CALIBRATION OF FUEL PERFORMANCE MODELLING USING METROPOLIS-HASTINGS-WITHIN-GIBBS

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ABSTRACT

This paper presents the calibration of a fission gas release model implemented in the fuel performance code Transuranus to commercial data from Westinghouse. Traditionally, calibration relied on conservative techniques, but there's been a shift towards adopting more best-estimate models with realistic uncertainties. However, model inadequacies can adversely impact calibration techniques, resulting in uncertainties that fail to capture prediction-measurement discrepancies. Previous research demonstrated the incorporation of model inadequacy in the model parameters by assuming a parameter variation across experiments and calibrating distribution parameters using a Metropolis-Hastings-within-Gibbs sampler. This work applies the technique to a more extensive dataset than previous work, i.e., cases from Westinghouse's calibration and validation database. The obtained result agrees with earlier findings for other datasets that the derived uncertainties adequately include the dispersion of the residuals when propagated.

1 Introduction

Fuel performance codes [1] predict key safety parameters, which are compared against corresponding safety limits to ensure the safe operation of nuclear power plants. These codes typically need calibration against physical measurements. Furthermore, it is essential to account for uncertainties to bolster confidence in the results from the fuel performance codes. Consequently, those who develop these codes must estimate modeling uncertainties as part of the calibration process.

In recent years, the combination of Markov Chain Monte Carlo (MCMC) and Gaussian Process ($\mathcal{GP}$) surrogate modeling has gained popularity for calibration as it directly provides the probability distributions for model parameters to facilitate subsequent uncertainty propagation. Previous research [2–4], however, demonstrated that these techniques underestimate uncertainties in fuel performance modeling, primarily due to model inadequacy. More specifically, the derived model uncertainties will not cover the spread of the residuals between code predictions and corresponding measurements unless the model inadequacy is addressed.

Previously, a novel approach [2, 3] was developed involving inflating uncertainties in the calibrated model parameters to cover the effect of model inadequacy. This method, referred to as "the margin method," is based on the assumption of Gaussian intrinsic irreducible uncertainty. It then uses MCMC to calibrate hyperparameters - means and standard deviations of the underlying distribution of model parameters - using a derivative-based approach under linearity assumptions, with differentiated Gaussian processes [5] supporting the process. Reference [4] expands this with an enhanced methodology to remove the necessity for assumptions relying on derivatives and linearity. In that work, a Metropolis-Hastings (MH)-within-Gibbs sampler was employed, showcasing its effectiveness in accurately capturing uncertainties without relying on linearity assumptions.

To demonstrate the practical applicability of this enhanced methodology, this work focuses on extending the testing of the method presented in the reference [4] to calibrate a fission gas release model implemented in the fuel performance code Transuranus [6][7] using Westinghouse's commercial database of fission gas release measurements. The calibrated model parameters yield derived uncertainties that, when propagated, effectively encompass the dispersion of residuals between code predictions and experimental measurements.

2 Application

To calibrate the fission gas release model in Transuranus we use 139 measurements from Westinghouse's commercial calibration and validation database that range from 2% to 35% fission gas release. The rods used for these measurements cover the typical operating range of commercial reactors, though the exact values are proprietary. The calibration methodology needs measurement uncertainties in the specifications of the likelihoods for each measurement, and we select those in accordance with [8] to be a relative uncertainty $\sigma = 5$% (we assume that 10% given in reference [8] corresponds to 2σ). In addition, we use a small absolute uncertainty of 0.1% for regularization purposes. It shall be noted here that a misspecification of the uncertainty will result in yet another model inadequacy. Therefore, the remaining uncertainty not covered by the measurement uncertainty is expected to be lumped into the parameter uncertainties.

Since the calibration methodology described in [4] is sampling-based and requires many samples to reach convergence, we use the same approach of ensembling $\mathcal{GP}$ surrogate models as presented in more detail in reference [5]. To train the surrogate models, we use the Dakota software [9] and Westinghouse's version of Transuranus to uniformly sample 300×4 calibration multipliers applied to various critical phenomenological components of the model, listed in Table 1, to obtain corresponding relative fission gas release predictions.

