncertainty component is independent of the others, and implies that the variation in parameters is normally distributed. For certain applications, these assumptions are justified while in others the method may significantly over-estimate the uncertainty in key output parameters.

For small simulation codes, a Monte Carlo sampling approach can be used directly. If the probability distribution functions (PDFs) for the input parameters are known, they can be sampled directly to generate many simulations to permit PDFs for the output parameters to be created. The method accounts for propagation of uncertainties from the input to the code outputs, does not account for correlated inputs, but allows uncertainties in output parameters to be extracted from their PDFs. If only the key input parameters are sampled (*i.e.*, negligible correlation), the uncertainties in output parameters are better defined. The number of simulations required can be decreased if stratified sampling methods (*e.g.*, latin hypercube (2)) are employed.

For larger simulation codes, response surface techniques (2) in which key input parameters are related to selected output from a series of simulations to create a simplified analog (*i.e.*, response surface) of the simulation code. The response surface is then treated as a small simulation code as in the preceding paragraph. Since the response surface is an approximation of the simulation code, the "goodness" of the uncertainty analysis is limited by the "goodness" of the approximating response surface.

Two other methodologies have been investigated with limited success; adaptive control theory analog (3) and interval arithmetic (4):

1) The adaptive control theory analog (*i.e.*, Kalman filter) uses the difference between experimental measurement and the simulation as the error signal in the adaptive control (Figure 2).

2) Interval arithmetic provides a means of accounting explicitly for ranges of variables (both input and output) during a solution. The approach has been demonstrated for simple, steady-state systems but tends to become divergent for time series analyses.

An uncertainty analysis methodology has been developed for the French CATHARE system thermal hydraulics code. The technique is referred to as the Discrete Adjoint Sensitivity Method (5). The method requires two simulations for a complete uncertainty assessment; one a normal simulation, the other an adjoint simulation. The technique is under assessment for use with Ontario Hydro's larger simulation codes.

While other methods are being investigated, uncertainty analysis is being performed using linear error propagation (6). In this method, a set of input parameters, $\{x_i\}$, with uncertainties, Δx_i, are used to estimate the uncertainty in an output parameter, C, by combining the uncertainties and the sensitivities, $\partial C/\partial x_i$, using the expression:

$$\Delta C = [\ \Sigma((\partial C/\partial x_i)\ \Delta x_i)^n]^{1/n}$$

where n = 2, if the x_i are independent and their uncertainties are normally distributed,
= 1, for a total derivative expression.

To approximate independence of the x_i only key input parameters are considered as the key parameters are most likely to form an independent set. The Δx_i are assumed to represent 95% confidence limits and are evaluated using formal methods or are based on high/low ranges determined by expert judgement/consensus.

5. IMPACT

There are several impacts arising from the requirements for validation and uncertainty assessment:

1) The validation methodology provides a rational and defensible basis for validating simulation codes.

2) Data sets which contain error and uncertainty information, and which are themselves validated, are required.

3) The validation matrices provide important evidence for the judicious selection of further experiments.

4) The significant effort required in validating a simulation code and its associated uncertainty assessment should keep the number of code versions to a small number (*i.e.*, incremental changes in codes should become a thing of the past).

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TABLE 1
SYSTEM THERMAL HYDRAULIC PHENOMENA RELEVANT TO ACCIDENT ANALYSIS

ID #	PHENOMENA	Large LOCA	LOCA/ LOECI	Small LOCA	LOF	LOR	Feed Water Line Break	Steam Line Break
TH1	Break Discharge	✓	✓	✓			✓	✓
TH2	Coolant Voiding Rate	✓	✓	✓	✓			
TH3	Phase Separation; Channels	✓	✓	✓	✓			
TH4	Phase Separation: Headers	✓		✓				
TH5	CHF & PDO Heat Transfer	✓	✓	✓	✓	✓		
TH6	End-fitting Blowdown	✓	✓					
TH7	End-fitting Heat Transfer	✓	✓	✓	✓	✓		
TH8	...							
TH9								
TH10								
TH11								

