

# Validation of Computer Codes Used in the Safety Analysis of Canadian Research Reactors by W. E. Bishop and A.G. Lee AECL 2251 Speakman Drive Mississauga, Ontario L5K 1B2 Phone: (905)823-9040, FAX: (905)403-7347

E-mail: leea@aecl.ca

#### Abstract

AECL has embarked on a validation program for the suite of computer codes that it uses in performing the safety analyses for its research reactors. Current focus is on codes used for the analysis of the two MAPLE reactors under construction at Chalk River but the program will be extended to include additional codes that will be used for the Irradiation Research Facility. The program structure is similar to that used for the validation of codes used in the safety analyses for CANDU<sup>®</sup> power reactors.

### 1. Introduction

There is a continuing trend towards the application of increasingly sophisticated computer codes to the safety analysis of nuclear reactors. The reasons are three fold; the industry need to use more realistic assumptions in establishing the consequences of postulated accidents and thereby demonstrate overall lower risk; the regulator's requirement for the analyses of increasingly lower frequency events that tend to involve phenomena that are difficult to model and for which little experimental data is available; and the availability of increasingly powerful computers. Regulators in the nuclear power industry have in recent years placed increasing emphasis on the validation of the computer codes used in the mechanistic analysis of accident sequences leading to public dose consequences. This has resulted in multi-million dollar expenditures for the industry. In Canada, the Atomic Energy Control Board, the AECB, has now turned its attention to the validation of analysis codes used in the safety analysis of research reactors, requiring the license applicant to have completed an approved validation program prior to the start of nuclear commissioning of the reactor and experimental facilities. AECL has initiated a formal validation program for its MAPLE reactors: the two MAPLE reactors being constructed for MDS Nordion Inc., the worlds largest supplier of medical isotopes and the proposed Irradiation Research Facility or IRF that will be the successor to the NRU reactor. The validation program for the MDS Nordion reactors is underway and that for IRF will be complete by 2001, coinciding with completion of the program for CANDU power reactors.

#### 2. The Goal of Validation

There are currently a number of codes, standards and guides dealing with "verification" and "validation" that attempt to define these two English language words, usually in the context of some regulatory obligation. So as not to be pre-occupied with precise and

explicit definitions yet again, the focus of the following will be on concepts as understood by the analysis practitioner.

Nuclear engineering is very much characterized by the mathematical representation of phenomena and the performance of tests to establish their representation (correlations) or to show that the representation captures reality under anticipated circumstances, albeit with some degree of uncertainty. Safety analysis attempts to predict the consequences of events in which the phenomena participate, using these correlations or models simply because, in most cases, the real events cannot be created because of their potential hazard (there have been some exciting representative tests in the past, related to rapid reactivity additions, in which special provisions have been made to minimize the hazard). The process that is referred to as validation provides a quantification of the uncertainty in the output of the analysis. When computer codes are used to perform the analysis, the programming of the correlations, their inputs, and outputs in computer language must be checked for correctness or verified.

Computer codes used in safety analysis generally model components and systems by the phenomena that characterize their behavior. For example, a thermalhydraulics code will represent the phenomena of resistance of flow through a pipe with an equation or a collection of empirical data derived from experimental data. The parameter that mathematically represents the phenomena is referred to as a resistance coefficient 'k' which defines the relationship between flow and pressure drop. A more complex example is the mathematical representation of the phenomena of heat transfer from reactor fuel to the coolant. The heat transfer model typically incorporates a large group of parameters from fuel geometry to inlet coolant conditions. The model might consist of a mathematical equation for a certain range of parameters and empirical, look up tables for another range. Quite often the heat transfer model of the fuel is coupled to a model of the coolant so that the phenomena of reactivity changes due to coolant/moderator density or temperature changes can be modeled. A single computer code might be designed to model a single phenomena or a host of interconnected modules each representing a phenomenon. Consequently when one refers to "code validation", validation of a single phenomenon or a group of phenomena is intended.

