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Original Article

Surrogate based model calibration for pressurized water reactor physics calculations

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ABSTRACT

In this work, a scalable algorithm for model calibration in nuclear engineering applications is presented and tested. The algorithm relies on the construction of surrogate models to replace the original model within the region of interest. These surrogate models can be constructed efficiently via reduced order modeling and subspace analysis. Once constructed, these surrogate models can be used to perform computationally expensive mathematical analyses. This work proposes a surrogate based model calibration algorithm. The proposed algorithm is used to calibrate various neutronics and thermal-hydraulics parameters. The virtual environment for reactor applications-core simulator (VERA-CS) is used to simulate a three-dimensional core depletion problem. The proposed algorithm is then used to construct a reduced order model (a surrogate) which is then used in a Bayesian approach to calibrate the neutronics and thermal-hydraulics parameters. The algorithm is tested and the benefits of data assimilation and calibration are highlighted in an uncertainty quantification study and requantification after the calibration process. Results showed that the proposed algorithm could help to reduce the uncertainty in key reactor attributes based on experimental and operational data.

1. Introduction

Any mathematical model is an approximate representation of the real phenomenon of interest. Therefore, it is a common practice within engineering research communities to improve the predictability of mathematical models via model parameter calibration. Model calibration is a mathematical tool based on solving an inverse problem using the connection between experimental and operational data on one side and the mathematical model and its parameters on the other. This connection is used to improve the performance of the mathematical model by calibrating the model's parameters, along with updating their uncertainties to improve agreement of model predictions with experimental measurements and operational data.

Model calibration (sometimes referred to as data assimilation) has been used in various engineering fields, including nuclear engineering, for the enhancement of the predictions made by mathematical models and simulations [1,2]. Although very useful, model calibration analysis is hindered by two major challenges. The first is the computational burden associated with the high fidelity models (i.e., reactor core simulators). The second is the curse of dimensionality associated with the number of model parameters that will need to be calibrated (e.g., nuclear data cross-sections libraries). Both challenges are further worsened given the fact that the model calibration is an inverse optimization problem that requires multiple model executions.

Model calibration, utilizing the long operational experience with light water reactors, could improve simulation fidelity. In this work, the delayed rejection adaptive Metropolis (DRAM) algorithm [3] will be used in conjunction with reduced order modeling based surrogates, such that the end result is a practical and applicable algorithm for model calibration for large scale reactor core simulation, overcoming the two major challenges mentioned above.

DRAM is an algorithm for minimizing the samples required versus using a Markov Chain Monte Carlo algorithm. The DRAM method performs sample rejection by combining both the delayed rejection and adaptive Metropolis methods. In the delayed rejection samples are not rejected directly by the Metropolis sampler; a second stage proposal sample is generated with an acceptance probability that is calculated to guarantee convergence to the posterior probability density function. This second stage proposal depends on the previous rejected samples, yielding partial

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adaptation of the proposed distribution at each step of the sampling chain; therefore, the next stage can generate more reliable sample points. These refinements are local in nature and are discarded after each step [4,5]. By contrast, adaptive Metropolis relies on global adaptation of the proposed covariance based on the previously accepted samples in the chain. At certain intervals, the proposed covariance is updated to adapt information gleaned from the previous samples. This process of adaptation is introduced to improve the mixing of the chain so that it covers the target distribution more efficiently for any given number of iterations.

Reduced order modeling can facilitate the two major challenges mentioned earlier (high computational cost and the curse of dimensionality). Mathematical surrogates can address the first problem (the computational burden associated with running the high fidelity reactor core simulators). By contrast, reducing the dimensionality of the parameters of interest by identifying the influential degrees of freedom (DoFs) using the algorithms presented in Chapter 2 and Chapter 3 of Ref. [6] will address the second problem (the curse of dimensionality).

