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Annual progress report 2014

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Bayesian Uncertainty Quantification of Physical Models in Thermal-Hydraulics System Code

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1. Objectives of research

The objective of the research is to quantify the uncertainty of physical model parameters implemented in a thermal-hydraulics system code. The physical models concerned are the ones describing the phasic interaction (heat and momentum exchange) in a complex multiphase flow during reactor transient especially for the *reflood* phase following a loss-of-coolant-accident. These models are parameterized either by physical or empirical tuning parameters which values are uncertain.

Conforming with the practice of statistical uncertainty propagation widely adopted in the field of nuclear engineering, probability theory is used to quantify the uncertainties related to each one of these parameters in a form of density function and/or its approximation. The derivation of this density is posed as an inverse statistical problem following a bayesian approach as the parameters themselves are not directly observable. To this end, a methodology to quantify model uncertainty will be developed combining probabilistic modeling with available relevant experimental data taken from various separate effect test facilities.

2. Work achieved in the past year (state of research)

The PREMIUM benchmark was an activity coordinated by OECD/NEA starting in 2012 with the to compare and advance the methods for quantifying the physical model parameters uncertainties in thermal-hydraulics system codes. PREMIUM put an emphasis on the derivation of the uncertainties (Phase III) and its assessment by blind-predictions with experimental data (Phase IV). The scope of the benchmark was limited to the physical models relevant to the simulation of reflood. The derivation of uncertainties was based on the experimental data taken from the FEBA test facility and the assessment was based on the PERICLES test facility. The LRS at PSI is a participant in the benchmark using the TRACE code and works related to this participation was part of the PhD research activity.

During the last year, following the development and validation of the FEBA and PERICLES models in TRACE code, the work on PSI contribution for PREMIUM was conducted successfully until the last phase of the benchmark (Phase IV). First, the derivation of uncertainties on the parameters was based on expert judgment and literature review from sources available at PSI. Final listing of important uncertain parameters summed up to 26 for FEBA and 34 for PERICLES ranging from initial condition, material properties, to specific reflood model parameters. This list may also serve as prior estimates for the next phase of the project. Second, these uncertainties were propagated by Monte Carlo sampling to obtain the bounding uncertainty band on the cladding temperature prediction. The results of both FEBA and PERICLES were then submitted to CEA as the organizer for the Phase IV of the benchmark. This submission concluded PSI contribution to the Phase IV of the benchmark ([1], [2]).

Following the submission, the results from other participants were disclosed by the organizer. The organizer of the benchmark presented a table summarizing the general results from all the participants and it is reproduced here in Table 1. It was noted that PSI results was in relatively good position compared to the other participants in terms of the width of the uncertainty band for all the tests.

Two other research activities were also carried out in the context of global sensitivity analysis as was planned. The first is related to the application of Morris Screening method for sensitivity analysis. The Morris method can be seen as the first step toward applying true global sensitivity analysis method on the reflood model of TRACE. In that particular work, sensitivity analysis was carried out for the TRACE model of FEBA facility considering 26 important parameters. A set of `python`-based scripts were developed to implement the Morris method. The screening results in approximately 5 most important model parameters with varying degree of indication in non-linearity and interaction. To further elaborate these results a work on applying the Sobol method for variance decomposition is currently in progress.

Table 1: Summary of the simulation uncertainty propagation results in PREMIUM Phase IV

General Results	Participant (Code)	Width of Uncertainty Band	No. of Parameters (FEBA) (PERICLES)
FEBA & PERICLES **well bounded**	IRSN, FR (CATHARE)	Very wide	3 3
	VTT, FI (APROS)	Wide	6 6
	UNIPI, IT (RELAP5)	Rather wide	5 5
	SJTU, CN (RELAP5)	Wide	4 4
	PSI, CH (TRACE)	Wide	26 34
FEBA **roughly** bounded	TRACTEBEL, FR (RELAP5)	Wide to Rather Wide	8 8
	CVRez, CZ (RELAP5)	Average	2 2
	OKBM, RU (KORSAR)	Rather Narrow to Average	2 2
FEBA **roughly** bounded PERICLES **not always**	OKBM, RU (RELAP5)	Very Narrow	3 3
	CEA, FR (CATHARE)	Rather Narrow to Average	3 3
	GRS, DE (ATHLET)	Wide	6 8
	Bel V, BE (CATHARE)	Very Narrow to Average	3 3
FEBA and PERICLES **not bounded**	KAERI, KR (COBRA)	Very Narrow to Narrow	4 4
	KINS, KR (MARS-KS)	Very Narrow	2 2

The second was related to a novel data analysis methodology applied to a typical reflood simulation results. The so-called *functional data analysis* (FDA) is a branch of statistics which analyzes data that is in a form of *functions* (defined by certain degree of inherent smoothness). The basic aim of the analysis is similar to the standard data analysis, *i.e.,* first and foremost summarizing data both in terms of central tendency and variability. This perspective of looking at data fits rather well to reflood simulation results (which consist of time series depicting cladding temperature evolution). As a proof-of-principle the method was applied to 100 random realizations of FEBA simulation.