In carrying out a safety analysis, a code or suite of codes is used to track the sequence of events that result from an initiating event in order to demonstrate that the design of the reactor and its systems either prevents or sufficiently limits the radiation exposure of onsite personnel or the general public. To do so within an acceptable level of uncertainty it is necessary to demonstrate that the model of the phenomena is representative for the range of parameters that occur during the event. Returning to the simple example of the pipe model, it is necessary to show that the equation used to calculate the parameter "k" is valid for the range of flows experienced during the event, from forced circulation to thermosyphoning, and that it is valid for the actual piping material to be used with its characteristic surface roughness, ovality, etc. The first step in validation is to examine the experimental basis for the model to ensure that the range of parameters are included. If not it would then be necessary to obtain additional experimental data that could be used to test the model or alternately used to generate a new model. Regardless of the outcome, the validity will be demonstrated but within a range of uncertainty arising from errors in the experimental data and/or the agreement between the calculated and measured value. The ultimate aim of the validation process is to quantify the uncertainty so that it can be taken into account in the sequence of events and its outcome. Typically the more important the phenomena, the smaller the range of uncertainty that is acceptable and the greater the need to demonstrate the validity of the representation. The tendency is to compensate for deficiencies in the representation of the phenomena by assigning a conservative uncertainty that makes the outcome worse and in many instances misrepresents real risk. The importance of the phenomena can change during the sequence of events. For example, pipe resistance can be a governing phenomena during an event in which thermosyphoning through a piping system prevents fuel failure during decay heating but of lower importance during forced circulation.

The scope of validation can be expected to expand as conservative assumptions are replaced by mechanistic analysis to reduce uncertainty and to better quantify and not overstate the risk of an event.

# 3. The Application of Codes to the Safety Analysis of MAPLE Reactors

The MDS Nordion reactors are dedicated to isotope production and consequently are the simplest MAPLE reactor configuration with a compact core surrounded by a volume of heavy water which acts as both a reflector and a moderator for irradiation facilities outside of the core. The core consists of an arrangement of 19 vertical fueled flow tubes that are supplied with light water coolant from a plenum located beneath the core. The reactor structure is located at the bottom of a light water filled pool. The fuel consists of bundles of elements containing  $U_3$ Si dispersed in an aluminum matrix that is surrounded by a co-extruded aluminum sheath. Reactor control is achieved by the insertion of hafnium tubes into the core. Shutdown is achieved by dropping similar tubes into the core or by partially removing the heavy water surrounding the core. The reactor pool is located in a reactor hall which is vented to a filtration system and a tall remote stack, all of which constitute a confinement boundary. The reactors are under construction at the Chalk River Laboratories where the outer security gate that defines the exclusion boundary is about 8 kilometers from the reactors.

The primary code used in accident analysis is a thermalhydraulics code, CATHENA, which incorporates a point kinetics model for the core. Reactivity effects arising from control and shutoff rod motion, heavy water dump, moderator density and temperature changes, for example, are modeled using input data generated by other codes such as WIMS-AECL/3DDT and MCNP. The heat transfer model is based on correlations developed from electrically heated fuel element simulators. The parallel fueled channels are grouped according to fuel bundle power and the bundle and element with the highest linear power rating is identified. The focus of the analysis of a particular event is the critical heat flux ratio experienced as critical heat flux is the primary criteria chosen for fuel failure. The most severe group of accidents analyzed is the rapid interruption of flow to the reactor fuel caused by pump seizure, rapid isolating valve closure or guillotine failure of the primary cooling piping. The reactor has a single primary cooling circuit that is supplemented by a pressurized accumulator which supplies cooling water during the transition to thermosyphoning flow.

The Irradiation Research Facility reactor is the most complex MAPLE reactor configuration as high pressure and temperature test facilities, beam tubes and a liquid

hydrogen cold source are incorporated. Not only do these individually add their own contribution to the suite of accidents analyzed, but the distributed and separated core configuration leads to potential loss of regulation accidents arising from non-symmetric control rod movements. CATHENA is again the primary transient analysis code and is well developed to analyze events associated with the test facilities that operate at CANDU<sup>®</sup> conditions. The model integrates the reactor and its systems with those of the experimental facilities so that any impact of a failure in a test loop on the core reactivity or other system, e.g., the primary cooling system, is correctly captured. In addition, the point kinetics model of the core is replaced by a dynamic multidimensional physics code which is capable of analyzing flux and power distribution with time. This code, which is still in a developmental phase, is interfaced with CATHENA thus providing the capability to analyze events where non-symmetric flux effects occur. As the IRF will be used to develop CANDU<sup>®</sup> fuel, two types of fuel must be modeled for fission product inventory, and different failure criteria applied in the analysis. Also whereas fission products from the reactor fuel are released to the pool water, those from test fuel are released to the test coolant loop and in the event of a failure of the coolant boundary, to the loop room. Consequently two models are required for fission product release and transport.

