OUTPUT UPDATING IN SEVERE ACCIDENT UNCERTAINTY ASSESSMENT; A BAYESIAN FRAMEWORK

Mohammad Pourgol-Mohammad[1], Seyed Mohsen Hoseyni[2],

[1] *Department of Mechanical Engineering, Sahand University of Technology, Tabriz, Iran, pourgolmohammad@sut.ac.ir*
[2] *Department of Basic Sciences, East Tehran Branch, Islamic Azad University, Tehran, Iran, m.hoseini@srbiau.ac.ir*

Abstract

Uncertainty depends on different types and sources of uncertainties in thermo-hydraulics and severe accident calculations for nuclear power plants (NPPs). Methodologies for the treatment of these uncertainties are categorized as "input based" and "output based" approaches. A hybrid approach is introduced here where an input based method is augmented with Bayesian correction of the output. The proposed methodology takes output uncertainties obtained from the input phase to be corrected upon the availability of separate information about the figure of merit. Concretely, as part of a broader objective to develop a comprehensive severe accident uncertainty analysis methodology, a Bayesian framework is developed using MCMC (Monte Carlo Markov Chain) for incorporating different types of new evidences to update the output distributions. The methodology will be applied to LP-FP-2 severe accident experiment of LOFT test facility.

I. INTRODUCTION

Severe accident phenomena are very complex and our knowledge is still limited in some areas especially for the late phases of the accident. Application of conservative approach is proved to be unacceptable for management of severe accident uncertainties therefore the use of best estimate method is recommended. A best estimate approach indeed requires a framework for dealing with the related uncertainties. Three major sources of uncertainty in accident analyses have been identified and are discussed for the accident analysis in detail in Reference [1], as follows:

(1) Code or model uncertainty, which is associated with models and correlations, the solution scheme, model options, not modeled processes (completeness uncertainties), data libraries and deficiencies in the codes;

(2) Simulation or Representation uncertainty, associated with the inability to model the real plant exactly due to simplification of the complex geometry, three dimensional effects, scaling effects, simplification of systems, etc.;

(3) Plant uncertainty, associated with errors in measuring and monitoring the real plant behavior, such as reference plant parameters, instrument errors, system component set points, etc.

In 1988, USNRC revised the ECCS licensing rules to allow the use of "best estimate" computer codes [2]. This requires explicit quantitative assessment of the uncertainties of the thermal-hydraulics (TH) calculations in the licensing and regulatory processes. To support this licensing revision, USNRC developed the code scaling, applicability, and uncertainty (CSAU) methodology to demonstrate the feasibility of a best-estimate plus uncertainty approach. Thereafter, a number of research efforts over the past 20 years were focused on methods and procedures to address thermo-hydraulics code uncertainties. Among these methodologies, several have proposed uncertainty quantification at input level while others are concentrated on the output uncertainty quantification. Recently developed IMTHUA approach however is an integrated method for thermo-hydraulics uncertainty evaluation that utilizes all available sources of data and information at both input and output level in an effective way.

Characterizing uncertainty in severe accident progression is first studied by Khatib-Rahbar [3] where an ensemble of computer codes known as the Source Term Code Package (STCP) was used. The methodology named QUASAR and its basic approach of this methodology is to:

1) Identify the code input parameters, sensitivity coefficients, and modeling options that describe or influence the predicted quantity of interest,

2) Prescribe likelihood descriptions of the potential range of these parameters, and

3) Evaluate the code predictions using a number of random combinations of parameter inputs sampled from the likelihood distributions.

They applied this methodology to some severe accident problems namely core melt progression, containment challenges and fission product release. This method only assesses the parameter uncertainty and is limited to the input based uncertainty analysis.

Sandia National Laboratory (Developer of MELCOR code) introduced an uncertainty analyses tool in 2004 that is coupled with MELCOR for the quantification of uncertainty but this tool only considers input uncertainty assessment. Model uncertainty, output uncertainty and integrated treatment of the uncertainty are not in the scope of this engine and more work is needed in this area.

