Reliability Engineering and System Safety 169 (2018) 422–436

Contents lists available at ScienceDirect

Reliability Engineering and System Safety

journal homepage: www.elsevier.com/locate/ress

Kriging-based inverse uncertainty quantification of nuclear fuel performance code BISON fission gas release model using time series measurement data

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A R T I C L E I N F O

Keywords:
Inverse uncertainty quantification
Metamodel
Kriging
Nuclear fuel performance analysis
Principal component analysis

A B S T R A C T

In nuclear reactor fuel performance simulation, fission gas release (FGR) and swelling involve treatment of several complicated and interrelated physical processes, which inevitably depend on uncertain input parameters. However, the uncertainties associated with these input parameters are only known by “expert judgment”. In this paper, inverse Uncertainty Quantification (UQ) under the Bayesian framework is applied to BISON code FGR model based on Risø-AN3 time series experimental data. Inverse UQ seeks statistical descriptions of the uncertain input parameters that are consistent with the available measurement data. It always captures the uncertainties in its estimates rather than merely determining the best-fit values. Kriging metamodel is applied to greatly reduce the computational cost during Markov Chain Monte Carlo sampling.

We performed a dimension reduction for the FGR time series data using Principal Component Analysis. We also projected the original FGR time series measurement data onto the PC subspace as “transformed experiment data”. A forward uncertainty propagation based on the posterior distributions shows that the agreement between BISON simulation and Risø-AN3 time series measurement data is greatly improved. The posterior distributions for the uncertain input factors can be used to replace the expert specifications for future uncertainty/sensitivity analysis.

1. Introduction

The development of advanced computational platforms allows the simulation of sophisticated multi-physical phenomena within nuclear reactors in a coupled fashion. Current physical phenomenon involved in nuclear reactor modeling include neutron transport, thermal-hydraulics, fuel performance, and coolant chemistry. Indeed, although the modeling of nuclear reactor systems has made tremendous progress, there are always discrepancies between an ideal *in silico* designed systems and real-world manufactured ones. As a consequence, uncertainties must be quantified along with the simulation outputs to facilitate optimal design and decision making, ensure robustness, performance or safety margins. The propagation of input uncertainties to the response Quantities of Interest (QoIs) is known as Uncertainty Quantification (UQ) [1], which plays a vital role in the validation process [2] of a computer model.

Nuclear reactor fuel performance analysis studies the thermo-mechanical behavior of fuel rods and verifies their compliance with safety criteria under both normal operation and accidental conditions. Various complex phenomena need to be considered in nuclear reactor fuel performance analysis [3], for example: (1) for fuel: fission product swelling, densification, thermal and irradiation creep, fracture, and fission gas production and release; (2) for cladding: cladding plasticity, irradiation growth, and thermal and irradiation creep; (3) for others: gap heat transfer, mechanical contact, and the evolution of the gap/plenum pressure with plenum volume, etc. Examples of some popular fuel performance codes are BISON [3], TRANSURANUS [4], ENIGMA [5], FRAPCON [6] and FALCON [7].

In this work, we focus on the behavior of the fission gases xenon and krypton in uranium dioxide fuel, which significantly affect the thermo-mechanical performance of the nuclear fuel rods employed in current Light Water Reactors (LWRs) due to the following reasons [8,9,10]:

1. The fission gases tend to precipitate into bubbles after production which results in fuel swelling and promotes fuel rod gap closure and the ensuing Pellet-Cladding Mechanical Interaction (PCMI).
2. The released fission gas accumulates in fuel rod free volume, causing pressure build-up and thermal conductivity degradation of the fuel rod filling gas.

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https://doi.org/10.1016/j.ress.2017.09.029
Received 4 May 2017; Received in revised form 28 September 2017; Accepted 30 September 2017
Available online 3 October 2017
0951-8320/

3. The precipitated gas bubbles in fuel rod also have a negative effect on the fuel thermal conductivity, and consequently the temperature distribution in the fuel pellet.
4. The increase of fuel temperature will in turn lead to higher amount of released fission gases which forms a positive feedback, potentially leading to fuel rod failure due to cladding ballooning and cladding burst under accidental reactor conditions.

The accurate modeling of fission gas behavior in nuclear fuel performance simulation is vital considering its detrimental nature. However, the numerical analysis of fission gas release (FGR) and swelling involves treatment of several complicated and interrelated physical processes, which inevitably depend on uncertain input parameters. For example, the state-of-the-art fuel performance code BISON [3,11,12,13] incorporates an advanced physics-based FGR model that depends on several model parameters whose uncertainties are only known by expert judgment [10]. This poses difficulties and leads to inaccuracies in uncertainty and sensitivity analysis of BISON.

The objective of this paper is to inversely quantify the uncertainties associated with such model parameters in BISON FGR model based on available experimental data. *Inverse UQ* seeks statistical descriptions of the uncertain input model parameters that are consistent with the observed data, which is sometimes referred to as inverse problem, parameter estimation/inference, or Bayesian calibration. *Calibration* is the process of adjusting a set of code input parameters so that the agreement of the code calculations with a chosen set of experimental data is maximized [14]. *Deterministic calibration* finds the best-fit point estimation while *Bayesian calibration*, also called *statistical calibration* [15,16,17], provides statistical descriptions like the distributions. Bayesian calibration and inverse UQ employ the same idea especially when Bayesian inference and Markov Chain Monte Carlo (MCMC) are to be used. However, we would like to address the subtle difference between them. Calibration aims at reducing the difference between experiment and model prediction[1], while inverse UQ emphasizes quantifying the uncertainties in input parameters. When the computer model produces results that agree very well with measurement data, we may conclude that no calibration is needed. However, the inverse UQ is still required because the underlying uncertainties in random input parameters have to be quantified. In essence, in cases where there is no need to do Bayesian calibration, inverse UQ may still be necessary and useful.