Blockage of a single fuel channel can be postulated to occur in both the MAPLE and the IRF reactors. This accident is analyzed using CATHENA to determine the minimum size of the blockage with other methods used to analyze fission product release. Since dose consequences are the major concern, the codes used to analyze the event focus on fission product retention, dispersion and dose consequences.

TABLE 1 provides a summary listing of the codes used in the safety analysis of MAPLE reactors.

4. Code Validation for MAPLE Reactors

For its research reactors, AECL has chosen to adopt to the extent practical, the code validation methodology that it and the Canadian nuclear power industry is applying to the safety analysis of the CANDU<sup>®</sup> power reactor. The method involves five steps.

Preparation of a Technical Basis Document

The Technical Basis Document or TBD identifies the phenomena which govern the sequence of events that occur in the various accidents that are to be analyzed. Firstly, the safety concerns arising from accidents are identified. These typically would be the release of fission products from fuel to the environment with dose consequences. Where heavy water is utilized in the reactor, the release of tritium is also a concern. Working with a selection of bounding events established from a systematic review of components and systems and their operation, the sequence of events through the stages of the accident are examined to identify the phenomena that govern their outcome. The parameters that define the phenomena are also identified along with their range. It is helpful to associate the phenomena with a particular discipline to assist in the preparation of the subsequent Validation Matrix and Validation Plan and as a cross check for completeness by comparison with phenomena. As an example of the methodology, for a primary cooling pump seizure, the safety concern is melting of the fuel and consequent fission product

release. The governing thermalhydraulics phenomena is heat transfer to the coolant as the flow regime transfers from forced to thermosyhoning. The parameters are the power in the elements and the surface heat flux, the coolant flow, pressure, and inlet temperature. The governing physics phenomena are coolant reactivity feedback and the negative reactivity effects from the movement of the shutoff rods. The parameters are coolant density and temperature, the reactivity worth of these for a given core configuration, and the position of the shutoff rod at a point in time and the reactivity worth of the rods as a function of position, again for a given core configuration.

Discipline	Code	Application
Physics	WIMS-AECL	2-D neutron transport code for preparing multi-
		group macroscopic cross sections and diffusion
		parameters
	3DDT	3-D neutron diffusion code for calculating core
		power distributions, reactivity worths of
		assemblies, reactivity changes as functions of
		fuel burn up, control rod position, coolant
		temperature, coolant void and fuel temperature
	MCNP	3-D neutron Monte Carlo code for calculating
		element powers, core power distributions,
		reactivity worths of assemblies, neutron flux
	TANK	distributions and gamma dose rates
	TANK	2-D neutron kinetics code for simulating
	DONJON	asymmetric reactivity transients
	DONJON	A dynamic 3-D neutron diffusion code that can
		be coupled with thermalhydraulic analysis code to provide physics parameters on a time step
		basis.
	ORIGEN-S	fuel depletion and fission product inventory code
	ORIGEN-5	ruer depiction and rission product inventory code
Thermalhydraulics	CATHENA	1-D thermalhydraulics code for steady-state and
		transient thermalhydraulic behaviour, includes
		point kinetics model for neutron feedback
Dose Dispersion	PEAR	Fission product dispersion and dose calculation

TABLE 1: List of Codes Used in Safety Analyses for the MAPLE Reactors

Preparation of Validation Matrix

The Validation Matrix is a two dimensional matrix of primary phenomena and experimental data against which the mathematical model is to be validated. Where a particular phenomena could occur within different ranges of parameters, multiple entries are made. Several diverse sets of data for each phenomena are advisable. Identifying appropriate data is extremely important and key to efficient completion of validation exercises. As an example of a matrix entry, the fuel heat transfer model used in CATHENA for establishing critical heat flux conditions will be validated against a series of heat transfer experiments.

## Preparation of Validation Plan

An important step in establishing budget and schedule, the Validation Plan identifies the validation exercises that will be carried out using existing data or the experimental programs needed to create the data.

