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BAYESIAN CALIBRATION OF EMPIRICAL MODELS COMMON IN MELCOR AND OTHER NUCLEAR SAFETY CODES

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ABSTRACT

In modern scientific analyses, physical experiments are often supplemented with computational modeling and simulation. This is especially true in the nuclear power industry, where experiments are prohibitively expensive, or impossible, due to their extreme scales, high temperatures, high pressures, and the presence of radiation. To qualify these computational tools, it is necessary to perform software quality assurance, verification, validation, and uncertainty quantification. As part of this broad process, the uncertainty of empirically derived equations must be quantified. In this work, three commonly used thermal hydraulic models are calibrated to extensive sets of experimental data. The empirical equations are used to determine single phase friction factor in smooth tubes, single phase heat transfer coefficient for forced convection, and the transfer of mass between two phases. Bayesian calibration methods are used to estimate the posterior distribution of the parameters given the experimental data. In cases where it is appropriate, mixed-effects hierarchical calibration methods are utilized. The analyses presented in this work result in justified and reproducible joint parameter distributions which can be used in future uncertainty analysis of nuclear thermal hydraulic codes. When using these joint distributions, uncertainty in the output will be lower—and therefore more accurately represent the state of knowledge for these phenomena—than traditional methods of determining parameter uncertainty.

KEYWORDS
Calibration, Friction, Heat Transfer, Bayesian Analysis

1. INTRODUCTION

In the classical scientific method, the reciprocity between explanatory hypotheses and physical experiments was used to make conclusions. In recent decades, this paradigm has been enhanced through the introduction of the modern computer. The new scientific process allows predictive computational models to explore and analyze events at scales and with precision that was previously unattainable. However, before physical experiments can be supplemented with computational simulation, the accuracy of computer models must be established.

Rigorous evaluation of computer models has been outlined throughout the literature, for example in [1, 2]. These processes include software quality assurance, verification, validation, and uncertainty quantification. This work focuses on calibration, which is a process related to uncertainty quantification during the uncertainty in empirical models is addressed. In general, calibration is performed individually on empirical models in the code to assess both parameter and experimental uncertainties.

In this work, two different statistical models are employed where appropriate. The first model is a fixed effects analysis, which is very commonly employed [3]. In this case, all experimental data is governed by a single law or physical model without variation between individual experiments. In some cases where

individual experiment(s) exhibit deviations from the population, fixed effects models are insufficient. In these cases, mixed-effects analyses are necessary. One example of mixed-effects analysis has consistently been used to demonstrate mixed-effects tools in computational packages (e.g., R, Matlab, etc.) [4]. In this example, the circumferences of five orange trees are measured over time. Though the trees are all governed by the same growth pattern, they each have individual growth rates determined by sun exposure, nutrition, disease, etc. Therefore, the circumference of all the trees are fit to a logistic growth model and the mixed-effects model is used to account for variations between the individual trees.

Mixed-effects analysis is common in many fields, but it has only recently received attention for engineering applications. For example, a mixed-effects model has been fit to experimental data for the degradation of nuclear reactor pipes [5] and dating of crystals through the process known as *fission track dating* [6]. In this work, these ideas are extended to common practical nuclear engineering problems. It is our intent to introduce these methods to a wider audience and make them more accessible for general applications.

The Bayesian calibration techniques employed in this work are introduced in Section 2. Example applications are outlined in Section 3, which includes three common nuclear engineering models: friction factor, heat transfer coefficient, and mass transfer coefficient between phases. The work concludes with a discussion and outline of future work.

2. BAYESIAN CALIBRATION

Bayesian analysis assumes a joint prior parameter distribution, $\pi_o(\theta)$, which incorporates knowledge previously known about the distribution. The goal of Bayesian calibration is to combine the information provided by the prior with some new experimental data y. This is done by determining the posterior distribution $\pi(\theta|y)$, which uses the likelihood function $\mathcal{L}(y|\theta)$ to incorporate information about both the prior and experimental data. The posterior and prior functions are related through the likelihood function through Bayes formula.

$$\pi(\theta|y) = \frac{\mathcal{L}(y|\theta)\pi_o(\theta)}{\int \mathcal{L}(y|\theta)\pi_o(\theta)\, d\theta} \tag{1}$$

Combinations of parameters that are more likely to have generated the observed data are associated with greater likelihood values. The direct solution of Bayes formula is either impossible or very computationally intensive for most practical applications. Therefore, sampling methods are generally used to approximate it [7]. This general class of methods, Markov Chain Monte Carlo (MCMC), construct a sampling-based chain whose stationary distribution is the desired posterior. Bayesian calibration provides a joint posterior distribution that is consistent with experimental data, justifiable, reproducible, and not constrained to any predefined distribution.