The calibration parameters we employ are multipliers to the Matzke diffusion coefficient [10] and the athermal release fraction due to recoil and knockout effects suggested by Turnbull [11]. We also apply calibration parameters as multiplicative factors to the standard values of the grain boundary saturation limit and the burnup threshold to activate the modeling of the high burnup structure. All calibration parameters are implemented in the standard strategy for modeling fission gases (fispro = 1) and are listed in Table 1.

We divide the generated data into 75% for training and 25% for testing. The test points are plotted against the Transuranus predictions in Figure 1, and the mean error of the surrogates is 7.2E-3% fission gas release, and the root mean square error is 0.18% fission gas release. This indicates an accurate and unbiased model. The derived surrogates replace the simulation code in this application and are used in calibration and validation in the coming sections. Note here that the models calibrated are confidential and not presented in detail in this paper. Still, some details regarding the standard strategy of modeling fission gas in Transuranus are given in [5].

Tab 1: Calibration parameters in terms of multipliers applied to the important phenomenological components of the calibrated fission gas release model.

Multiplier	Description	Lower Limit	Upper Limit
x_1	Diffusion coefficient	0.05	50
x_2	Athermal release	0.02	10
x_3	Grain boundary saturation limit	0.02	2
x_4	High burnup structure	0.8	1.2

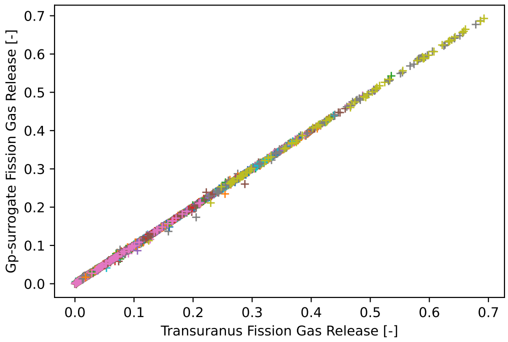


Fig 1: Predictions vs. Transuranus calculations for the independent test data. The different colors represent different measured data points.

3 Calibration Methodology

In this work, we will apply the calibration method already presented in [4] to evaluate how it performs for a different model and more extensive dataset. Therefore, the purpose is not to reiterate the method itself, and we present only a brief overview. More details can instead be found in the original reference.

As demonstrated in [2–4], one way of addressing model inadequacy is to increase the uncertainty of the calibration parameters to adapt its effect. As also demonstrated earlier, that is to assume that the calibration parameters are allowed to vary between experiments. This is opposed to standard calibration, where parameters are considered unknown but physically fixed and have an uncertainty that decreases with the induction of more independent data.

For the four calibration parameters in this paper, such a probabilistic relationship is described as a Bayesian network in Figure 2. The picture shows that instead of having four calibration parameters $\{x_1, x_2, x_3, x_4\}$, it is assumed that there are four calibration parameters $\{x_{i,1}, x_{i,2}, x_{i,3}, x_{i,3}\}$ specific to each experiment i. Those are, in turn, bounded over all experiments according to Gaussian distributions with their own mean μ and std. deviation σ. Under this probabilistic model, we can use the local parameters $\{x_{i,1}, x_{i,2}, x_{i,3}, x_{i,3}\}$ in model $\mathcal{M}_i$ to model each observed experiment y_i. Given a population of measurement values $\{y_1, y_2, ..., y_n\}$, we can further evaluate the Bayesian posterior probability of the entire model and infer both the local parameters and the hyperparameters (means and std. deviations). Previous work [4] has demonstrated that such a probabilistic model can be efficiently sampled using an MH-within-Gibbs sampler despite the high number of free parameters.