In the following Hybrid of Input-Based and Output-Based Uncertainty Assessment will be presented for the severe accident calculations. The research will assess code output uncertainties associated with identified structural and parametric uncertainties at input and sub-model levels. The research will evaluate the available data in sub-models and overall plant performance for the figure of merit. The second stage updates the obtained input level uncertainty distribution with any available integrated experimental data and validation information. This "output uncertainty correction" phase is intended to at least partially account for code user choices (user effects), numerical approximations, and other unknown sources of uncertainties (model and parameter) not considered in the first phase.

II. Overview of the Integrated Methodology for Severe Accident Uncertainty Analysis

This research develops a comprehensive methodology to assess the uncertainties in calculation of severe accidents for nuclear power plants. Flowchart of the proposed methodology is illustrated in Figure 1. Details of input phase are elaborated in the previous papers of the authors [4], [5], [6].

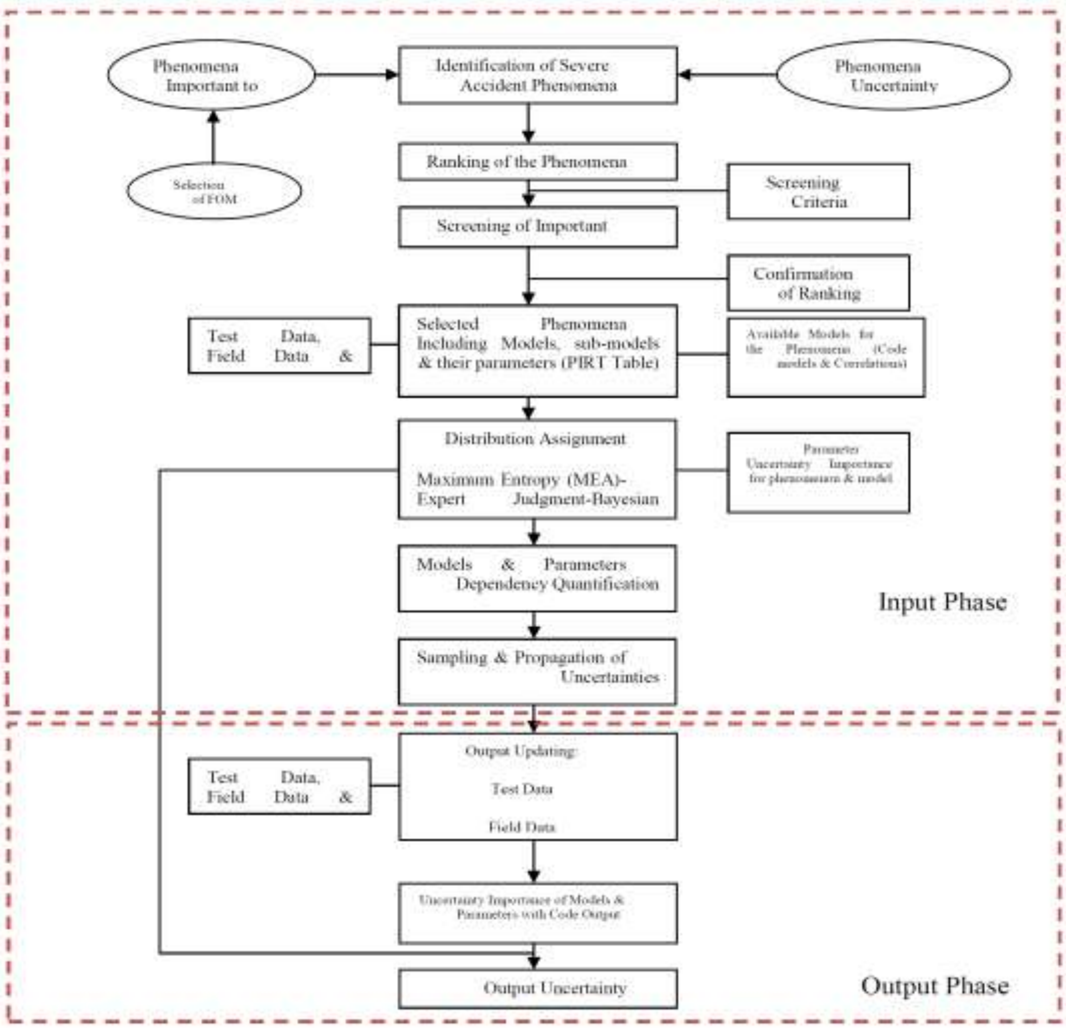

Figure 1: Flowchart of the proposed methodology

Table 1 summarizes the 2 phases of the proposed methodology and its practical steps. This is elaborated in more details in the following sections. Here, we will concentrate on output phase of the methodology and refer the interested readers to the previous works of the authors. Section III describes the output phase of the methodology in detail.

Table I: Phases of Integrated approach and its practical steps

Phases of Methodology	Practical Steps
INPUT PHASE: Input parameter and Model uncertainty of severe accident	1.Identification of uncertainty sources through modified PIRT 2. Input parameter uncertainty quantification 3. Structural treatment of model uncertainty in the code internal 4. Uncertainty importance analysis and ranking of uncertainty sources
OUTPUT PHASE: Output updating using experimental data and new evidences	1. Prior distribution assignment to code calculations and experimental data 2. Output updating using available data and new evidences through MCMC approach