2.1. Fixed Effects Analysis

In most cases, empirical models represent data which is governed by the same physical law or theory. In such cases, the same parameter distributions describe the whole population. These types of analyses are indicative of *fixed effects* statistical models.

$$y_n = f(x_n, \theta) + \varepsilon \tag{2}$$

Here, the n-th experimental data point y_n is associated with the state variable(s) x_n and f is the model to be fit to the experimental data. The observational error ε is generally assumed to be identically,

independently, and normally distributed with a mean of zero, $\varepsilon \sim N(0, \sigma^2)$ [3]. The model parameters θ and observational error variance σ are unknowns to be statistically inferred.

For fixed effects analyses, this work employs the Delayed Rejection Adaptive Metropolis (DRAM) algorithm, which an MCMC method [8]. DRAM improves upon basic MCMC by updating the covariance matrix throughout the simulation [9] and by allowing second stage candidates to be proposed [10]. Both improvements increase the efficiency and robustness of the algorithm.

To accurately sample from the posterior distribution, the Bayesian chains must be converged. To achieve a converged solution, the MCMC algorithm is run for an initial convergence period, or *burn-in*, which is excluded from the final analysis. In this work, 10^6 burn-in samples are used, which is relatively large compared to other analyses in the literature [3,11]. This large burn-in period is required because no effort is made to provide the DRAM algorithm with accurate initial values of the parameter distribution or observational error. The DRAM code used in this work was implemented by Marko Laine [12].

2.2. Mixed Effects Analysis

Some physical processes require mixed-effects analysis. This statistical model allows the population to be governed by some physical model while individuals in the population exhibit variations. The mixed-effects statistical model has *random effects* for each laboratory β_l [11].

$$y_{nl} = f(x_n, \theta + \beta_l) + \varepsilon \tag{3}$$

Here, the *global effects* θ account for the overall behavior of the model whereas the random effects β_l account for variations between the l individuals. In this work, a hierarchical Metropolis-within-Gibbs Bayesian framework is employed to estimate both the global and random effects. Gibbs sampling is an MCMC method for sampling a posterior distribution that is either unknown or difficult to sample and is therefore well-suited to the hierarchical framework [11]. With this method, the parameters are given prior distributions $\theta \sim N(\theta_o, \Sigma_o)$, $\beta \sim N(\beta_o, \Psi)$, $\Psi \sim W^{-1}(\psi_o, \rho_o)$, and $\sigma^2 \sim InvGamma(\nu_o, \tau_o)$ [11]. Here, $W^{-1}(\psi_o, \rho_o)$ indicates the inverted Wishart distribution with scale matrix ψ_o and degrees of freedom ρ_o.

For this work, the same implementation is used as the fixed effects analyses [12]. Mixed-effects models converge slowly, and therefore 10^6 burn-in iterations are used. Prior distributions and starting values for the chains are determined using the Matlab function `nlmefit`.

3. APPLICATIONS

In this section, Bayesian calibration methods are applied to three empirical models used in MELCOR [13]. These models are also common in other nuclear safety codes, such as the subchannel code COBRA-TF [14] and the system code RELAP [15].

3.1. Single Phase Friction in Smooth Tubes

The analytical derivation of friction factor f requires that the velocity distribution within the pipe is known. The is only practical for flows with low Reynolds numbers, where the fluid flows in parallel layers without lateral mixing. Under this *laminar flow* condition, the friction factor can be analytically calculated for incompressible Newtonian fluids in smooth tubes [16].

$$f = \frac{64}{Re} \tag{4}$$

For Reynolds numbers greater than about 2000, turbulence causes chaotic changes in the velocity field, which makes analytical calculation of the friction factor impossible. Under these conditions, the friction factor is determined empirically. For high Reynolds numbers, where *turbulent flow* exists, a variety of equations exist for determining the friction factor. One of the most widely used is the McAdams relation [17,18].

