Proceedings of the ASME 2010 3rd Joint US-European Fluids Engineering Summer Meeting and
8th International Conference on Nanochannels, Microchannels, and Minichannels
FEDSM-ICNMM2010
August 1-5, 2010, Montreal, Canada

FEDSM-ICNMM2010-31263

THERMAL HYDRAULICS STRUCTURAL UNCERTAINTY ANALYSIS; APPROACHES AND CHALLENGES

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ABSTRACT

Model uncertainty is a relatively new topic of discussion in TH code calculations, despite being often the major contributor to the overall uncertainty and a challenging practice in uncertainty analysis. The Integrated thermal-hydraulics uncertainty analysis (IMTHUA) methodology, developed by the authors, treats the TH code structural uncertainties (generally known as model uncertainty) explicitly by treating internal sub-model uncertainties, and by propagating such model uncertainties in the code calculations, including uncertainties about input parameters. This paper presents systematic model uncertainty of thermal-hydraulics system codes as part of IMTHUA methodology. The objective is to demonstrate effectiveness and practicality of the methodology on complex thermal-hydraulics system codes calculations and discuss the challenges dealing with these types of uncertainty sources. TH codes are an assembly of models and correlations for simulation of physical phenomena and behavior of system parameters in temporal domain. In some cases, there are alternative sub-models, or several different correlations for calculation of a specific phenomenon of interest. There are also “user options” for choosing one of several models or correlations in performing a specific code computation. Dynamic characteristics of TH calculations add more complexity to the code calculation, meaning for example, that specific code models and correlations invoked are sequence-dependent, and based certain (dynamic) conditions being satisfied. Structural uncertainty assessment (model uncertainty) for a single model will be discussed by considering “correction factor”, “bias” , and also through Bayesian sub-model output updating with available experimental evidence. In case of multiple alternative models, several techniques including dynamic model switching, user controlled model selection, model mixing, will be discussed. This paper discusses the challenges in treatment of the structural uncertainties in Thermal-Hydraulics system codes. Subjectivity and dependency on expert judgment in some of the solutions leaves some concerns on context of such systematic solutions to utilize imperfect and partially relevant data and information.

Keywords: Model Uncertainty, IMTHUA, Thermal-Hydraulics System, Code Structure.

INTRODUCTION

The integrated thermal-hydraulics uncertainty analysis (IMTHUA) methodology is developed for assessment of the uncertainties for applications to “best estimate” analyses of complex thermal hydraulics (TH) system codes [1-2]. The goal is to develop a comprehensive method to make such codes capable of supporting the uncertainty assessment with the ability to handle important accident transients. Model uncertainty is a relatively new topic of discussion in TH code calculations by its community, despite being often the major contributor to the overall uncertainty. The IMTHUA methodology considers the TH code structural uncertainties (generally known as model uncertainty) explicitly by treating internal sub-model uncertainties, and by propagating such model uncertainties in the code calculations, including uncertainties about input parameters. This paper presents on systematic thermal-hydraulics application of IMTHUA methodology model uncertainty portion only. The objective is to demonstrate effectiveness and practicality of the methodology on complex thermal-hydraulics system codes calculations. Special attention is given for the techniques of thermal-hydraulics model uncertainty treatment and their application on some practical examples. These codes are

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an assembly of models and correlations for simulation of physical phenomena and behavior of system parameters in temporal domain. In some cases, there are alternative sub-models, or several different correlations for calculation of a specific phenomenon of interest. There are also "user options" for choosing one of several models or correlations in performing a specific code computation. Dynamic characteristics of TH calculations add more complexity to the code calculation, meaning for example, that specific code models and correlations invoked are sequence-dependent, and based certain (dynamic) conditions being satisfied. Structural uncertainty assessment (model uncertainty) for a single model will be discussed by considering "correction factor", "bias" , and also through Bayesian sub-model output updating with available experimental evidence [3]. In case of multiple alternative models, several techniques including dynamic model switching, user controlled model selection, model mixing, will be discussed. This paper will discuss the challenges in treatment of the structural uncertainties in Thermal-Hydraulics system codes.