Ref. [1] introduced high order predictive model calibration algorithms and applied them to relatively large scale applications, while Ref. [2] performed model calibration for a few thermal-hydraulic parameters using a lower order surrogate to replace the actual thermal-hydraulics simulator. This work will employ polynomial surrogate models to substitute for the original coupled models in the virtual environment for reactor applications-core simulator (VERA-CS), which uses MPACT (Michigan Parallel Characteristics Transport Code) as a neutronics model, COBRA-TF (COolant-Boiling in Rod Arrays-Two Fluids) as a sub-channel thermal-hydraulics model, and ORIGEN (The Oak Ridge Isotope Generation) for the depletion of the fuel [7]. Therefore, this work performs model calibration for a three-dimensional core depletion problem with thermal-hydraulics feedback. Finally, cross-sections (high dimensional parameter) will be calibrated along with the few thermal-hydraulics parameters considered here. Verification is completed using synthetic data, that is, data generated using VERA-CS with perturbed parameters, to determine if the actual parameter perturbations can be assessed and ultimately used to enhance the uncertainty associated with the responses of interest [5].

2. Surrogate based data assimilation and model calibration

Referring to Ref. [3], it can be noted that several steps make DRAM limited to small-to-medium parameter dimensionality problems with reasonable computational burden. If the model is complex and characterized with high computational cost, then DRAM is no longer a practical algorithm. Therefore, in this section, a subspace-based surrogate model with a smaller number of DoFs will be used to replace the original model of interest, VERA-CS. Ref. [6] proposes gradient-based and gradient-free algorithms for identifying the important and influential DoFs for single and multi-physics modeling. Since the gradient calculation capability is not always available, the gradient-free approach will be used in this work to identify the influential DoFs in the form of basis vectors.

Once, the basis is determined (**U**), a second order goal-oriented surrogate will be constructed as follows:

$$f \approx \tilde{f} = \bar{S}_1^T \Delta\bar{x} + \left(\bar{S}_2^T \Delta\bar{x}\right)^2$$

where f is the response of interest (e.g., multiplication factor, maximum fuel pin power, and maximum fuel pin temperature), and $\Delta\bar{x}$ is the variation in the parameters of interest from the reference values (e.g., cross-sections, fuel pellet-clad gap conductivity, and grid loss coefficient).

In order to reduce the number of model runs required to construct the surrogate form, the gradient-free approach mentioned before is used to calculate the basis matrix (**U**) of the lower dimensional subspace approximation for the parameters' space. The columns of matrix **U** represent the influential DoFs. Before discussing how the matrix **U** is used in constructing the surrogate, it is worth mentioning that once the influential DoFs are determined, the remaining DoFs are actually ignored, which obviously introduces a source of error in the algorithm. Fortunately, the error introduced by this truncation process can be quantified and upper bounded using the theory presented in Ref. [8] and used in [2,6]. To summarize this error upper bound equation, let us assume that vector $\bar{y}$ (represents some physical quantity) is assumed to vary along the DoFs or basis represented by the columns of matrix $\mathbf{U_F}$; then if only the influential DoFs are identified and collected in matrix **U** (which is a sub matrix of the full matrix $\mathbf{U_F}$) then the error in representing the variations in the physical quantity $\bar{y}$ via **U** can be upper bounded via the following expression:

$$\varepsilon_{upper} = 10\sqrt{\frac{2}{\pi}}\max_{j=1,\ldots p}\left\|\left(\mathbf{I}-\mathbf{U}\mathbf{U}^T\right)\bar{y}_j\right\|_2$$

This upper bound (ε_{upper}) is guaranteed with a success probability of $1-10^{-p}$ [8] where p is the number of extra snapshots used to compute that upper bound. For more information about the theory behind this error upper bund estimation and its applications, refer to [6,8].

The goal of the surrogate here is to employ it to perform model calibration analysis, so that the uncertainty and mean of each parameter might be updated. The implication is that the parameter perturbations ($\Delta\bar{x}$) generated to determine the influential DoFs and surrogate model are random within the interval of interest. This contrasts with an uncertainty quantification application, where parameter perturbations would be based upon sampling the parameters' probability distribution functions.