$$f = 0.005 + 0.5Re^{-0.32} \tag{5}$$

This equation is valid for $3 \cdot 10^3 < Re < 3 \cdot 10^6$. In the turbulent regime, the friction factor is also a function of pipe roughness; however, this dependence is not generally treated in nuclear safety codes. Due to manufacturing processes, radiation damage to materials, and the buildup of corrosion materials on reactor surfaces, it is nearly impossible to determine the effective roughness of a surface in a normal operational reactor. This uncertainty is even larger in MELCOR, since the roughness of severe accident materials (debris, core melt, etc.) are unknown. Therefore, surface roughness will not be considered in this work.

Between laminar and turbulent flow, there exists a *transition region*. In this work, the transition region is modeled as a combination of the laminar and turbulent relations.

$$f_{trans} = (1 - S)f_{lam} + Sf_{turb} \tag{6}$$

Here, S is the logistic function

$$S = \frac{1}{1 + e^{-a(Re-b)}} \tag{7}$$

Where the two parameters a and b determine how quickly the transition happens and where it is centered. The parameters have approximate values of 0.01 and 2500, respectively. In this section, the friction factor is parameterized with two random effects and five global effects.

$$f = \left(1 - \frac{1}{1 + e^{-(\theta_1+\beta_{1l})(Re-(\theta_2+\beta_{2l}))}}\right)\frac{64}{Re} + \frac{\theta_3 + \theta_4 Re^{-\theta_5}}{1 + e^{-(\theta_1+\beta_{1l})(Re-(\theta_2+\beta_{2l}))}} \tag{8}$$

Here, the parameters that determine the transition regime are modeled using mixed-effects. The transition to turbulence is strongly influence by laboratory-dependent factors such as entry geometry, development length, and pump vibrations [19]. Recent studies have even suggested that the transition to turbulence depends upon microscopic motions of molecules, meaning that the selected working fluid also plays a roll [20]. Therefore, the laminar-turbulent transition is dependent upon the experimental facility and there are biases that lend themselves to mixed-effects analyses.

Experimental data sources for the friction factor calibration are shown in Table I and Figure 1. Note that the figure shows the transition and turbulent regimes separately, but the two models are continuous and smooth. The data is restricted to friction factors below 0.05, since the laminar solution is analytical. Any error in this region can therefore be attributed to model form, which is not related to the calibration process. We also restrict the data to $Re < 2 \cdot 10\text{^}6$, which is representative of nuclear reactor conditions and is well within the range of applicability for the McAdams equation. In total, 453 data points from five experiments are used for the calibration.

The mixed-effects Bayesian calibration is performed, and the resulting 95% prediction intervals are shown in Figure 2. The intervals enclose the appropriate proportion of the experimental data and have

Table I. Data sources for single phase pressure drop in smooth pipes

Year	Author	Pipe	Fluid
1914	Stanton & Pannell [21]	brass	water, air
1932	Nikuradse [22, 23]	brass	water
1969	Patel & Head [24]	brass	air
2002	Swanson et al. [19]	stainless steel	gases, liquid He
2017	Everts & Meyer [25]	copper	water