LOCA Loss-of-Coolant Accident
LOECI Loss of Emergency Coolant Injection
LOF Loss of Flow
LOR Loss of Regulation

TABLE 2
SYSTEM THERMAL HYDRAULIC PHENOMENA and RELEVANT DATA SETS FOR CODE VALIDATION

ID #	PHENOMENA	IN 1	IN 2	IN 3	IN 4	IN 5	IN 6	IN 7	IN 8	IN 9
TH1	Break Discharge Characteristics			□			□	○		
TH2	Coolant Voiding Rate			□			□	○		
TH3	Phase Separation: Channels			□	□				○	
TH4	Phase Separation: Headers									
TH5	CHF & PDO Heat Transfer								○	
TH6	...									

□ primary source
○ seconadry source

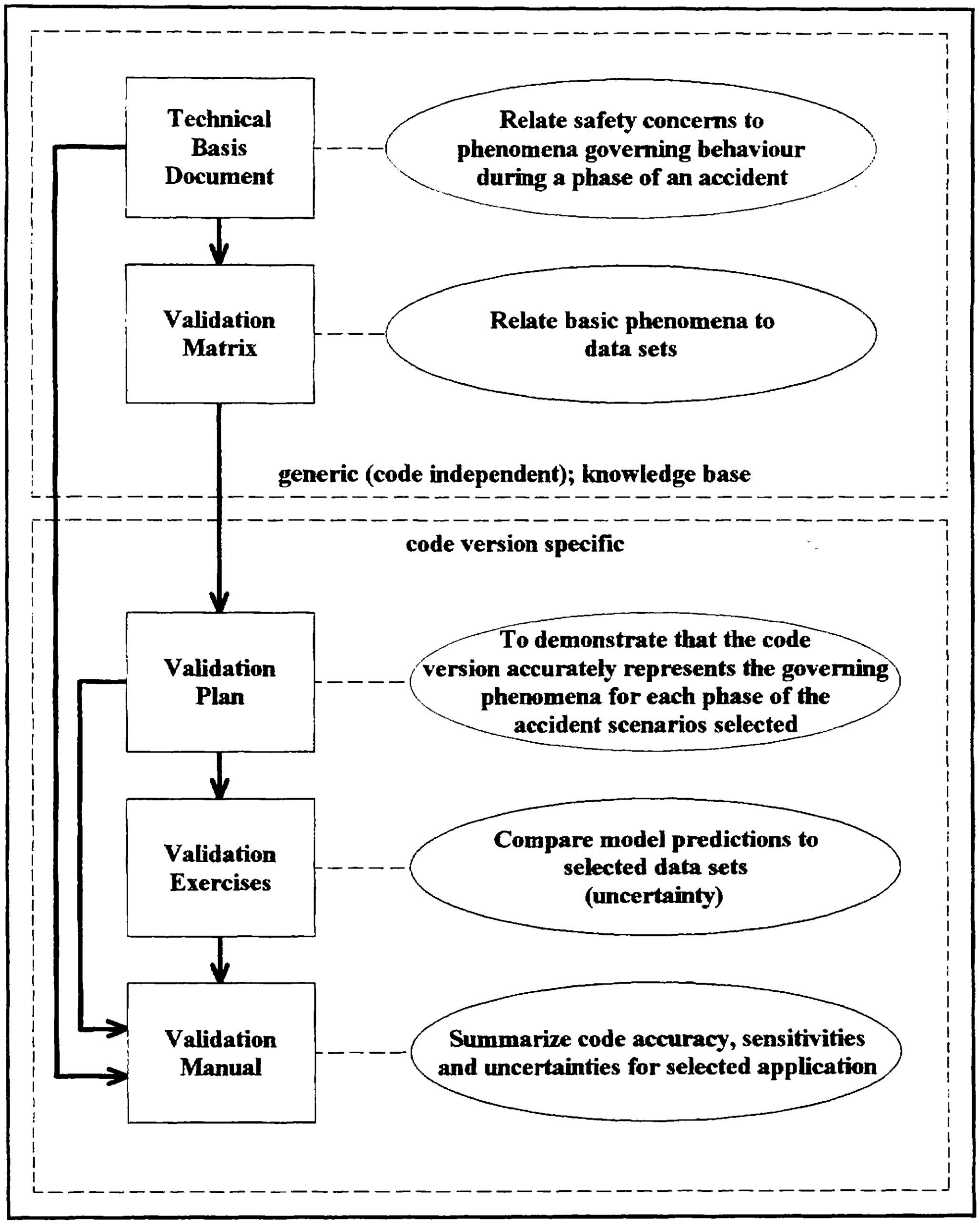

FIGURE 1

VALIDATION METHODOLOGY

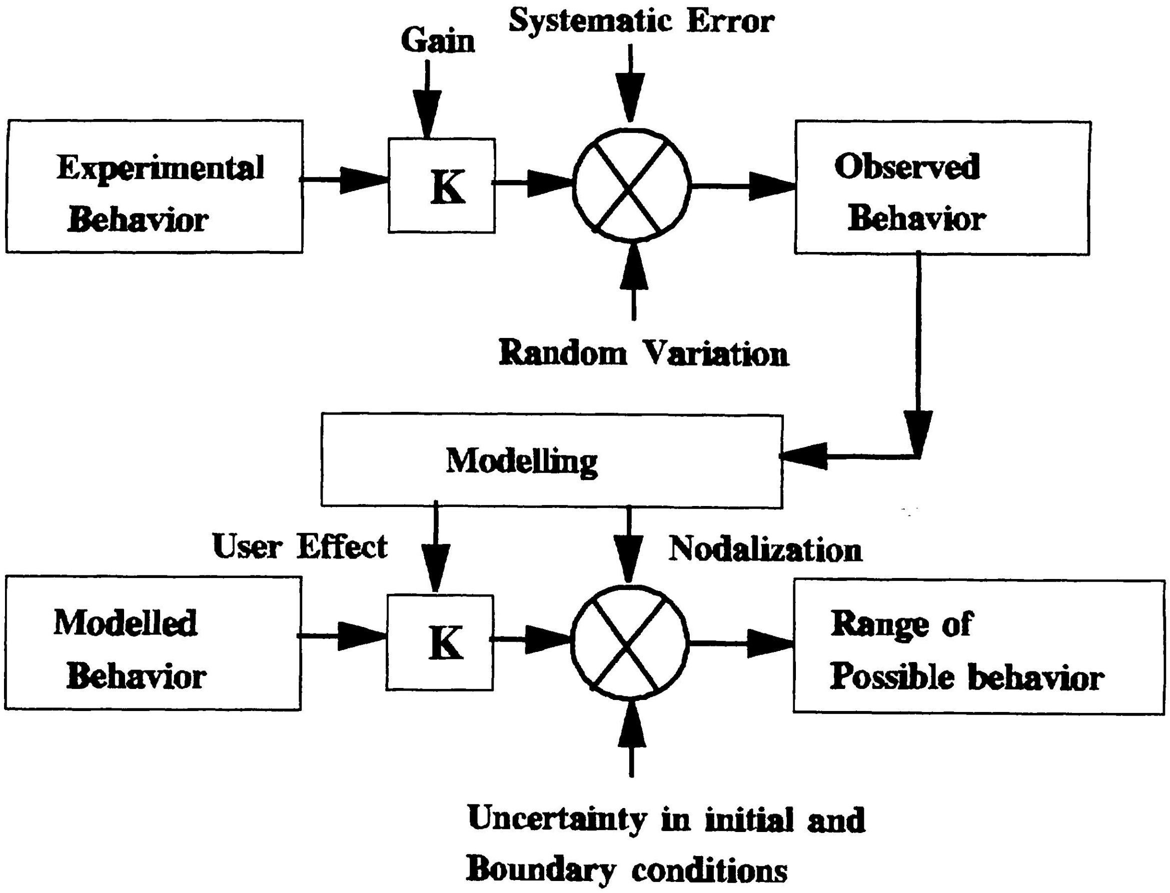

FIGURE 2

COMPONENTS OF UNCERTAINTY