An efficient goal-oriented surrogate can be constructed as follows:

$$f \approx \tilde{f} = \overbrace{\bar{\beta}_1^T\mathbf{U}}^{\bar{\beta}_{1,r}^T}\ \overbrace{\mathbf{U}^T\Delta\bar{x}_{rand}}^{\Delta\bar{\alpha}} + \left(\overbrace{\bar{\beta}_2^T\mathbf{U}}^{\bar{\beta}_{2,r}^T}\ \overbrace{\mathbf{U}^T\Delta\bar{x}_{rand}}^{\Delta\bar{\alpha}}\right)^2$$
$$= \bar{\beta}_{1,r}^T\Delta\bar{\alpha} + \left(\bar{\beta}_{2,r}^T\Delta\bar{\alpha}\right)^2 \quad (1)$$

where $\Delta\bar{x}_{rand}$ is an input vector generated by randomly sampling the parameters. Given that $\mathbf{U}\in\mathbb{R}^{n\times r}$ and $\Delta\bar{\alpha} = \mathbf{U}^T\Delta\bar{x}_{rand}\in\mathbb{R}^r$, $\bar{\beta}_{1,r}^T = \bar{\beta}_1^T\mathbf{U}\in\mathbb{R}^r$ and $\bar{\beta}_{2,r}^T = \bar{\beta}_2^T\mathbf{U}\in\mathbb{R}^r$, in order to determine the unknown elements of $\bar{\beta}_{1,r}$ and $\bar{\beta}_{2,r}$ the model needs to be run $2r$ times so that the coefficients are determined (where r is the number of influential DoFs or the rank of matrix **U** which is the dimension of the identified subspace).

The surrogate based algorithm proposed here depends on two main points: first, identifying the important DoFs via methods of subspace analysis (refer to Chapter 3 in [6]). Second, once the important DoFs are determined in the form of the basis of a subspace, these bases can be used to form surrogate models $\tilde{f}$ (e.g., polynomial or Gaussian process) which can replace the original computationally expensive model f. The following is a summary of the algorithm for Surrogate Based Model Calibration (SBMC): (1) Construct the basis of the lower dimensional subspace approximation of the parameter space (**U**); (2) construct the goal-

oriented surrogate model ($\tilde{f}$); (3) solve the data assimilation problem (e.g., DRAM) with the surrogate model $\tilde{f}$ with the reduced parameter space $\mathbb{R}^r$; and (4) after the convergence of the data assimilation algorithm, the updated reduced parameters (i.e., space $\mathbb{R}^p$) are mapped to the original input parameter space ($\mathbb{R}^r$).

In the following sections, the SBMC will be used to perform parameters' calibrations. The parameters of interest are the nuclear data cross-sections (high dimensional parameter) and two thermal-hydraulics parameters (fuel pellet-clad gap conductivity and grid loss coefficients). In this work, we deal with the model calibration algorithm (i.e. DRAM) as a black box; our contribution is by replacing the original high fidelity model with a surrogate that has negligible computational cost to run and reducing the number of model parameters to deal with by considering the influential DoFs only.

3. Case study: 3-dimensional core depletion problem

The problem of interest is one of the Consortium for Advanced Simulation of Light Water Reactors (CASL) progression problems. The problem is a core wide problem represented by Watts Bar Nuclear Unit 1 for Cycle 1 with depletion (CASL Progression Problem Number 9) [7]. In this case study, a few parameters are calibrated performed via the Surrogate Based Model Calibration (SBMC). The core simulator of interest is VERA-CS. Fig. 1 presents the models that make up VERA-CS. Referring to the figure, the parameters of interest—in this case study—are the pellet-clad gap conductivity (h_{gap}), and the grid loss coefficient (g_{loss}). In this example, the cross-sections of interest are the fission, absorption, and scattering cross-sections for a few isotopes. The number of energy groups in the VERA-CS cross-sections library used is 47. Therefore, the number of parameters to be calibrated is 846 cross-section parameters and two thermal-hydraulics parameters. The DRAM–QUESO algorithm (encoded in DAKOTA 6.2 [9]) will be employed to solve the inverse problem using 100,000 samples per chain (after burning the first 30,000 samples in the chain).