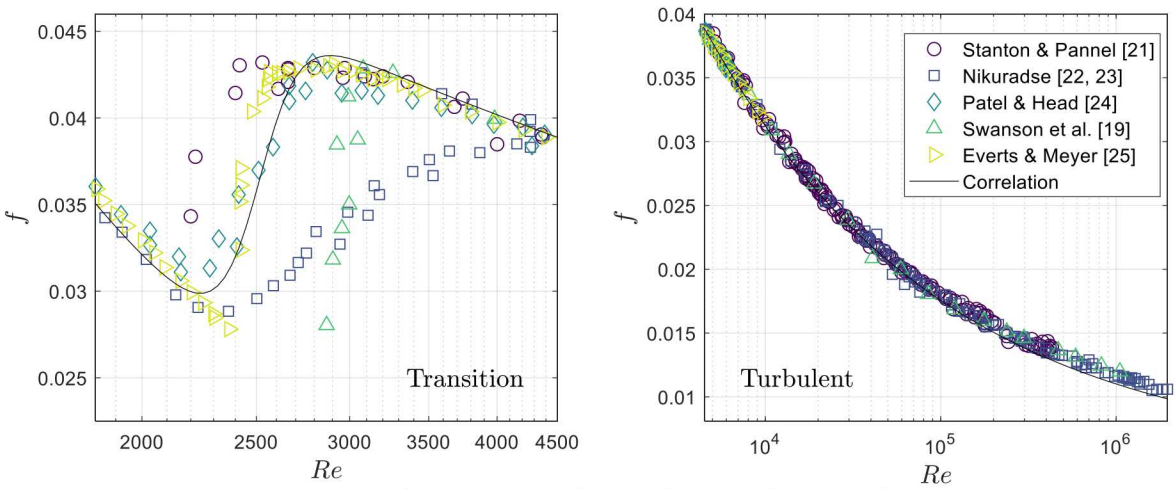

Figure 1. Experimental data for the friction factor calibration

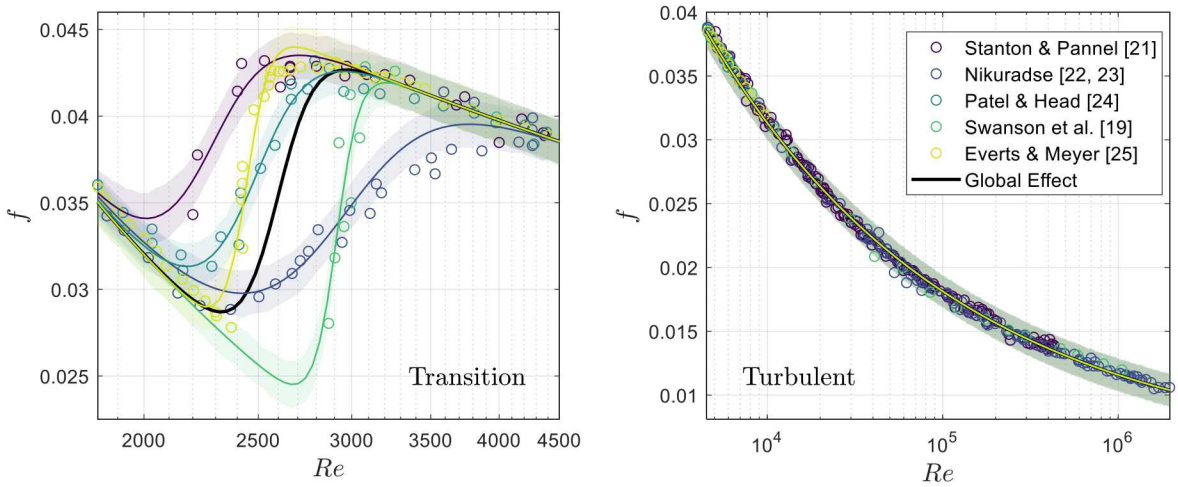

Figure 2. Calibration results for friction factor calibration

reasonable levels of uncertainty. Additionally, the variable behavior of the transition regime is appropriately accounted for by the mixed-effect statistical model. The parameters in the turbulent regime are all global, so there are no differences between the results for the different experiments. The calibration results in an overestimation of uncertainty at high Reynolds numbers, since the friction factor at low Reynolds numbers is much higher. To account for this, the observational error could be scaled with the friction factor prediction at the corresponding Reynolds number [3].

3.2. Single Phase Forced Convection Heat Transfer

Heat transfer coefficients can be analytically derived in situations where the temperature and velocity distributions are known. However, this is generally only possible for laminar flow conditions. For transition and turbulent flow, the heat transfer coefficient must be determined empirically. For forced convection flow through smooth tubes, the Dittus-Boelter equation [26], which is based on the experimental data of Morris and Whitman [27], is generally used.

$$Nu = 0.023\, Re^{0.8} Pr^{0.4} \tag{9}$$

The Dittus-Boelter equation is formed into a three-dimensional calibration model, where all three parameters have both global and mixed effects.

$$Nu = (\theta_1 + \beta_{1l})\, Re^{(\theta_2+\beta_{2l})} Pr^{(\theta_3+\beta_{3l})} \tag{10}$$

Data from three different sources is gathered for the Dittus-Boelter calibration; they are listed chronologically in Table II and shown in Figure 3.