# Validation Exercises

Validation exercises involve the modeling of the experiments and the comparison of predicted and experimental results in order to quantify the uncertainty to be applied in a specific application of the code. Although this might appear to be straightforward, in practice the interpretation of the differences in results can be quite complex. The uncertainty in the data, random and systematic errors, must be quantified using statistical techniques that are appropriate for the quantity of available data. Although the model might be tuned slightly to provide better agreement between measured and predicted results, the underlying assumptions in the model must be examined carefully to ensure that they are valid. For example the assumption that heat transfer correlations based on local conditions at a fuel element predict bundle behavior could indeed be invalid should the predicted and measured results disagree significantly after all experimental uncertainties have been accounted for. The deliverable of the exercise is a report that quantifies the uncertainty to be applied to analysis results.

# Validation Summary

The validation summary provides a guide to the analyst for the uncertainty that should be applied to the results of the analysis of a particular scenario or sequence of events. The summary will also include a sensitivity analysis that shows the variation of key output parameters to variations in key input parameters. The summary document will identify the computer program or code that was validated and refer to the Technical Basis Document, the Validation Matrix, Plan and Exercises. It will identify the scenarios for which the code was validated and the range of parameters for each scenario. It will also tabulate the simulation error for each key output parameter, both a best estimate and a 95% confidence level. Any unusual behaviors or constraint on code usage will also be noted.

## 5. Validation Activities for MAPLE Reactors

The Technical Basis Document, Validation Plan for the codes used in the analysis of the MDS Nordion MAPLE reactors have been completed and validation exercises are underway. Preparation of the TBD for the IRF reactor has begun and will proceed in concert with that being prepared for CANDU facilities.

The validation exercises for the static physics codes that are used to provide fuel power and reactivity coefficients will use experimental data derived for validation by other users of the codes in the nuclear industry. The most important data comes from the suite of static and dynamic commissioning tests performed for the HANARO reactor. It is proposed to use a dynamic physics code for the IRF reactor because the core and reactivity mechanism geometry can result in dynamic and non-symmetric changes in flux during some events. The selection of the code and the requirements for validation are currently under review.

The heat transfer correlations used in CATHENA to predict temperature and void reactivity feedback and fuel temperature, determine the sequence of events for all loss of cooling and loss of regulation accidents. The most important of these, predicting local conditions at fuel element, have been derived from experiments conducted with single electrically heated fuel element simulators. To provide data for the validation of these correlations when applied to a bundle geometry, AECL has conducted a series of tests in which critical heat flux (CHF) is reached in an electrically heated bundle assembly. Validation exercises using this data are underway.

The blockage of flow to a fuel channel in the MAPLE core can result in the release of fission products from the aluminum fuel. Confinement or containment has been incorporated into the facility design to mitigate against this event. To provide realistic predictions of dose consequences, the transport of fission products from the fuel, from the pool water and ultimately to the environment, is tracked using various correlations and calculational methods. Validation exercises for these are underway.

As noted earlier the IRF incorporates test facilities that replicate CANDU<sup>®</sup> fuel channels with appropriately scaled heat transport systems. Consequently many of the event sequences analyzed for CANDU<sup>®</sup> reactors apply to these systems and the associated phenomena and their identifiers have been incorporated into the TBD for the IRF. The sequences can be more complex because of the strong reactivity coupling of the experimental channels and the reactor core. The suite of codes used in the analysis of events therefore includes a combination of those used for the MDS Nordion MAPLE and CANDU<sup>®</sup> reactors and the IRF validation plan incorporates the validation exercises for both and will benefit from the exercises currently underway.

### 6. Conclusion

The validation of computer codes used in the safety analysis of research reactors is coming under increasing scrutiny by the Canadian regulator. To support the licensing case for the MDS Nordion MAPLE reactors and the proposed Irradiation Research Facility, AECL has established a validation program for the suite of physics, thermalhydraulic and fission product transport codes that it uses. The IRF reactor incorporates experimental CANDU<sup>®</sup> fuel channels and the validation of the codes used to analyze related accidents has been incorporated into the Canadian industry wide validation program. The program for the MDS Nordion MAPLE reactors is underway and the completion of the program for the more complex IRF reactor will coincide with that for CANDU<sup>®</sup> power reactors in 2001.