Effective uncertainty distribution (range) is defined here as one developed by applying all available knowledge, including data, models, and expert opinion at a specific confidence level. In the case of TH code uncertainty analysis, this requires a number of qualitative and quantitative steps to consider any given information for any aspect of the problem. A partial listing of such steps are shown in Refs. [2-3]. Some of these steps are demonstrated in CSAU [4], UMAE [5-6], and IMTHUA [2] (in the form of qualifications), and are defined as "reasonable uncertainty ranges" by AEA Technology [7-8]. The IMTHUA method is designed to incorporate the qualitative and quantitative information in a formal and systematic way. The information is used (1) to assess and propagate the uncertainties about various parameters, (2) to assess and propagate model and sub-model uncertainties, and (3) to adjust the resulting uncertainties on TH code output based on the previous two steps, by adding whatever information is available for overall code performance. This paper discusses IMATHUA's [2] main techniques for dealing with code structure uncertainties.

2. STRUCTURE OF TH SYSTEM CODES

The structure of the TH codes is similar to those of the other computational codes, with the exception that the TH codes were based on regulatory needs, available experimental data, and other information from the nuclear industry. They have limitation on detail calculation, due to the relatively small number of nodal points in the computational model. Limitations in computers' computational power (which has improved over time, along with code performance) and in necessary resources are important considerations for code structure characteristics. A general discussion of TH model uncertainty and its complexities are necessary before there can be any description of TH code structure and methods of treatment.

2.1 Structure of TH Codes and complexities

TH code is capable of modeling a wide range of systems, from configurations as simple as single pipes in small-scale experimental facilities to ones as complex as nuclear reactor plants. These codes are an assembly of models and correlations for simulation of physical phenomena and behavior of system parameters in temporal domain. In some cases, there are alternative sub-models, or several different correlations for calculation of a specific phenomenon of interest. RELAP5 has models for thermal hydraulics phenomena, including non-condensable gas transport, control systems, heat transfer to and from solid surfaces, and nuclear reactor kinetics [1, 9]. The models are built up from volumes connected by junctions with associated heat structures attached to them. The most difficult part of the solution is to solve the thermal-hydraulic behavior of the fluid and the coupling to the fuel/structural heat transfer through the HTCs, mainly because there are more coupled field equations associated with describing the fluid (more independent variables) and more phenomena to be considered, and the HTCs are also very dependent on the fluid properties and velocities. TH codes are relatively difficult to understand because of their structures' inherent complexity, which is described below:

i. Complexity of understanding (Knowledge-Based)

- Lack of control over code structure by user as well as developer
- Lack of appropriate data and information about models, sub-models, and actual variables, such as HTC

ii. Complexity of Phenomena (Inherent)

- Many Models and Correlations (thousands) involved in the computations

- Dynamic code behavior; only a portion of the code models involved in the calculations depend on fulfillment of conditions
- Many Horizontal and Vertical regime phases in the code calculation, with fuzzy borders between them
- Deficiency in field equations that solve precisely for specific configurations due to large average nodes. In case of choked flow phenomena, use of relatively large nodes dominating some microscopic scale phenomena leaves field equations unable to reach a solution with the requisite precision. The code calls for a choked flow model for velocity calculation if the momentum equation calculation result is unsatisfactory and replaces it with a calculation for choked flow model. TH codes are coupled with CFD codes for the sake of precise calculation where needed.

The complexity in TH dynamic behavior emerges in a spectrum of possible LOCAs and other types of transients, with a spectrum of associated PCTs as a figure of merit for most analyses. Each scenario has its own sequence of events, resulting in observations of different sets of phenomena, while modeling for these phenomena produces different sets of models and correlation involvements in simulating the system behavior, which depends both on time and on the progress of the transient. This dynamic behavior adds more complexity to the uncertainty analysis. Uncertainty grows in time step advancement, which means that uncertainty in code output as clad temperature of given rod accumulates with progress of transient and involvement of models and correlations in the calculation which different level of accuracy and credibility was assigned to each of them. The ideal way to quantify uncertainty in a code's temporal output (e.g., core temperature and vessel pressure) is to propagate the uncertainties by calculating uncertainty statistics (e.g., standard deviation or coefficient of variance) from time step to next time step. These statistics are evaluated for their updating in each time step. But this becomes more difficult in complex simulations of complex NPP transient cases. The practical alternative is to utilize a Monte Carlo-type propagation, which has been found to be effective approach in TH code calculations.