Inverse problems have received increasing attention in the modeling & simulation community in practically all branches of engineering [19,20,21,22,23]. Representative applications in nuclear engineering are [24,25,26,27,28,29,30]. Inverse UQ formulation adopts a Bayesian setting [31] and its solutions are the posterior distributions. MCMC [32] is usually used to explore the posterior distributions and normally tens of thousands of samples are required, which poses challenges for computationally prohibitive models as each MCMC sample requires a full model execution. This issue is frequently bypassed by using metamodels.

Metamodels are approximations of the input/output relation of a computer code/model. They are also called *surrogate models, response surfaces* or *emulators*. Metamodels are built from a limited number of runs of the full model at specially selected values of the random input parameters (the so-called experimental design [33,34]) and a learning algorithm. Metamodels usually take much less computational time than the full model while maintaining the input/output relation to a desirable accuracy. Constructing the metamodels normally requires limited number of full model runs. Once validated, metamodels can be used to perform uncertainty and sensitivity analysis, validation, optimization, etc. See [35,36] for detailed reviews of surrogate models.

In the current research we built kriging metamodel (also known as Gaussian Process emulator) [37,38] for the BISON code during inverse UQ. The uncertainties in the model parameters of BISON FGR model are inversely quantified based on Risø-AN3 benchmark FGR time series data [39,40]. Because the shapes of FGR time series between measurement and BISON simulation are significantly different, we propose to perform the inverse UQ process in a reduced space formulated with Principal Component Analysis (PCA), thereby avoiding the issue of dealing with high-dimensional output and difficult convergence of MCMC sampling.

This paper is organized in the following way. Section 2 presents the Bayesian formulation for inverse UQ. In Section 3, the theory for kriging will be presented. BISON FGR model and Risø-AN3 benchmark will be introduced in Section 4. Section 5 briefly discusses how PCA for dimension reduction is implemented in the current research. Sections 6 and 7 present the results and conclusions, respectively.

2. Inverse UQ problem formulation

Consider a forward computer model $\boldsymbol{y}^M = \boldsymbol{y}^M(\mathbf{x}, \boldsymbol{\theta})$ where $\boldsymbol{y}^M$ is the model output which can be either a scalar or vector, $\mathbf{x} = [x_1, x_2, \dots, x_r]^{\mathrm{T}}$ is the vector of *controllable input variables* (also called *design variables*), and $\boldsymbol{\theta} = [\theta_1, \theta_2, \dots, \theta_d]^{\mathrm{T}}$ is the vector of *calibration parameters*. Examples of design variables are initial conditions (ICs) and boundary conditions (BCs). Calibration parameters, according to the definition in [15,41], are physical parameters that are specified as inputs to the computer model but are unknown or not measureable when conducting the physical experiments. Another broader definition for calibration parameters has also been used, e.g. [23], which include physical constants, context-specific constants, and tuning parameters that are needed to make the model perform well. Examples of calibration parameters are physical model parameters like material properties, and tuning parameters like multiplicative or additive factors. Design variables are usually required by both model simulation and field experiments, while calibration parameters are only needed by the former. In the current research the calibration parameters in BISON FGR model we are interested in are all multiplication factors.

Suppose that we have experimental observation $\boldsymbol{y}^E(\mathbf{x})$ which directly corresponds to the computer model output. Denoting the real or true value of the QoIs by $\boldsymbol{y}^R(\mathbf{x})$, we have:

$$\boldsymbol{y}^E(\mathbf{x}) = \boldsymbol{y}^R(\mathbf{x}) + \boldsymbol{\varepsilon} \tag{1}$$

where $\boldsymbol{\varepsilon} \sim \mathcal{N}(\boldsymbol{\mu}, \sigma_\varepsilon^2 \boldsymbol{I})$ represents the measurement error. Note that there can be multiple measurements and it is widely accepted to have homoscedastic experimental errors, which means that σ_ε^2 is same for different measurements. Also, $\boldsymbol{\mu} = 0$ is frequently used. Since $\boldsymbol{y}^R(\mathbf{x})$ represents the unknown reality, we only have an approximation of it by the computer model:

$$\boldsymbol{y}^R(\mathbf{x}) = \boldsymbol{y}^M\left(\mathbf{x}, \boldsymbol{\theta}^*\right) + \delta(\mathbf{x}) \tag{2}$$

where θ^* is the exact but unknown value for the calibration parameters, the learning of which is the goal of inverse UQ process. $\delta(\mathbf{x})$ is the *model bias*, also called *model discrepancy, model inadequacy* or *model uncertainty* [15,41,42]. The model bias term always exists because all computer models are reduced representations of the reality. Causes of the model bias are incomplete description of the underlying physics, numerical approximations, and other inaccuracies that would exist even if all the parameters in the computer model were known. The model bias is first addressed in the seminal work of Kennedy and O'Hagan [15]. It is important to consider model bias as otherwise we would have an unrealistic level of confidence in the computer model predictions (model will equal reality in Eq. (2) if model bias is not considered). By accounting

[1] Unlike deterministic calibration, Bayesian calibration does not necessarily result in estimation of calibration parameters that can reduce the discrepancy between model simulation and field data. This is because Bayesian calibration depends on both prior and the likelihood. In cases when the priors give model results that are very different from the field data and the data is very limited, Bayesian calibration is unlikely to produce posteriors that are consistent with the data, because the data is insufficient for the posteriors to "forget" the influence of the priors. See [18] for a recently developed approach called "consistent Bayes" which only tries to find parameters which yield model results close to the field data.