The method was able to expose the variability of the functional dataset through 5 scalars describing the principal modes of variations. These scalars can be used as quantities of interest for sensitivity analysis characterizing in a parsimonious way variability within a set of functional data (*i.e.,* a set of reflood curves) The first 3 aforementioned scalars are given in Table 2 along with their loose interpretations. These interpretations came from the effects of perturbing the mean function by the principal modes as shown in Fig. 1.

The results of these 2 activities were summarized in two separate conference papers submitted to the 10^{th} International Topical Meeting on Nuclear Thermal-Hydraulics, Operation, and Safety (NUTHOS-10). Both papers were accepted and will be presented in the middle of December 2014 ([3], [4]).

Table 2: Principal modes and their interpretation

Modes	Explained Variability	Interpretation
1^{st}	50.05%	Vertical shift in the amplitude of temperature transient prior to quenching
2^{nd}	34.38%	Convexity/concavity of the temperature descent
3^{rd}	4.68%	Vertical shift of the quenching temperature

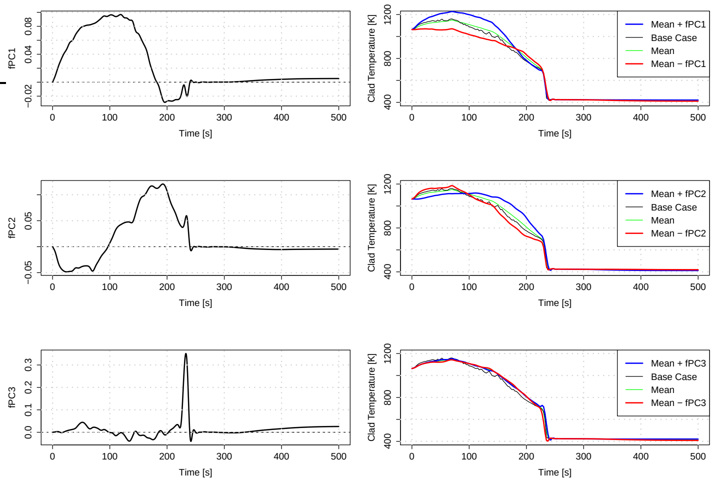

Figure 1: Principal modes and their effects on the mean function

3. Current state of work

The current state of research during the year are summarized in Table 3 shown below.

Table 3: Current state of research in relation to the previously submitted (1^{st} year) work plan

Phase	Task Description	Planned Outcome	Current State of Work
1	Comprehensive reviews of post-CHF flow closure laws in TRACE and externalization of important model parameters	1 Technical Report (PSI)	1. Important reflood model parameters externalized 2. PSI contribution to OECD/NEA PREMIUM Benchmark finalized
2	Global sensitivity analysis of important based on FEBA test facility	1 Technical Report (PSI) & 1 Journal Article	1. A paper on Morris screening method for NUTHOS-10 2. Another paper on an application of functional data analysis for NUTHOS-10 3. One abstract on global sensitivity analysis method submitted to NURETH-16
3	Definition of error and specification of probabilistic error model; Calibration of TRACE reflood model based on the FEBA facility; Approximation of the posterior distribution by Markov-Chain Monte Carlo;	1 Technical Report (PSI) & 1 Journal Article	–
4	Calibration of TRACE reflood model based on another reflood test facility	1 Conference Paper	Possible candidates of reflood facility with adequate specification and experimental data are available (*e.g.*, SEFLEX, NEPTUN, ACHILLES)
5	Consolidation of the calibration results based on 2 facilities and validation based on another reflood test facility	1 Journal Article	–
6	Thesis write-up	Thesis	–

The work in the application of global sensitivity analysis using FDA-derived metrics as the quantities of interest is currently in-progress. The Sobol method for variance decomposition is a step forward in extending the global sensitivity analysis where parameter importance are ranked by the nature of their interactions. Combining these developments, further insight into the behavior and performance of the reflood model in TRACE can be gained especially in terms parameters interaction. The interpretation of these aspects of the model are important to avoid ill-posedness in a parameter estimation problem.

Following a better understanding of model behavior and model parameter interactions through global SA, the work will continue on defining an appropriate probabilistic error model as well as the likelihood function for a reflood model. This model and the function should be derived on the basis of probability theory and, at the same time, should also be consistent with the underlying models describing the reflood phenomena.