First, the goal-oriented surrogate is constructed in the form represented by Eq. [1]. The surrogate, constructed as described in the previous section, is evaluated via examining the norm of residuals (i.e., difference between VERA-CS and surrogate predictions) and their distributions. In this case study, the measured attributes are: the multiplication factor (k_{eff}), and the relative fission reaction rate axial distribution at the in-core detector radial locations (**FR**). The matrix **FR** is equivalent to measuring the fission rate over 49 axial levels (within the 56 axial levels of the core simulator model). Synthetic data will be used instead of real data for the purpose of proof of concept. Using the synthetic data implies that the actual solution of the model calibration problem is known *a priori* enabling the model calibration method to be verified. Five depletion steps (6 depletion points) are used to generate the synthetic measurements of interest. Hence, each response is measured at each of the depletion steps (0, 9, 32, 45, 120, 160 Effective Full Power Days (EFPD)). The values of the measurements of k_{eff} are: 1.000443, 1.00012,1 1.00013, 0.999951, and 0.99991 with a constant uncertainty of 60 pcm corresponding to a typical measurement uncertainty of the multiplication factor. The relative fission rates at the core center are: 1.9321, 1.8962, 1.8212, 1.7612, and 1.7312 with an assumed measurement uncertainty of 0.02 (the complete incore detector readings are used in the data assimilation; however, these measurements are mentioned here to exemplify their values). In generating the synthetic data values, the uncertainties were applied by randomly sampling a normal distribution using the above stated standard deviation values.

The surrogate is constructed using VERA-CS with the perturbations generated randomly within the intervals of interest [h_{gap} (±50%), g_{loss} (±4%), cross-sections (±5%)]. As noted earlier, the surrogate form-related uncertainty is related to the uncertainty in the surrogate coefficients determined by the fitting process (refer to Table 1 for details about the surrogate error analysis). Note that the RMS for the **FR** reflects the Root Mean Square (RMS) of a vector formed from the matrix storing the relative fission rate; that is, $\epsilon_{\mathbf{FR}} = RMS(vec\{\mathbf{FR}\})$, where *vec* is a process that transfers a matrix into a vector. Due to the computational resource limitation, a 2nd

Table 1
Surrogate error analysis.

Surrogate order	RMS	Surrogate form–related uncertainty
2nd order	14.4 pcm 0.0332	35.0 pcm (percent milli) 0.0093 (Maximum)

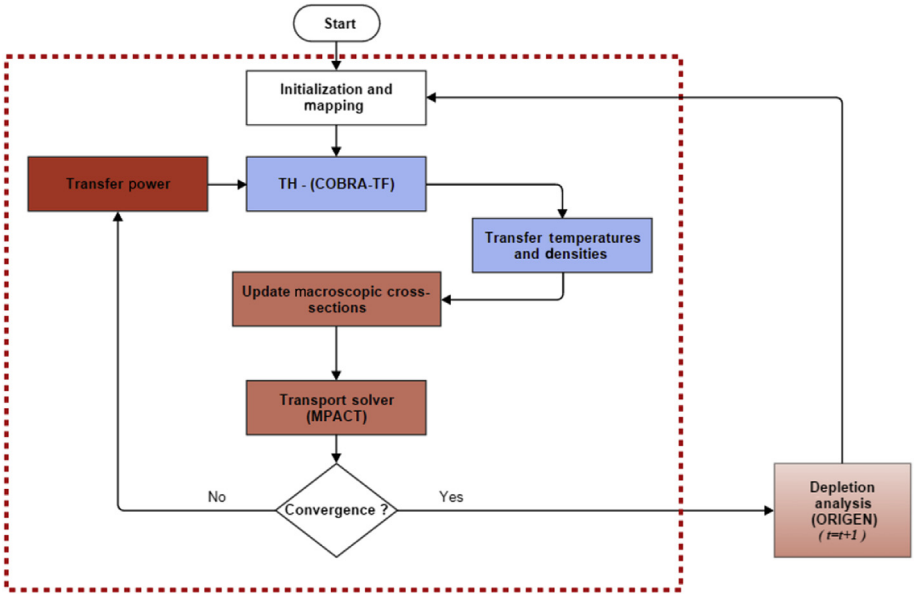

Fig. 1. Virtual environment for reactor applications-core simulator (VERA-CS) scheme.