Applying an MH-within-Gibbs sampler to the problem above generates samples from the posterior distribution of both means, standard deviations, and local parameters given observed experimental values. The uncertainties can be transferred using the posterior of μ and σ and the assumed Gaussian relationship for a new unobserved experiment. This is practically gen-

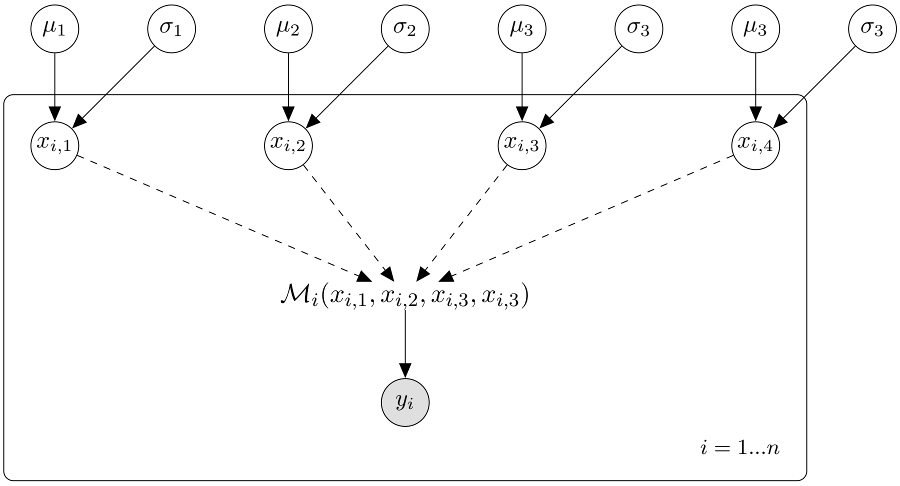


Fig 2: Bayesian network depicting the probabilistic calibration model.

erated after the calibration by sampling one sample from a normal sample for all samples of the hyperparameters. This is the final result of the method as it can be propagated through the model to obtain the uncertainty related to a new prediction and is the main result presented in this paper.

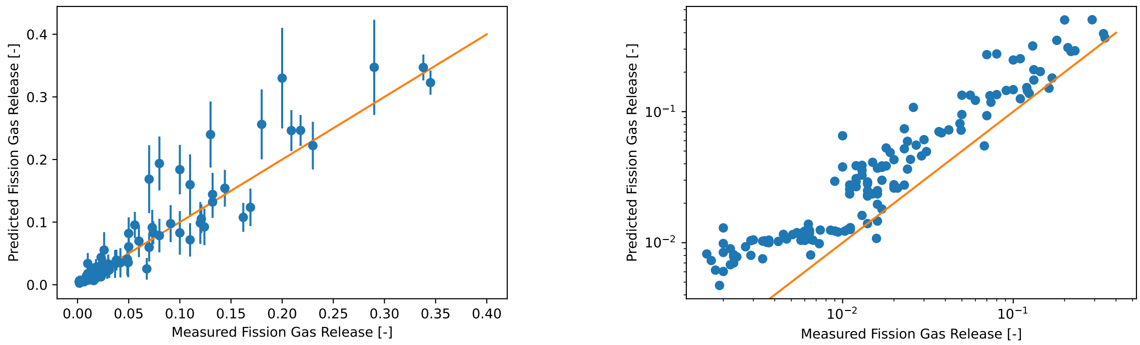
4 Results

This section presents the application of the calibration method to calibrate Transuranus against Westinghouse's fission gas release calibration and validation database. The entire dataset is used in the calibration, and the derived final distribution of the model parameters is presented in Figure 4.

The results indicate that the diffusion coefficient and the thermal release fraction require amplification relative to the standard model and that the diffusion coefficient, in particular, exhibits substantial uncertainty. Conversely, the grain boundary saturation limit and the high burnout threshold multipliers are approximately centered around one. This can be attributed to applying calibration factors to standard values, which have already been pre-optimized.

To investigate the effect of the derived uncertainty on the output, we have propagated the uncertainties to the outputs and generated 1-σ uncertainty bands, see Figure 3a. We also calculate a $\chi^2 = 1.0$, indicating a good fit from this figure. Note here that the validation is inherently stochastic, meaning that exact replication of the process doesn't yield identical results. Consequently, numerical outputs like chi-square values will fluctuate upon repetition.