4. Calendar of upcoming work

Table 4: Calendar of upcoming work (year 2015)

Time Frame	Task Description	Publication Outcome
Mid. Jan. - Mid. March	Application of Sobol Method for reflood simulation on FEBA SETF; Development of nodalization tool to fastened model development; Coursework	NURETH-16 Conference contribution
Feb. - Apr.	Comprehensive review on TRACE reflood closure laws including the functions call stack structure from inside the source code; Development of nodalization tool to fastened model development; Coursework	1 Technical report (PSI)
Apr. - Mid. Jun.	Consolidated studies of the model review, global sensitivity analysis results (Morris and Sobol) using FDA-derived quantities of interest; Preparation of a master thesis proposal on FDA-based GSA and UQ for the Achilles reflood facility; Coursework	1 Journal publication (an extension of the contribution to NURETH-16) & a Master Thesis Proposal
Jul. - Mid. Aug	TRACE assessment on the basis of FEBA complemented with development of an appropriate error model for functional (transient) output; Coursework	1 Technical report (PSI)
Mid. Aug. - Sep.	ACHILLES TRACE modeling and assessment; Participate in NURETH-16 conference; Preparation for the master student's semester work (*if applicable*)	1 Technical report (PSI)
Oct. - Dec.	Development of probabilistic error model and simple proof-of-principle on the application of Bayesian updating for reflood model in TRACE; Supervision of student's semester work (*if applicable*)	1 Technical report (PSI) & 1 Conference publication

5. Other activities and remarks

5.1 NES PhD Student Day

A poster was prepared and presented at the annual PhD Student Day of the Nuclear Energy Safety (NES) Department, Paul Scherrer Institut and co-sponsored by the *Nuklearforum Schweiz*. The poster [5] was presented along with 11 other PhD students within NES Department to general audience. The presentation was well-received and was selected as the best poster by a panel of jury.

5.2 Nuclear Computation Lab (ETH-531)

A teaching activity during the year 2014 was carried out for a part of the Nuclear Computation Lab. course given at PSI (one chapter out of six). The course was part of the block courses offered to the EPFL/ETHZ Nuclear Engineering Master Program. A single day was dedicated for lecture session followed by a hands-on computer simulation sessions. 12 students participated in the course this semester.

In preparation for the course, the available lecture slides was fully revised for a better structure and added with more clarifying examples. Part of the lab. manual has also been updated for this period. Finally, the simulation session was slightly extended with more freedom given to the students to set up their own model. Helped by students' enthusiasm and interactions, the overall experience was positive.

6. Scientific publications, conference contributions, and presentations

[1] D. Wicaksono, O. Zerkak, and A. Pautz, "PSI Contribution to PREMIUM Phase IV," Paul Scherrer Institut, Tech. Rep., 2014.

[2] ——, "PSI Contribution to PREMIUM Phase IV – Post-Test Uncertainty Quantification of FEBA and PERICLES Reflood Tests," Paul Scherrer Institut, Tech. Rep., 2014.

[3] ——, "Exploring variability in reflood simulation results: an application of functional data analysis," in *Proceedings of the 10th International Topical Meeting on Nuclear Thermal-Hydraulics, Operation, and Safety (NUTHOS-10)*, Okinawa, Japan, 2014.

[4] ——, "Sensitivity analysis of a bottom reflood simulation using the Morris Screening Method," in *Proceedings of the 10th International Topical Meeting on Nuclear Thermal-Hydraulics, Operation, and Safety (NUTHOS-10)*, Okinawa, Japan, 2014.

[5] D. Wicaksono, *Bayesian uncertainty quantification of physical models in thermal-hydraulics system code*, NES PhD Student Day - Poster Presentation, 2014.

Comments by the thesis advisor(s)

Prof. A Pautz

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O. Zerkak

Damar can be credited with a prolific and promising first phase of his research project. Despite unavoidable initial difficulties, Damar could assimilate the topic and rapidly become independent. He proposed a solution approach of his own, that he will need to implement and test for the reflood problem next year. His approach of combining FDA with a solution method for Bayesian inference problem (such as Markov Chain Monte Carlo sampling) is very original in the nuclear engineering field. I should also add that Damar has proved very reliable in executing PSI contribution to the OECD/NEA PREMIUM project.

Signatures

Thesis advisor ....

Thesis co-advisor ....
(if officially nominated)

With his signature, the candidate confirms that he took note of the above comments.

Candidate ....

Date ....

To be returned to: EPFL-EDPY / Station 3 / 1015 Lausanne / Suisse