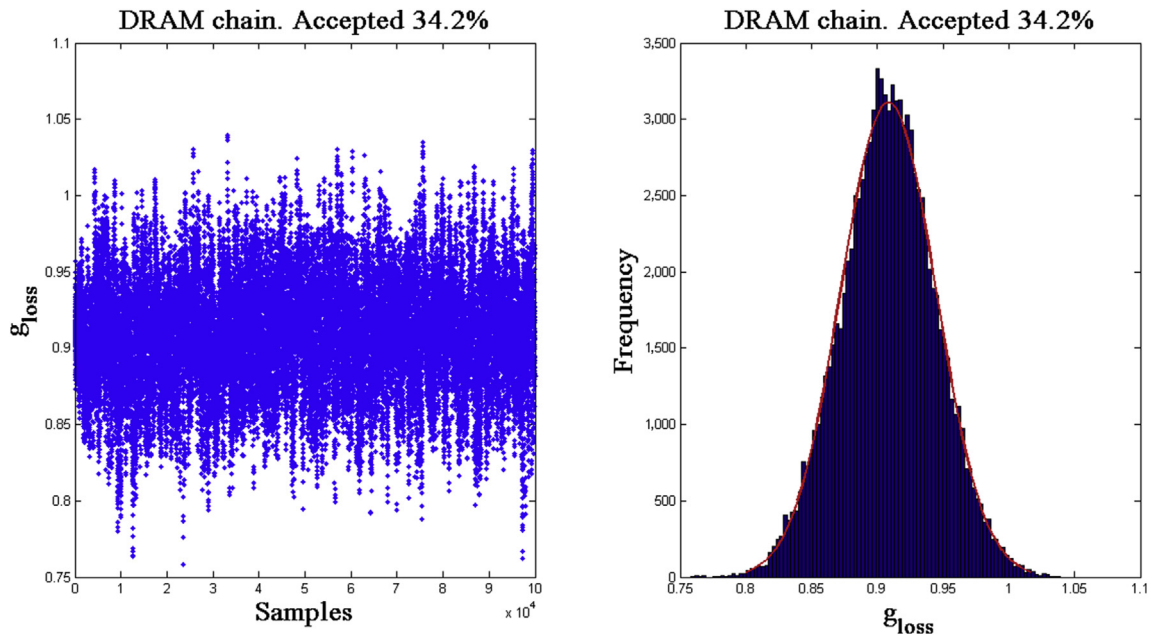

Fig. 2. Grid loss coefficient chain (all points). DRAM, delayed rejection adaptive Metropolis.

polynomial surrogate is used as previously described. For the surrogate model to be useful, the residual errors need to be an order of magnitude smaller than the experimental uncertainties. The other form of uncertainty to be taken into consideration is the surrogate form related uncertainty, which reflects the effect of the uncertainty in the surrogate coefficients into the responses of the surrogate.

The surrogate is constructed for each of the modular components of VERA-CS (MPACT-COBRA-TF-ORIGEN) due to the computational burden of constructing a surrogate for VERA-CS at once (which was done in a previous work for an assembly problem [10]). The implication is to capture feedback effects between the modular components. The outputs of one component, which serves as inputs to another component, are represented by surrogate models the variables of which are the inputs from another component. In this example, the inputs are: the nuclear data-cross-section library (MPACT), gap thermal conductivity, spacer grid coefficient, and the pin power distribution (COBRA-TF).

The surrogate is then used for simultaneous calibration of the thermal-hydraulics parameters along with the cross-sections of interest. The synthetic measurements are first generated via the high fidelity simulator (VERA-CS) where specific known parameters' perturbations are used. Next, model calibration is completed using the surrogate, starting with unperturbed parameter values. Therefore, as noted above, the ideal solution to the model calibration problem is known *a priori* and the performance of the SBMC can be evaluated by comparing the known perturbations and the