III. OUTPUT PHASE: Bayesian updating of code output using experimental data

This phase of the methodology which is the main area covered in this paper enables output uncertainties obtained in the previous steps, by sole reliance on the input contributors of uncertainty, to be modified when a new piece of evidence arrives at an integral level (same level as the model prediction). The driving tool for this updating is a set of Bayesian methods for incorporating different types of new evidence into the output distributions.

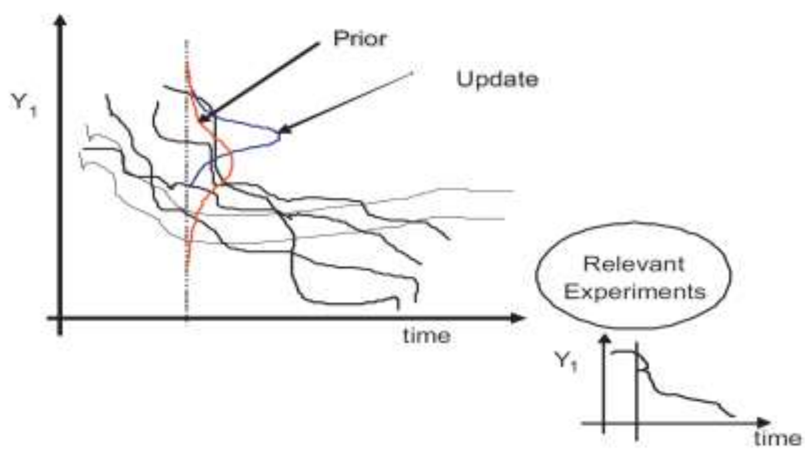

Figure 3: Schematic demonstration of output updating

Fig. 3 illustrates the output updating concept in a schematic way. Y1 is the uncertain figure of merit, obtained by the propagation of various input and sub-model uncertainty contributors to TH code predictions. The distribution of Y at a specific time (e.g. t=t0) is updated utilizing measured values (for the same time) from relevant experiments for Y1. The parametric distribution fitted to the data for t0 (prior) and updated distribution (posterior) is also shown in Fig. 3.

The format of information available and the nature of the variable of interest (Y) are determining factors in the choice of specific Bayesian method to be used. Before moving forward, we describe the types of data considered and then present the mathematical formalism and examples. In the case of severe computer codes for nuclear power plant accident analysis, applicable experimental data come from scaled-down facilities, such as SET or ITF. SET facilities are designed for the assessment of specific models or correlations corresponding to various phenomena or system components. ITF are designed for the assessment of the behaviour of a reactor system. Depending on the way the data are collected and the nature of the underlying experiments, the relation between the ITF data points and the severe accident code-calculated results can be characterized in two ways: ''paired'' and ''non-paired.'' Each category could additionally be characterized by the level of applicability of the information to the case being considered.