2.2 TH System Codes

There are different levels of approaches to modeling in relation to inputs and output[s]. It may be as a black box model, with no knowledge of the code structure, or as a white box model, which does have knowledge of the code structure. A structural, or "white box" test uncertainty assessment, allows the user to peek inside the "box," focusing specifically on internal knowledge of the code to guide the use of data and knowledge. The degree of model uncertainty varies among available methodologies, and is treated as a weight assignment for the alternative models and correlation in the GRS methodology. Code assessment is used in CSAU and ASTRUM methods for treating model uncertainties. IMTHUA considers the code structure shown schematically in Figure 1 with a white box by treating the code's sub-models and alternatives models, as well as the interaction between them [2, 10]. With many models and correlations interacting with each other, this type of modeling is complex, and depends to availability of resource and information.

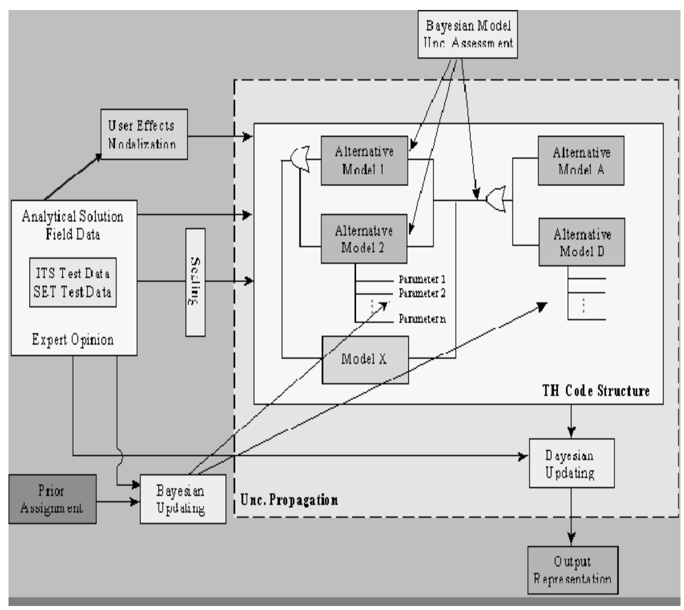

Figure 1: Code Structure Treated in IMTHUA Methodology for Uncertainty Quantification

3. CODE MODEL UNCERTAINTY

Code structure uncertainties are crucial sources of uncertainty in TH analysis results. The "structure" refers to such model features as the assembly of sub-models and correlations for simulating the various physical phenomena, system components for fluid and structural simulation, and cases where different sub-models are available for code calculations. Reliance on subjective expert opinion is not inevitable when there is interest in the performance assessment of nuclear core calculations and radioactive waste repositories, for which the models' predictive capabilities cannot be verified over the time frames and spatial scales to which they are required to apply (with limitation of experimental data discussed in previous). As the analyst cannot obtain empirical confirmation of the validity of a model from observations (this is especially the case with nuclear power plant test data, with most of data on scaled-down facilities), so that the model evaluation must rely exclusively on the subjective interpretation of the information available at the time of the analysis. This leads to the conclusion that any attempt to address the issue of model uncertainty in a quantitative manner will rely on expert judgment. This subjective assessment of is one of the concerns in adequate quantification of uncertainty.