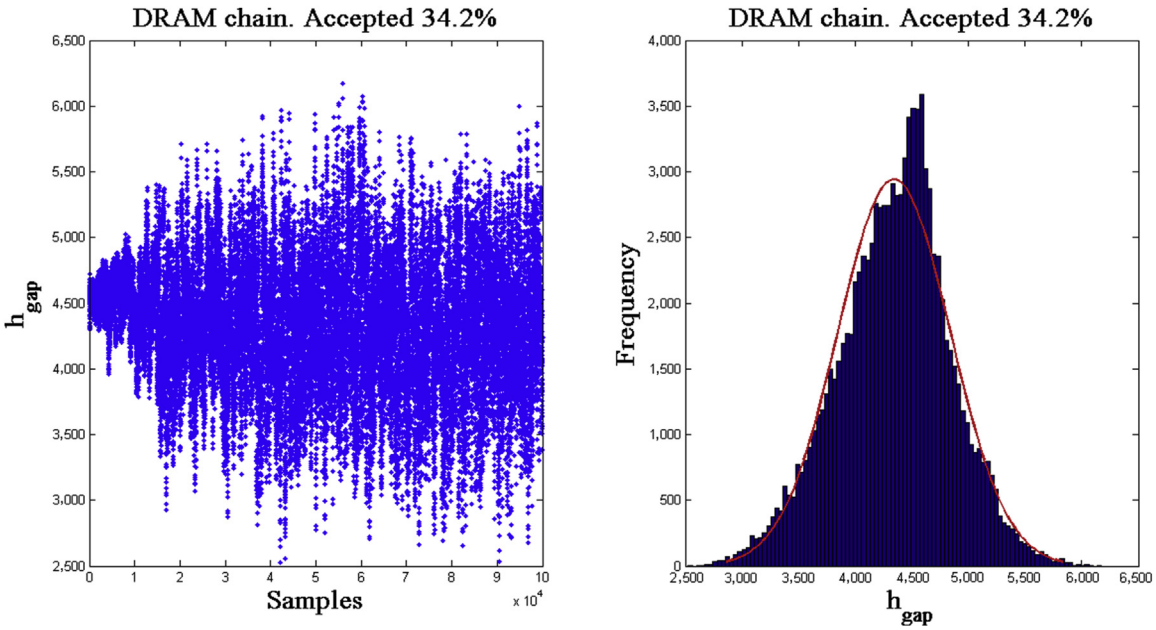

Fig. 3. Gap conductivity chain (all points). DRAM, delayed rejection adaptive Metropolis.

Table 2
Model calibration results for a few important parameters.

Parameter	Prior value & uncertainty	Perturbed value	SBMC posterior value & uncertainty
h_{gap}	4500 ± 2250	4359.91	4109.2 ± 504.1
g_{loss}	0.907 ± 0.03628	0.9123	0.9088 ± 0.035
Σ_f^{U-235} (0.0306–0.012396) eV	1125.219 ± 2.66	1258.435	1267.01 ± 1.11
Σ_f^{U-238} (2.2313–1.3534) MeV	0.43297 ± 0.00528	0.42523	0.4212 ± 0.00243
Σ_f^{Pu-239} (0.0306–0.012396) eV	1363.475 ± 16.03	1441.313	1436.2 ± 6.11
Σ_s^{H-1} (0.0306–0.012396) eV	75.35 ± 0.07	82.47610	78.72 ± 0.0382
Σ_s^{O-16} (0.0306–0.012396) eV	4.33 ± 0.0434	4.629821	4.611 ± 0.0211

mean variations generated by DRAM in conjunction with the surrogate (SBMC).

For the thermal-hydraulics parameters, a uniform distribution was used as *a priori* distribution sampled using the uncertainties reported earlier with the reference values of the parameters. Figs. 2 and 3 show the chains and their distributions for the thermal-hydraulics parameters (grid loss coefficient and gap conductivity). The variations in the grid spacer loss coefficient are not identifiable using the current responses of interest, due to the fact that there is a weak, if any, correlation between the grid spacer loss coefficients and either the multiplication factor or the relative fission rate.

Table 2 shows that the SBMC calibrated parameters and their uncertainties are modified, and while the introduced perturbations are not exactly retrieved, the perturbations are in the correct direction. In addition, the updated uncertainties seem to be smaller than the *a priori* values, which mean that if real experimental measurements are used in the model calibration analysis, then the updated uncertainties can be used to requantify the uncertainty in responses of interest. This benefit will be explored in the next section.

4. Benefits of model calibration

In this section, the benefits of model calibration are highlighted. Among these benefits are the enhancement of the model predictability and further understanding of the physical parameters and their uncertainties and correlations.

In order to exemplify the enhancement of uncertainty estimation via methods of model calibration, the problem discussed in the previous section is used. Uncertainty quantification is first performed before model calibration using the *a priori* uncertainty distributions, and then the uncertainty quantification is recompleted using the posterior uncertainty distributions.