In an ideal platform (paired data), each experimental data $P=\{T_M^1, T_M^2, ..., T_M^n\}$ where n=m and TiM is a prediction of TiD . When such paring of experimental and predicted data points is not possible, then the two data sets are called ''non-paired''.

The work presented in reference [7] represents application of output updating on the basis of model (code) uncertainty for non-nuclear applications. In this work a methodology capable of opening up a fire simulation code following a "white-box" uncertainty analysis is presented. Similarly, the black-box used to differentiate the level of analysis performed. The simulation code output results from the white-box approach for both sub-models will be updated using experimental results following a similar method presented in the previous black-box research.

III.1 Paired data output updating

This would be simplest case to manage the uncertainties. Reference [8] offer a Bayesian methodology for model uncertainty based on paired data. This approach can be used to directly obtain the uncertainty associated with a given figure of merit (e.g. temperature, T) given the code-calculated figure of merit. In order to apply the methodology, the model is executed for each experimental data set to produce a single model prediction that can be paired with the corresponding test data. In the next step, Bayesian approach produces an uncertainty distribution of the figure of merit of interest given a code prediction, utilizing such paired data on model performance. In case of continuous output parameters, the method requires the pairing of experimental data and code calculation results. Additive or multiplicative error models can be applied to develop the likelihood function.

III.2 Non-paired data output updating

The nonpaired data situation, requires special treatment. The data used should be different from those used in the input assessment phase and should be in the form of integral experimental data about the code output. The procedure is as follows [2]:

1. Specify parametric distribution forms for model predictions and for distribution of the test data.
2. Apply all previous subjective knowledge to build prior distribution for output. This is done by estimating prior distribution for parameters associated with the output variable.

III.3 Partial Relevant Data

A Bayesian weighting process has been developed [8] for considering partially relevant information. Criteria for assigning the weights for the case of severe accident experiments are based on an assessment of the degree of similarity between the test conditions under which the data are collected and the conditions simulated by the code. Some attributes of scenario and experimental facilities for applicability assessment include distortion resulting from scaling, location and size of break, rate of power, scaling ratio of the facility, involved safety systems, nuclear core configuration, and so on. These attributes should be compared pairwise for applicability and relevance assessment. The value of φ factor ranges from 0, for ‘‘absolutely not applicable,” to 1, for ‘‘absolutely applicable.” This factor is utilized in modifying the likelihood function of the data ‘D’ according to the Bayesian process proposed by.

$$\pi(T \mid IM, D) = \frac{\left[L(IM, D \mid T)\right]^{\varphi} \pi(T)}{\int_T \left[L(IM, D \mid T)\right]^{\varphi} \pi(T) dT} \qquad (1)$$

IM is information about the model, and D is the data. The degree to which the data influences the strength of the data used to modify the uncertainty distribution of the code (or model) output from π(T) to π (T|IM, D) can be controlled by using different values of φ. When φ is in range (0, 1), it will defuse the likelihood, resulting in the partial effect of the data on the posterior.

Although the proposed approach is subjective, it paves a systematic methodology for consideration of imperfect data, which is the premise in effective uncertainty assessment, to utilize all data and information. Likelihood adjustment method is another alternative to using the u factor for updating of the output distribution. The ϕ factor comes from source data, as discussed above. A shape was assumed for Likelihood (e.g. normal), and objective adjusts the distribution parameters (e.g. μ, σ) for data and information implementation as

$$\left[L(IM, D \mid T)\right]^{\varphi} = \left[L(IM, D \mid \mu, \sigma)\right]^{\varphi} \qquad (2)$$

or by substitution of a statistics of μ, σ such as mean or mode, we arrive at a simple relation for output distribution.