3.1 Single Model Uncertainty Treatment (Prediction Expansion)

In prediction expansion, a single model is chosen as the best one to represent the system; however, it is recognized that this model has drawbacks, and may represent some system characteristics better than others. Sensitivity studies are performed on the various assumptions to analyze the effects on the model output. The associated uncertainty is handled by the application of a random adjustment factor (uncertainty factor) to the model results. This factor may be multiplicative or additive, or both. The uncertainty factor (UF) method [11], also known as the error factor approach, accounts for model uncertainty by modifying the prediction given by a single "best" model (also called the reference model) by means of a correction factor, which is usually uncertain [12]. However, it is not clear if the technical exercise of quantifying the gap between reality and the model (i.e., the quantification of the adjustment factor distribution) is feasible in practical analyses. Furthermore, a question arises on the reasoning behind this approach: if there is information that leads the expert to say something about the error in a model prediction, its correction can simply be considered as a modification of the original model [13-14].

Comparison of code calculations with available data from plants and tests in different scales show biases in model performances. The film de-entrainment model for ECC bypass and upper plenum de-entrainment calculations is an example of full-scale conservative biases in TRAC code calculation [15]. "Bias" can be defined as the average of the measured quantity divided by the same code-calculated quantity. Ref. [15] discusses S. Dederer's finding that the TRAC natural choking model had an average bias of 1.2, where the bias is the average of the measured test flow rate divided by the code-calculated flow rate for several different tests, test configurations, and test diameters. A bias of 1.2 means that, on average, the TRAC-PD2 model overpredicts the measured critical flow by 20 percent. The biases may be caused by scaling and/or intrinsic bias in the model, and should be evaluated one by one in models and correlations.

i. Bayesian Method

In the case of a single sub-model with available data from calculations and experiments, non-paired method $Y_i \neq Y'_i$ and/or $N \neq M$ setup for output updating may be used for uncertainty quantification for code sub-models. The method depends on the availability of experimental data for sub-model output. The method basis and procedure are discussed in detail in Ref. [2]. It is illustrated in the following example of a choked flow model, supplemented by data from the Marviken test facility.

The critical flow test was chosen to demonstrate the methodology, with the aim of obtaining critical flow data. The Marviken test facility is a blow-down vessel separate effects test facility. In the tests, the vessel was filled with degassed water up to a certain level, which varied between the tests (16.7 m above vessel bottom). A pre-test warm-up period produced a temperature profile along the vessel height. After a stabilizing period of several hours, the test was initiated by failing the discs in the rupture disc assembly. Measurements were recorded in the vessel, discharge pipe, and test nozzle, while the vessel fluid was discharged through the test nozzle into the containment and then through the exhaust pipes to the ambient atmosphere. The test was terminated when the ball valve began to close, or when pure steam entered the discharge pipe. (For further details, the reader may refer to [16] about details of the test facility and data). Experiments are considered reference points for this application. The effects of possible experimental errors are not considered; however, maximum errors calculated in experiments were based on the manufacturer's specifications. These were discussed with some statistical quantities, such as error limits and their confidence, and also probable error. See Ref. [17] for details on experimental errors. This approach was tested for Marviken test [16-17] facility tank temperature. The result is shown in Figure 2a. To find the distribution of a given parameter (tank temperature here), mode or mean value of the distribution of parameters b and σ are used as in Eq. (1), with results shown in Figure 2b.

$$f(T) = f(T \mid \bar{b}, \bar{\sigma}) \quad \textbf{(1)}$$

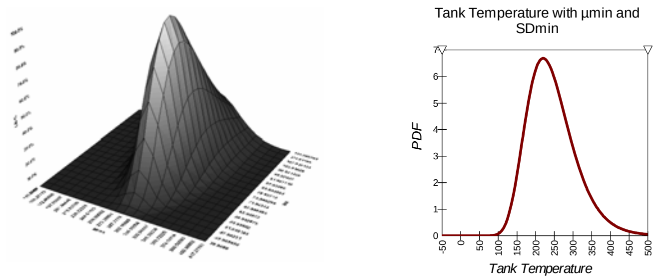

Figure 2: (a) Joint Distribution of σ, and b (b) Tank Temperature Distribution using mean of σ, and b