Figs. 4–6 compare the uncertainties in the quantities of interest prior and posterior to model calibration. The multiplication factor (k_{eff}), maximum fuel pin power (P_{max}), and the maximum fuel pin temperature (T_{max}) are the responses of interest for this case study. In all cases, the posterior uncertainties for the quantities of interest are reduced from their prior values. Note that the uncertainties (σ_R) are generally reduced along with the uncertainty in those uncertainties ($\sigma_{\sigma R}$), represented by the shaded area in the figures, caused by the uncertainty in the surrogate model. This is due to the

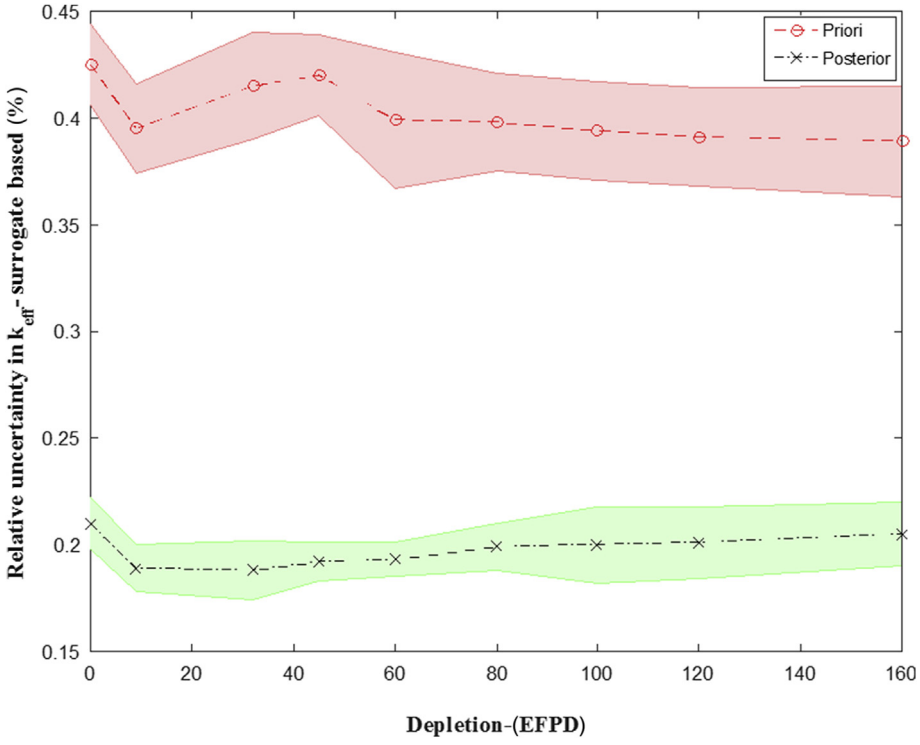

Fig. 4. Prior versus posterior uncertainty in k_{eff}. EFPD, Effective Full Power Days.