Assume that μ_M and σ_M are parameters of the normal distribution of an output variable YM calculated by the code. We can also use μ_M and σ_M as the parameters of the normal distribution of test data YD. Other forms of distributions may be assessed for the data, but analytical formulation may not be possible. In those situations, a numerical solution (e.g., MCMC-type approaches) may be used. We recall from applied statistics that if YD and YM are represented by a bivariate normal distribution, then the conditional distribution of $Y_M \mid Y_D$ will be normal:

$$f(T_M \mid T_D) \sim N(\mu_{M|D}, \sigma_{M|D})$$

The conditional mean and variance of YM, given YD, are

$$\mu_{M|D} = \mu_M + \rho \frac{\sigma_M}{\sigma_D}(T_M - \mu_D)$$

$$\sigma_{M|D} = \sigma_M \sqrt{1-\rho^2}$$

$$correlation(T_D, T_M) = \rho \qquad (3)$$

The development of a Bayesian solution requires that we first select parametric forms for the distributions of code predictions and test data, then select a parametric form for their joint distribution, and assume values for inestimable parameters associated with this joint distribution and a joint prior distribution for the estimable parameters. Finally, the simulated posterior distribution calculates an adjusted model prediction Y_{new}^{D} based on a new model prediction generated by the SA code.

IV. APPLICATION OF THE PROPOSED METHODOLOGY ON LOFT-LP-FP-2 EXPERIMENT

The LOFT experimental facility was designed to simulate the major components and system response of a current-generation PWR during a LOCA. The experimental subsystems include the reactor vessel, the intact loop, the broken loop, the blow-down suppression tank (BST) system, and the ECC systems. The arrangement of the major LOFT components for test LP-FP-2 is shown in Figure 5. LOFT is a PWR model with a rated power of 50 MW(th), including all systems and components needed to simulate the accident under study.

The LOFT FP-2 test was a relatively large scale experiment to determine fission product transport and the effect of steam supply and reflood for a severely damaged core assembly. The LOFT-FP project, completed in 1985, was conducted by the Idaho National Laboratory (INL/INEL, USA) on an assembly of 121 UO2 rods with nuclear heating (in-pile) core. It consisted of tests on rod degradation and fission product release, and involved temperatures up to 2400 K (locally). Steam cooling was used, followed by water reflooding.

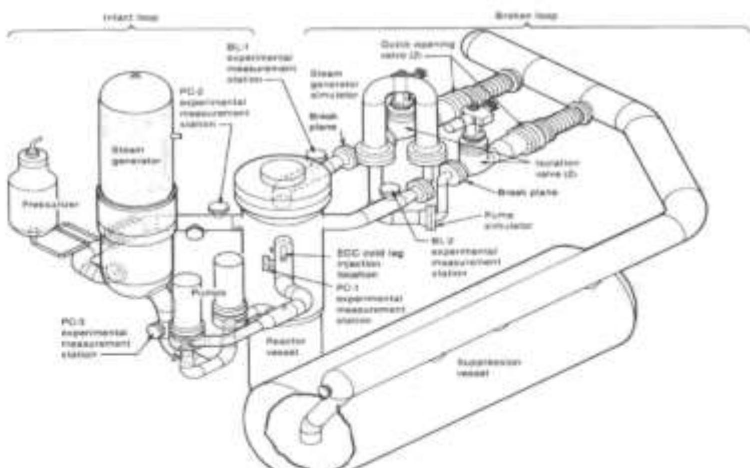

Figure 4: Schematic Diagram of the LOFT Test Facility for Experiment LP-FP-2 [9]

IV.1 Input Phase Uncertainty

Considering the LOFT-FP-2 experiment, its significance is clear especially for fission product release. For the application of interest to this article, FP release data were selected for further assessment. Therefore MELCOR code performance is examined for the prediction of the mentioned phenomena. The code merges the radio-nuclides into the so called classes based on their chemical properties (16 classes by default). The selected figures of merit are three classes as follows:

- Class 1: Xenon
- Class 2: Cesium
- Class 4: Iodine

The reason for their selection is their significant importance from safety point of view since these are the most volatile fission products. The other decisive factor is availability of data about the release of RN classes.