3.2 Alternative Model Uncertainty

There are several situations where the user and the code are able to choose one of the alternative models available. Depending on the data available and the situation itself, there are varieties of treatment options. Weighting and combining models, and switching between them as well, are among the cases discussed in detail below. Expert judgment plays an important role in these decisions. In multiple model cases, the characteristics of the system under consideration are analyzed, and models are created in an attempt to simulate the system based on ease-of-fit criteria. The models may use different assumptions and require different inputs. Each model has its own limitations on and ranges of applicability. In such cases, if the results from alternative models (using other data, information, knowledge) yield similar results to a problem, then one can be more confident that the results obtained from the model are realistic in the presence of uncertainty. If, however, alternative models yield different conclusions, further model evaluation might be required. One evaluation may involve verifying model estimations with the actual observations, or from experiments. Sometimes the uncertainty associated with the risk model assumptions is characterized by sensitivity analysis. These models might then combine to produce a meta-model of the system. Several methods have been proposed regarding the construction of this meta-model, including mixture [2, 18] and Bayesian updating [19-20]. Dynamic Model Switching, Change of Code Models by User in Same Run, Model Mixing, Maximization/Minimization and Bayesian Updating are the techniques discussed in this paper [2].

Case 1: Dynamic Model Switching

Model switching, as shown in Figure 3, is one option in using alternative sub-models in the code. A model switch can be made dynamically when certain pre-specified conditions (condition X in Figure 3) are present at any time. Once sub-model ***A*** is executed, say at time t, depending on the set of conditions (Condition ***X1*** or ***X2***), either sub-model ***B1*** or sub-model ***B2*** is called. Model switching is a way to reduce prediction error, and is not, strictly speaking, an uncertainty assessment.

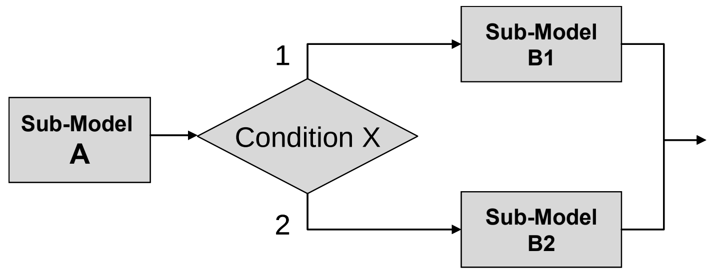

Figure 3: Model Switch Based on a Given Set of Conditions

One example is flow phase-change in an ongoing transient affecting conditions for the choked-flow phenomena. The transient will change conditions from the single-phase choked flow to the two-phase choked flow model due to the change in flow conditions. This is illustrated for the calculation of mass flow of the Marviken blow-down scenario in Figure 4. This approach may encounter problems in the continuous behavior prediction of phenomena, as seen in the application example discussed in [19]. Careful attention is required if model switching is utilized. Expert justification is needed for proper application, and the switching conditions.

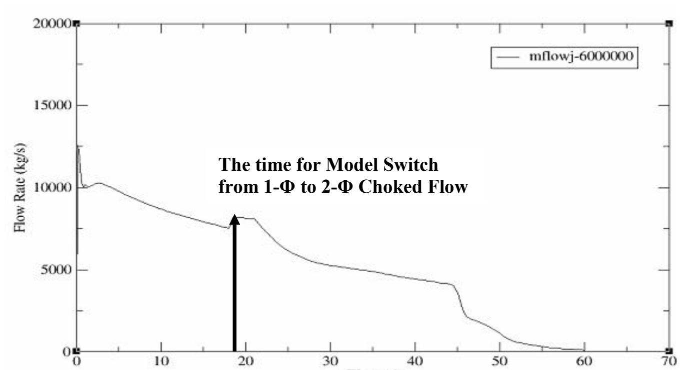

Figure 4: Model Switch from Single-Phase Choked Flow to Two-Phase Choked Flow-Marviken Blowdown Calculation