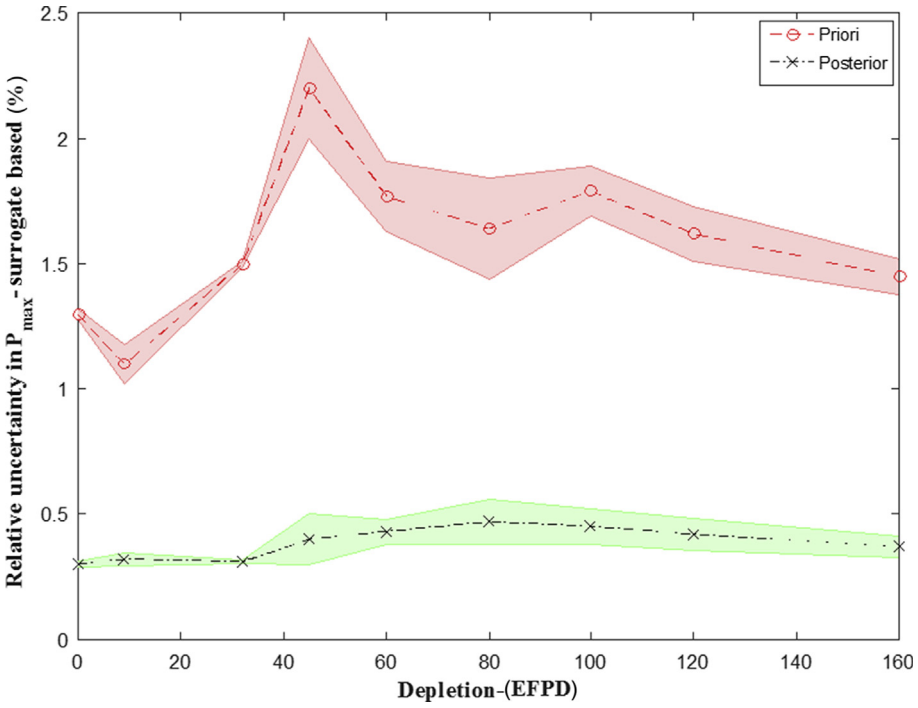

Fig. 5. Prior versus posterior uncertainty in P_{max}. EFPD, Effective Full Power Days.

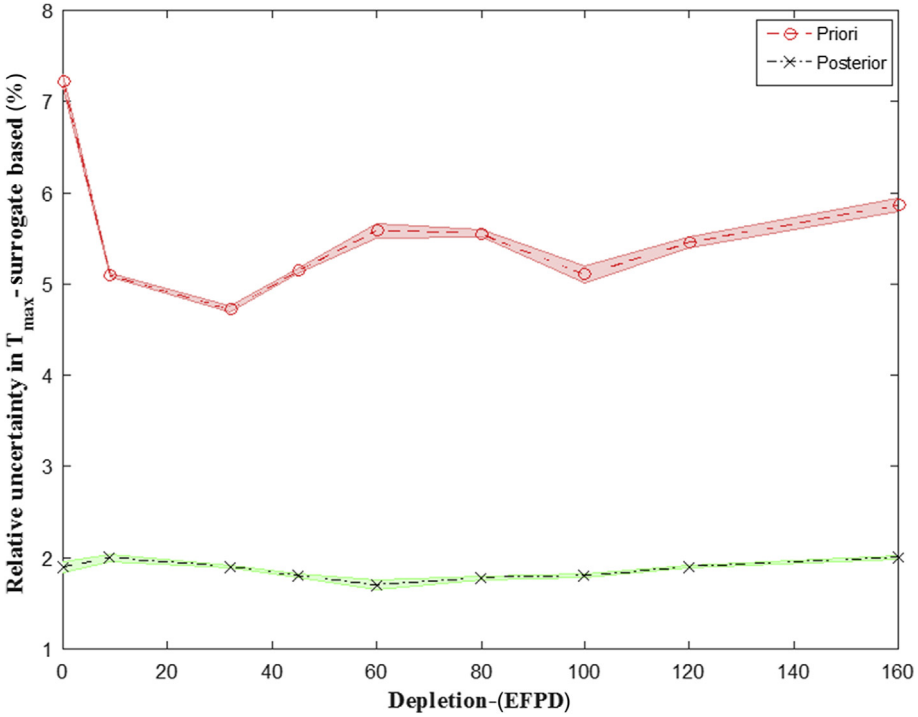

Fig. 6. Prior versus posterior uncertainty in T_{max}. EFPD, Effective Full Power Days.

fact that the updated uncertainty intervals are reduced, and this affects the uncertainty in the surrogate model when predicting the quantity of interest.

5. Conclusion

In this work, surrogate based model calibration has been introduced as an efficient tool to utilize experimental and operational data for model performance enhancement. A previously developed gradient-free algorithm based on reduced order modeling techniques is used to identify the influential DoFs. Once determined, these DoFs are used to recast the problem in terms of these DoFs in the form of mathematical surrogates that can replace the original model.

CASL Progression Problem Number 9 (3 dimensional core depletion problem with thermal-hydraulics feedback) is used to

test the SBMC. The surrogates were constructed for each VERA-CS component (MPACT, COBRA-TF, and ORIGEN) separately due to the limitation in the computer allocation available. Therefore, the presented algorithm can be used to perform model calibration studies with a reasonable computational cost.

This work indicates that model calibration can be used for core simulator problems to enhance thermal-hydraulic and neutronics parameters along with their uncertainties. Moreover, the benefits of model calibration have been explored with regard to uncertainty requantification, which enabled a considerable reduction in the uncertainties of the quantities of interest (about 50–85%), as depicted in Figs. 4–6.

Conflicts of interest

All authors have no conflicts of interest to declare.

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