In addition to the prediction intervals, we have generated one-sided 95/95 prediction limits (including the derived uncertainties and the measurement uncertainty), which are crucial when conservative predictions are compared against safety limits. Those are presented in Figure 3b (log scales are used on the axes for a better interpretation), and the number of unbounded points is 4 out of 139. When plotting predictions against measurements in log-scale, it is apparent that a group of points with low fission gas release has a more flat relationship than the equality line. This disparity hints at a systematic inadequacy in the predictions, particularly evident in scenarios characterized by minimal fission gas release. Such instances primarily stem from athermal processes and will not pose significant safety concerns since a very low fission gas release is expected to have a negligible effect on internal rod pressure and gap heat transfer.



(a) 1-σ prediction intervals

(b) 95/95 Upper Bound Prediction limits

Fig 3: Best-estimate and upper-bound predictions plotted against fission gas release measurements. In Figure 3a, corresponding 1-σ prediction intervals (includes both parameter and measurement uncertainties) accompany best-estimate predictions, and in Figure 3b, upper bound predictions (also includes both parameter and measurement uncertainties) are plotted in a log-log scale for better visualization of the bounding of low-fission gas release cases.

5 Discussion and Conclusions

In this paper, we have applied the calibration methodology from reference [4] to Westinghouse's commercial fission gas release calibration and validation database. The results show that the calibration methodology yields accurate uncertainties in that the dispersions between the predictions and measurements are covered within the calibration parameters. Compared to previous applications, this study includes a more extensive data set identical to that used to calibrate models for fuel licensing. The results thus confirm that the applied calibration method is suitable for calibrating fuel performance codes intended for industrial applications. However, the results in this work are to be considered preliminary in that the calibration method is applied to the entire database without using independent data for validation. Therefore, future work should include using cross-fold or hold-out validation.

The process is simpler and easier to apply than the previous methods using linearity assumptions. Moreover, the methods do not require pre-calibrating the means as the previous method, which is an improvement. Both previous methods and this method stem from the assumption of the hierarchical model, where the parameters have intrinsic variability, and we note that this is very similar to that assumption of calibrating aleatoric variables in reference [12]. Moreover, in this context of a hierarchical model, it is a drawback that the distribution type has to be user-specified, but using the MH-within-Gibbs sampler easily allows the use of any distribution as long as one can formulate an expression proportional to its logarithmic probability density function. Therefore, one topic for future research is to implement and test the use of other distributions, such as log-Gaussian, that allow for skewer behavior.

The sampler employs inner Metropolis-Hastings (MH) steps to update experiment-specific calibration parameters iteratively. These steps rely on proposal covariances, which were set at fixed values and remained unadjusted throughout this application. Therefore, a notable area for enhancement lies in integrating the calibration methodology with an automated tuning mechanism for proposal covariances. One promising approach involves leveraging adaptive proposal distribution methods [13–15] to dynamically adjust the covariances, thereby potentially enhancing the efficiency of the calibration process.