Table II. Data sources for forced convection heat transfer coefficient

Year	Author	Pipe	Fluid
1928	Morris & Whitman [27]	steel	water, oil
1931	Lawrence & Sherwood [28]	copper	water
1952	Deissler & Eian [29]	Inconel alloy	air
1963	Kays & Leung [30]	Inconel alloy	air

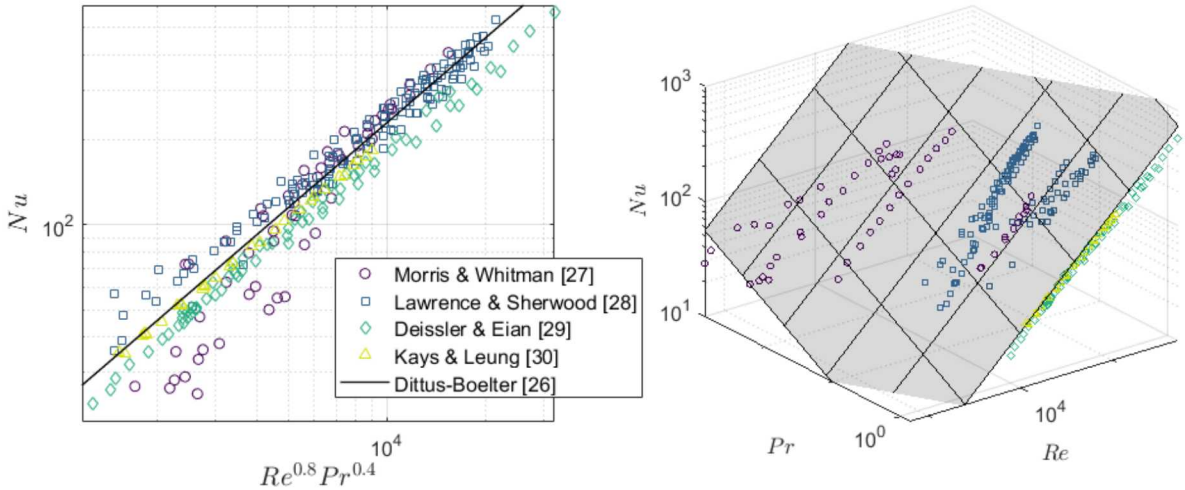

Figure 3. Experimental data for heat transfer coefficient calibration

The correlation is calibrated to the experimental data, yielding a three-dimensional mixed-effects result. Plotting intervals for the full three dimensions is very difficult, so instead two-dimensional slices are analyzed. Two slices are shown in Figure 2, where $Pr = 0.7$ and $Pr = 3.0$ are respectively representative of air and water. The random effects in this analysis are larger in this analysis than in the friction factor correlation, and therefore there are strong deviations of individual experiments from the global effects.