Case 2: Model Mixing

In the mixture approach, the set of plausible models and their probabilities of being correct are determined by the experts. The output distributions of the models are then linearly combined, with weights corresponding to the probabilities of correctness. The model distributions should be presented to the analysts before they are combined, allowing for an in-depth evaluation at the range of variabilities that are combined into the meta-model. This approach uses a weighted average of alternative models, as shown schematically in Figure 5. The same underlying data, but with different model structures, is the requirement for model mixing. An example is the countercurrent flow limitation (CCFL) model of the Wallis, Kutateladze, and Bankoff correlation available in RELAP5 code. A general CCFL model is used, allowing the user to select the Wallis form or the Kutateladze form, or a mixture of the Wallis and Kutateladze forms. This general form was proposed by Bankoff and is used in the TRAC-PF1 code, as well as in the RELAP5 code. A variable β specifies the level of mixing. When $\beta = 0$, the code uses the Wallis correlation, while the Kutateladze correlation is used for $\beta = 1$. For $0<\beta<1$, the Bankoff model, which is a weighting of the Wallis and Kutateladze correlations, is used. The Wallis (or Kutateladze) form is recommended for small (or large) diameters.

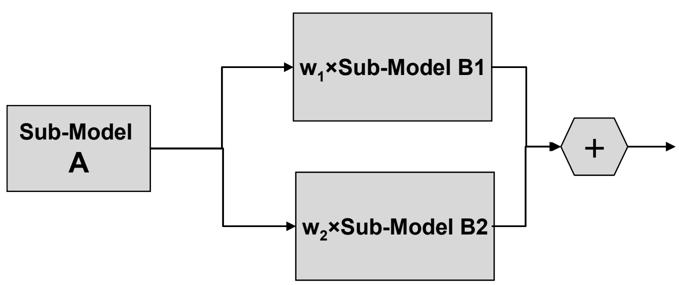

Figure 5: Model Mixing

An example for this case is given below. It discusses three different code executions of RELAP5 for LOCA calculation of a typical 4-loop PWR NPP, with CCFL models of Wallis, Kutateladze, and Bankoff correlations. A general countercurrent flow limitation (CCFL) model is implemented in RELAP5 code, allowing the user to select the Wallis form or the Kutateladze form, or a form in between the Wallis and Kutateladze forms, which was proposed by Bankoff and is used in the TRAC-PF1 and RELAP5 codes. There are several structures internal to RCSs, where gravity drainage of liquid can be impeded by upward flowing vapor. These include the upper core tie plate, downcomer annulus, steam generator tube support plates, and the entrance to the tube sheet in the steam generator inlet plenum. In the absence of experimental data for making decisions on correlation selection, expert justification will be crucial. The results are shown in Figure 6. High experience with the given correlation provides better basis for justification of model mixing which again depends on expert opinion and subjectivity.

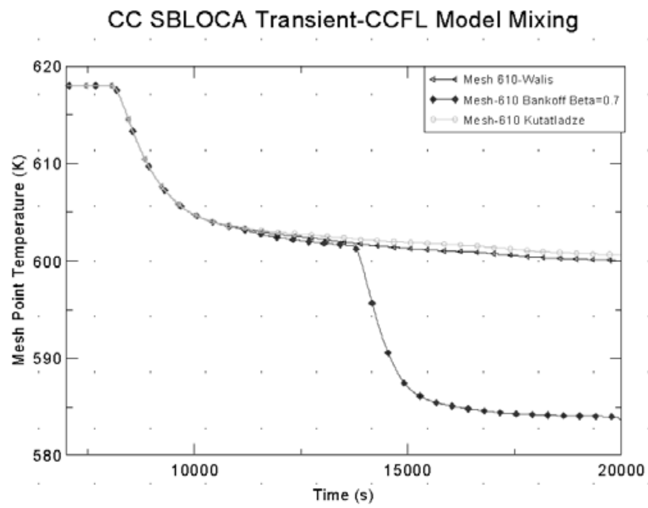

Figure 6: Model Mixing; (a) Wallis CCFL Model (b) Kutatladze CCFL Model (c) Bankoo Mix CCFL Model Beta=0.7

Case 3: Bayesian Mixing

In the Bayesian approach, the combination of the individual models is carried out using Bayes' theorem [21]. This method is able to incorporate both objective and subjective information in a probabilistic representation. The framework for the mixing varies based on the relationship between the models and the type of the data. Multiple models are classified as dependent or independent, with performance data as none, single, or multiple, and homogenous or non-homogenous.