There are four alternative models for release of fission products from fuel component (CORSOR options) in MELCOR SA code which are:

- CORSOR
- CORSOR-M
- CORSOR-Booth
- Revised CORSOR-Booth

These include the CORSOR and CORSOR-M models, each with and without a surface/volume correction term, and the CORSOR-Booth and revised CORSOR-Booth model with low- and high-burn-up coefficient sets, for a total of eight possible variations.

As indicated before, the CORSOR models are dependent on temperature. Three categories of parameters dominate the problem. These categories relate to different phenomena which are:

- TH phenomena
- Core damage phenomena
- Source term phenomena

The next step is the propagation of the samples through the code structure. The uncertainty propagation which maps the input parameters to analysis results is often the most computationally demanding part of the sampling-based uncertainty analysis. Then 100 code runs are made with the MELCOR code, each run using the generated input decks of sampling process from 1 to 100.

These 100 runs produce a sampling of the FP release fraction for each model, from which the statistical properties of the distribution of FOM is estimated.

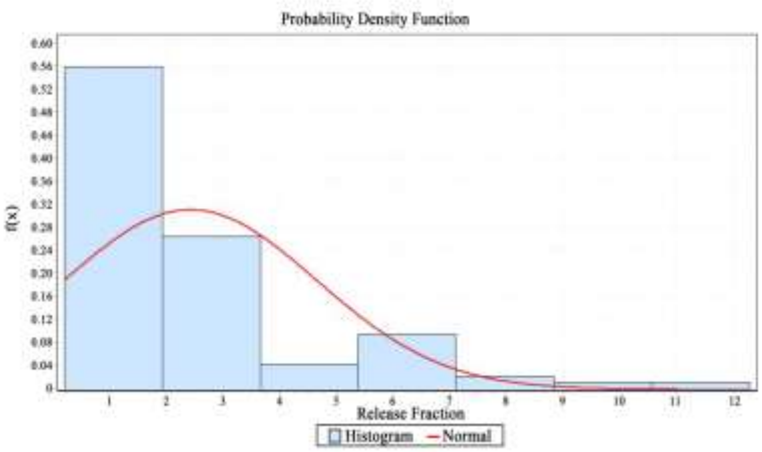

Figure 5: release fraction distribution for CORSOR with S/V Correction for Cs

In summary, given 8 CORSOR models, total of 800 calculations (100 for each model) were performed to obtain the uncertainty of output values of interest for each CORSOR model. The code calculated results are plotted for each modeling option in Figure 7 for 1 out of 8 available models. Once the calculations are carried out, the results are available for the characterization of output uncertainty. The goodness of fit tests (e.g., Kolmogorov-Smirnov test) could be used to select the distribution which best describes the obtained results. These tests show how well the selected distribution fits to the statistical data. For the case of LOFT application here normal distribution is the best fit to the output values. Easy fit software was used in this step and the best fits to the code data were selected. The final distribution of the output is plotted 1 out of 3 modeling options in Figure 7.

There are a number of references, which performed severe accident calculations for prediction of fission product release in different experiments or nuclear power plant scenarios. To overcome this deficiency, model averaging predicts unknown responses more reliably than each model by incorporating model-form uncertainty. This would not be captured if only a single model is considered. The proposed framework on model averaging is now implemented on the LOFT experiment since the probabilities of the model set and the code output statistics are known from the previous section. The outcome of BMA is summarized in Table II.