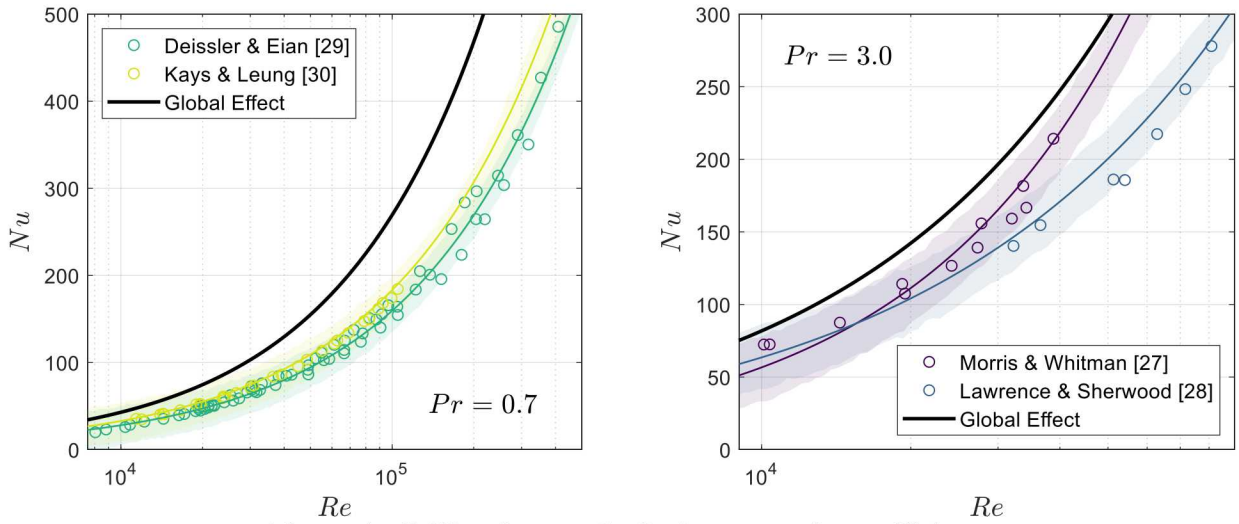

Figure 4. Calibration results for heat transfer coefficient

3.3. Mass Transfer between phases

As part of the boiling and condensation models in nuclear safety codes, the mass transfer between phases must be approximated. In addition, heat/mass transfer between other phases is treated using the same model in MELCOR. This empirical relation takes a form similar to the Dittus-Boelter correlation.

$$Nu = 2.0 + CRe^{0.5}Pr^{1/3} \tag{11}$$

It is derived through analysis of flow over spheres, where the value 2.0 is analytically determined and the remaining constants are semi-empirical. Values of C vary throughout the literature, but the most common values, suggested respectively by Froessling [31] and Ranz & Marshal [32], are 0.55 and 0.6.

Data is gathered from four sources, which are listed chronologically in Table III. The data is plotted in both two dimensions and three dimensions in Figure 5.

Table III. Data sources for interphase mass transfer relation

Year	Author	Fluid	Sphere
1938	Froessling [31]	air	analine
1940	Powell [33]	air	water
1952	Ranz & Marshall [32]	air	benzene, water
1960	Yuge [34]	air	steel, brass

For the calibration, the analytically determined parameter is held constant. Though the value may have model form uncertainty, we treat it as known for this analysis. The other three parameters are exposed, with only the first two having random effects.

$$Nu = 2.0 + (\theta_1 + \beta_{1l})Re^{(\theta_2+\beta_{2l})}Pr^{\theta_3} \tag{12}$$

The calibration is performed, and the resulting 95% prediction intervals for $Pr = 0.6$ and $Pr = 0.7$ are shown in Figure 6. The calibrated model agrees relatively well with the experimental data; however, the Powell data set appears to have larger experimental uncertainty than the other data sets. As such, an