Let us assume that n models $M_1, M_2, \ldots, M_n$ provide point estimates $x_1, x_2, \ldots, x_n$ about the quantity of interest X, and that there are multiple performance data sets for each model. Let $D_1=\{D_{11}, D_{12}, \ldots, D_{1n1}\}, \ldots, D_N=\{ D_{n1}, D_{n2}, \ldots, M_{nn}\}$ be the performance data sets on models $M_1, M_2, \ldots, M_n$, respectively, where $n_1, \ldots, n_n$ are the total number of data sets on each model. If $D=\{D_1, D_1, \ldots, D_n\}$, the posterior distribution of X is as follows:

$$\pi(x \mid x_1,...,x_n,D) = \frac{L(x_1,...,x_n,D \mid x)\pi_0(x)}{\int L(x_1,...,x_n,D \mid x)\pi_0(x)dx} \quad \textbf{(2)}$$

The likelihood function can be decomposed as:

$$L(\underline{x},D \mid x) = L(x_1 \mid x_2,...,x_n,D,x)...L(x_n \mid D,x)L(D_1 \mid D_2...D_n,x)...L(D_n \mid x) \quad \textbf{(3)}$$

A proposed way out consists of including the models in a meta-model parameterized with one index parameter φ, whose values (1,…,n) are associated to the different plausible models (M_1, M_2,…, M_n). With this method, uncertainty about the model can be converted into uncertainty about the value of the index parameter φ, which can be treated as a random variable whose uncertainty can be represented by a probability distribution. In practice, probability distributions can be assessed over the appropriate model structure and reinterpreted to be associated with the model index parameter. This also allows for a comparison of the impact of the model uncertainty to those of other uncertainties.

3.3 Code User and Input Deck

User effects for preparing the input deck for interactions with code structure have become a crucial point with respect to the quantitative assessment of the code uncertainties. The user has a significant influence on the input deck, given the many options for executable code preparations; the user also affects the computation in the various stages of code calculation, some of which are listed in Table 1, where user justification influences the overall calculation.

Table 1: TH Code Input Deck Preparation and User Options in Model Uncertainty [11]

User Domains	Impacts
System Nodalization	-Node Size -Component Selection -Node Numbers
Code Options	-Input parameters related to specific system characteristics -Input parameters needed for specific system components -Specification of initial and boundary conditions -Specification of state and transport property data -Selection of parameters determining time step size -Choice between engineering or alternative models, e.g., critical flow models -The efficiency of separators -Two-phase flow characteristics of main coolant pumps -Pressure loss coefficient for pipes, pipe connections, valves, etc.
Code Source Adjustments	-Multipliers -Choice between engineering or alternative models, e.g., critical flow models in a specific time -Numerical scheme

The case studies for evaluating user effects, especially ISP assessments, show a dominant effect on the predicted system behavior of the given figure of merit. They are reported in [22] as user effects on the number of nodes selection in input deck development, with different users estimating significantly different the value of a parameter of interest.

As some efforts (e.g., user training, improved user guidelines, and code improvement) are essential for user and input deck preparation quality, they do not eliminate the errors and uncertainties added to the calculation by user effects. Conditions vary greatly in dealing with choices and options faced by the user in preparing the input deck. The options' degrees of uncertainty are also different. Figure 7 shows these effects in code calculations for different users.