Table II: Results of BMA for release fraction of each class

	Xe	Cs	I
E (y|D)	1.911	2.120	2.751
VAR (y|D)	7.312	6.160	2.441
STD	2.704	2.481	4.938

IV.2 Output Updating Phase

Uncertainty quantification in input phase includes uncertainty of the code structure but screens out those sources which are identified as less important in the modified PIRT approach. As we discussed earlier output phase of the proposed approach tries to cover the uncertainty contribution from unidentified sources using Bayesian updating when a new piece of information arrives. The Bayesian solution for this problem needs to first know parametric forms for the distributions of code predictions and test data, then select a parametric form for their joint distribution, and assume values for inestimable parameters associated with this joint distribution and a joint prior distribution for the estimable parameters. As a result, the posterior distribution of the simulation will be of the following form:

$$\pi(\mu_M,\mu_D,\sigma_M,\sigma_D \mid T_D,T_M)=\frac{L(T_D,T_M \mid \mu_M,\mu_D,\sigma_M,\sigma_D)\pi_0(\mu_M,\mu_D,\sigma_M,\sigma_D)}{\int_{\mu_M,\mu_D,\sigma_M,\sigma_D} L(T_D,T_M \mid \mu_M,\mu_D,\sigma_M,\sigma_D)\pi_0(\mu_M,\mu_D,\sigma_M,\sigma_D)d\mu_M d\mu_D d\sigma_M d\sigma_D} \quad (4)$$

In practice, sufficient data are rarely available for pairing of the code predictions with their associated real values. For LOFT-LP-FP-2 experiment, two measured values are reported for the Xe release fraction at the end of the experiment (i.e. 2.5% and 2.8%); therefore the output updating problem here turns out to be of unpaired data type.

The WINBUGS14 [25] code was utilized to implement the Bayesian solution proposed. Bayesian inference using Gibbs sampling (BUGS), a basis and programming language for WINBUGS, is a program that carries out Bayesian inference on statistical problems using the MCMC method. WINBUGS assumes a Bayesian probability model in which all unknown parameters are treated as random variables. The model consists of a defined joint distribution over all unobserved (parameters and missing data) and observed quantities (data) it is necessary to place a condition on the data to obtain a posterior distribution for the parameters and unobserved data. Empirical summary statistics can be obtained from samples of the posterior and are used to draw inferences about the quantities of interest. Updated predictions of the model assuming bivariate normal distribution are obtained by maximizing the correlation between the code prediction and the corrected value as representative of the test data.

Figure 9 and table 7 below show result from fitting parametric normal distributions to code and experimental data. The statistics for the "Xe release fraction" as well as its mean and standard deviation parameters are shown in the tables beneath each distribution.

Table III: Summary of MCMC results

Parameter	Mean	SD	MC_error	Val5pc	median	Val95pc
expr	2.651	0.1094	0.001287	2.43	2.651	2.868
meand	2.651	0.04016	4.193E-4	2.572	2.65	2.73
meanp	2.653	0.437	0.004996	1.786	2.66	3.496
predu	2.58	4.48	0.04408	-6.252	2.569	11.23

The obtained results from MCMC calculations are substituted in the following formula to obtain the code updated output uncertainty:

$$pred\_new[i] = meand + \frac{\sigma_D}{\sigma_M}(pred[i] - meanp) \quad (5)$$

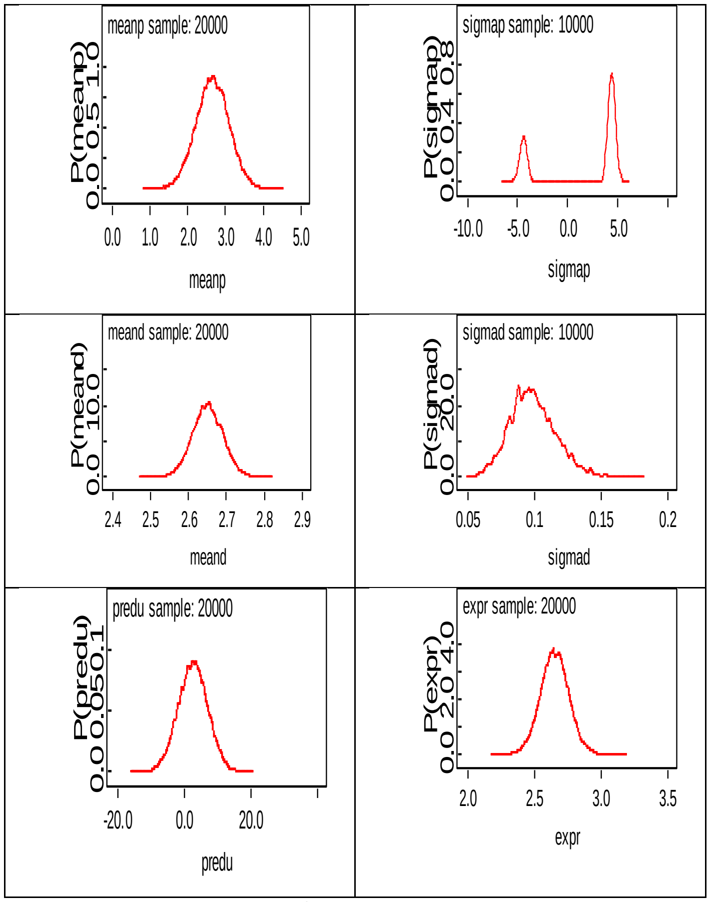

Figure 6: MCMC results for model parameters & experimental data

Figure 10 shows the prior and posterior distribution of the code results for “Xe release fraction”. Variance reduction is clearly observable here.

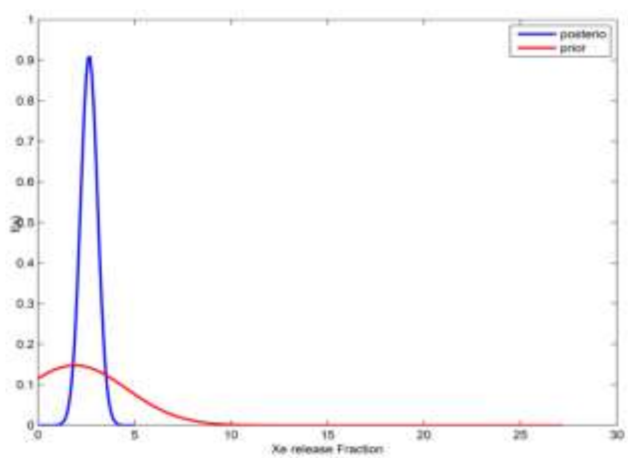

Figure 7: Output Updating for Xe release fraction

V. CONCLUDING REMARKS

A systematic approach for severe accident uncertainty assessment is presented and its application demonstrated on LOFT LP-FP-2 experiment. The proposed methodology is an integrated probabilistic approach where an input-driven white-box approach is augmented with output correction based on experimental results relevant to code output. It quantifies the observable sources of uncertainty in the severe accident modeling in input phase. Moreover it tries to explicitly take into account in output phase the uncertainty of unobservable sources through a Bayesian updating scheme when new evidence arrives. The unique feature of the proposed methodology is ranking of uncertain severe accident parameters with limited number of code simulations through a Bayesian ensemble of sensitivity measures. The whole features of the proposed methodology are fully implemented on the MELCOR modeling of LP-FP-2 severe accident experiment of LOFT test facility.

NOMENCLATURE

BMA	Bayesian Model Averaging
DCH	Direct Containment Heating
DSA	Deterministic Safety Assessment
ECCS	Emergency Core Cooling System
FMM	Finite Mixture Model
FOM	Figure of Merit
FP	Fission Products
HB	High Burn-up
IMTHUA	Integrated Methodology on Thermal-Hydraulics
INL	Idaho National Laboratory
ITF	Integral Effect Test
LB-LOCA	Large Break LOCA
LOCA	Loss of Coolant Accident
LOFT	Loss of Flow Test
LPIS	Low Pressure Injection System
MCMC	Markov Chain Monte Carlo
MLE	Maximum
NPP	Nuclear Power Plant
PIE	Post-irradiation examination
PIRT	Phenomena Identification and ranking Table
PWR	Pressurized Water Reactor
QUASAR	quantification and uncertainty analysis of source terms for severe accidents in light water reactors
RF	Release fraction
RN	Radio Nuclide
SA	Severe Accident
SET	Separate Effect Test
SNL	Sandia National Laboratories
TH	Thermal Hydraulics

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