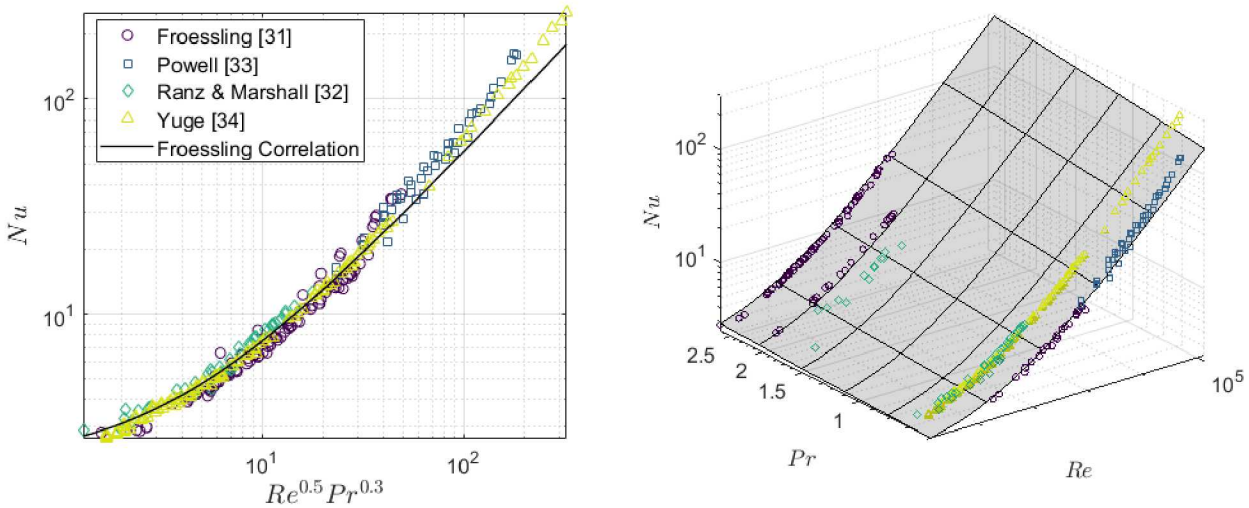

Figure 5. Experimental data for interphase heat or mass transfer calibration

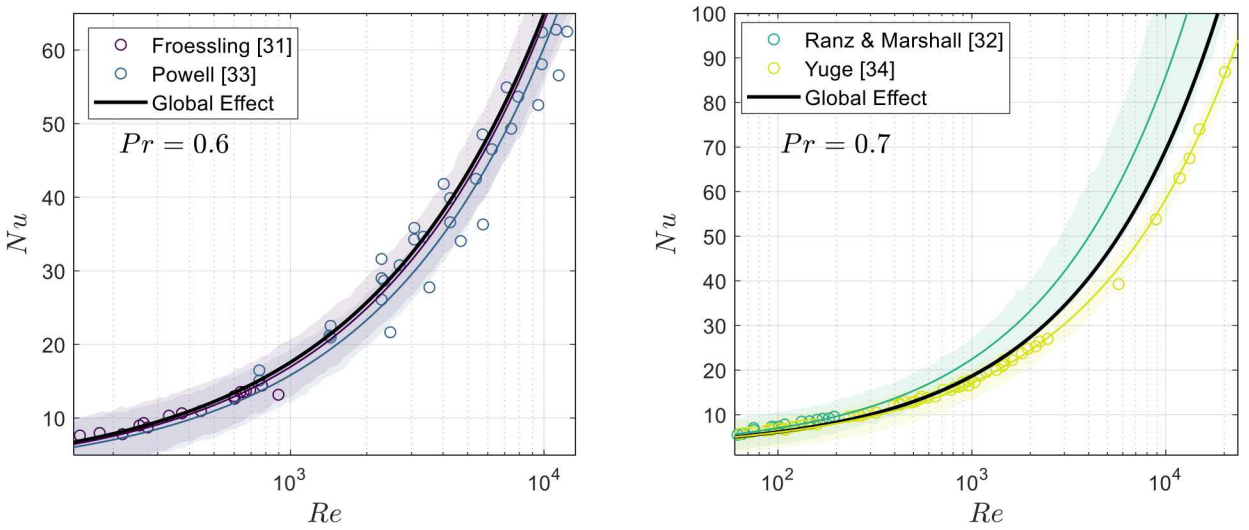

Figure 6. Calibration results for interphase heat or mass transfer

observational error which is different for each laboratory might be appropriate.

$$y_i = f(x_i, \theta + \beta_l) + \varepsilon_l \tag{13}$$

Such models are available in the literature and commonly used for such problems [3]; however, this extension is not performed here. Accounting for the variation in experimental error would have little effect on the global effects, which are the parameters of interest for propagation.

4. CONCLUSION

In this work, three empirical relations common to nuclear safety codes are calibrated to extensive sets of basic experimental data. The Bayesian methods lead to a justifiable and reproducible joint distribution of the parameters. The mixed-effects statistical model allows the calibration to account for biases between experiments, which are attributed to both physical phenomena and to unknown biases between the

experimental facilities. The resulting joint distributions can be used predictively by either (1) incorporating random parameters and analyzing additional experiments from the experimental facilities used in the calibration, or (2) excluding random parameters and using the global results to predict behavior in new facilities.

A few weaknesses of the currently employed Bayesian framework were exposed in this work. The two primary problems deal with the definition of the observational error, ε. The observational error is an absolute value, and therefore is not suitable for the calibration of models which vary many orders of magnitude. This was the case for both the Dittus-Boelter and the Froessling correlations. To fix this, the observational error should be scaled with the quantity of interest. The observational error also seemed to vary between different experiments, especially for the final calibration, where Powell's experiments had large uncertainties. To account for this, the observational error can depend upon the experimental facility, similar to the random effects.

In future work, similar methods should be extended to additional models in nuclear safety codes. With a thorough knowledge of individual models in the code, integral assessment of the code becomes possible. The analyses in this work can be incorporated into a hierarchical validation framework and used to incrementally improve a computational tool.

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