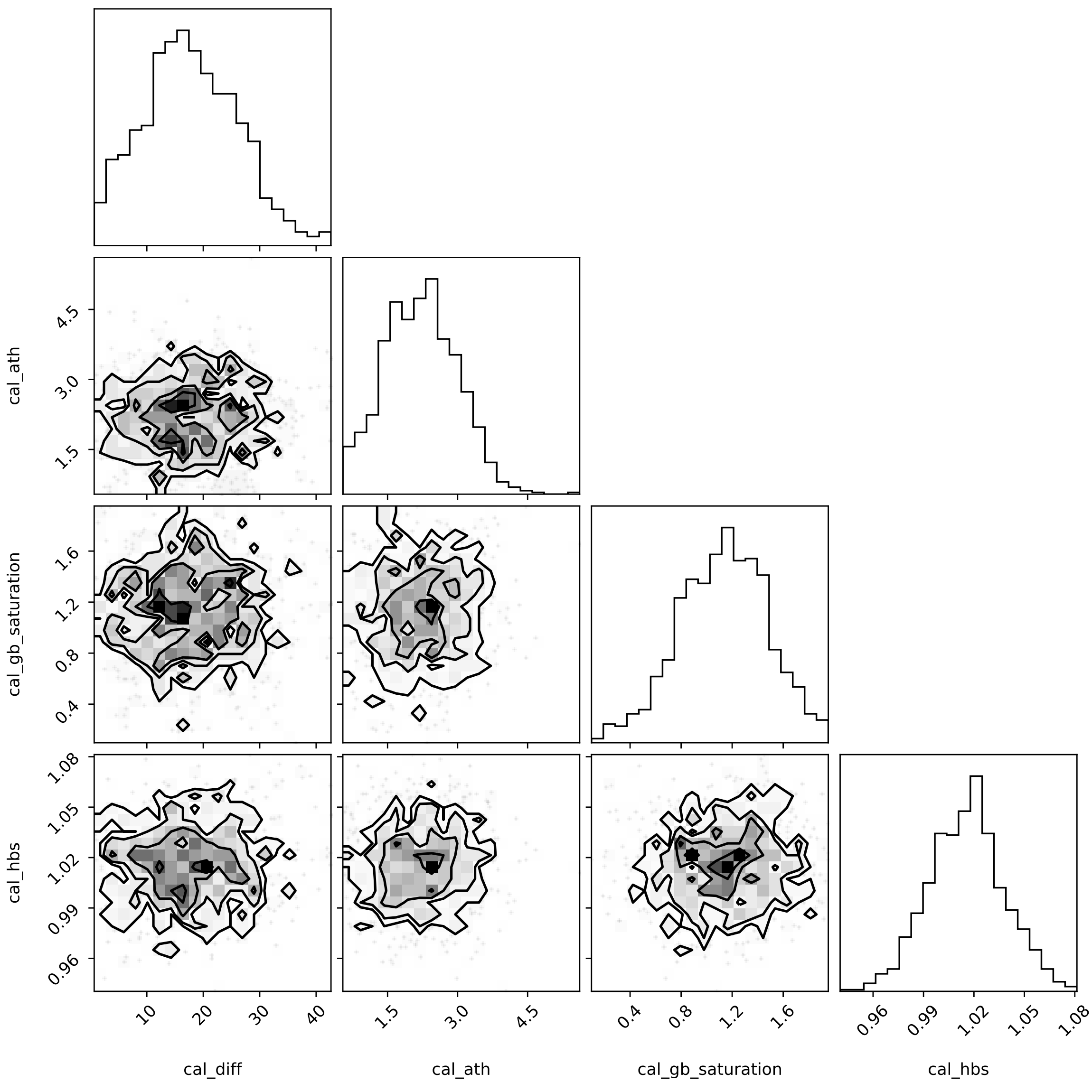


Fig 4: Derived inflated posterior distribution of the model parameters.

6 Acknowledgements

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A The APIS project

APIS is short for Accelerated Program for Implementation of Secure VVER fuel Supply. The objective of the APIS program is to create security of supply of nuclear fuel for Russian-designed pressurized water reactors (VVER) operating in the EU and Ukraine. The program is co-funded by the European Union through the Horizon program. It was started in January 2023 and has a duration of 36 months. Westinghouse is leading the program, supported by eleven different partners, including the affected utilities, another fuel manufacturer, fuel engineering, and research organizations.

The European partners in APIS from eight countries include utilities: CEZ AS - Czech Republic, Energoatom - Ukraine, Fortum - Finland, MVM Paks Nuclear Power Plant - Hungary, and Slovenske Elektrarne AS – Slovakia; fuel manufacturers: Westinghouse (Sweden) and Enusa (Spain); and fuel engineering and research organizations: JRC-Joint Research Centre-European Commission – Belgium, State Scientific and Technical Center for Nuclear and Radiation Safety of Ukraine, UJV REZ AS - Czech Republic, Uppsala University – Sweden, and VUJE, a.s., Slovakia.

The presented research is of general interest for all model calibration and, specifically all model calibration connected to fuel performance modeling. More specifically, this project is part of WP6- “Advance fuel performance modeling” in the EU-supported APIS project (https://apis-project.eu/), with the aim to deliver a new calibration methodology to the stakeholders.

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