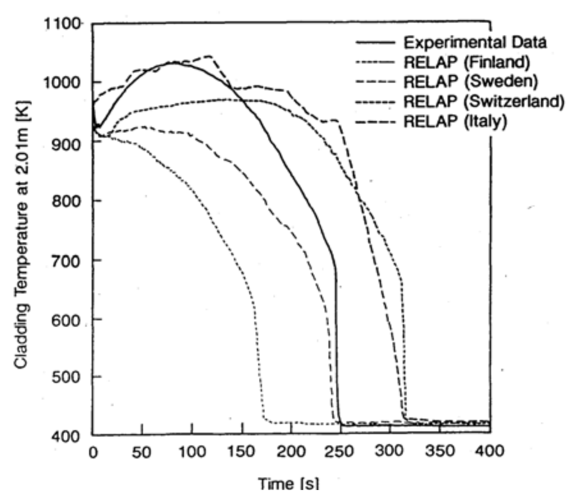

Figure 7: User Effects Study; Effects of Different Users on Code Calculation [22]

Credibility of code options are classified as follows:

i. Universally Recommended

There are some recommendations in the code for its execution for specific problem. This is the case when an option is strongly recommended for a specific condition. There should be strong evidence to confirm the hypothesis; if the evidence is not very supportive of such an expert decision, the overall uncertainty contribution to calculation results is not negligible. It is in a variety of conditions with recommendation on different models. The example is user choice for cross section area change (in pipes and elbows of nuclear power plant primary system); alternatives abrupt area change vs. smooth area change, or partial area change based on user justification. This is schematically depicted in Figure 8.

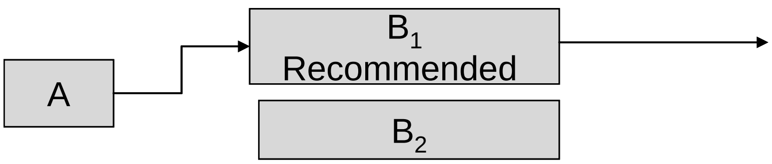

Figure 8: Run Code as Recommendation

ii. Recommended

As options and alternatives are not always universally recommended, there are situations where there is no consensus for a model selection. These options may be treated as a part of certain pre-processing approaches (e.g., PIRT [23]) for identification and classification with respect to their level of uncertainty importance. If uncertainty contribution is significant for a given option, it should be considered in the process of uncertainty quantification. If the effect is relatively insignificant, it is ignored in explicit uncertainty assessment. As discussed in [2], output uncertainty updates and missed or screened-out uncertainty sources can be considered in an implicit updating of output uncertainty processes.

4. CONCLUSION

Structure models make very important contributions to the final quantified results of TH code. This paper discusses strategies in structure model uncertainty assessment, and challenges in facing with these types of uncertainty sources. The main thrust of the methodology is to efficiently utilize all available types of data to identify important sources of uncertainty, and to assess the magnitude of their impact on the uncertainty of the TH code output values. Single sub-model uncertainties, as well as alternative models, were treatments and challenges in code structure are discussed. Depending on the conditions and on the availability of information and data, different solutions were proposed for uncertainty assessment of the models. Subjectivity and dependency on expert judgment in some of the solutions leaves some concerns. The solutions are the systematic way of utilization of such data and information. A Bayesian solution was proposed for single and multiple models' structure uncertainty assessment. Mixing, switching, maximization/minimization, and user effect consideration are proposed for alternative models.

NOMENCLATURE

CSAU	Code Scaling, Applicability and Uncertainty Evaluation
ECCS	Emergency Core Cooling System
GRS	Gesellschat Fur Anlagen- und Reaktorsicherheit
HTC	Heat Transfer Coefficient
IMTHUA	Integrated Methodology for TH Uncertainty Analysis
ITF	Integrated Test Facility
LBLOCA	Large Break Loss of Coolant Accident
LOCA	Loss of Coolant Accident
MCMC	Markov Chain Monte Carlo
PCT	Peak Clad Temperature
PIRT	Phenomena Identification and ranking Process
PWR	Pressurized Water Reactor
SET	Separate Effect Test
TH	Thermal-Hydraulics
UMAE	Uncertainty Analysis Methodology based on Accuracy Extrapolation
USNRC	United States Nuclear Regulatory Commission

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