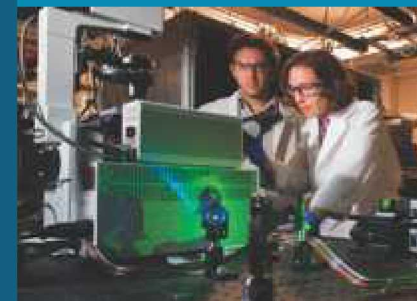
SAND2019-8178C xxC

Bayesian Calibration of Empirical Models Common in MELCOR and Other Nuclear Safety Codes



PRESENTED BY

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Motivation 1/2

- Empirical models used in reactor calculations are often based on data from decades ago.
- In many cases, these correlations are constructed using disparate data sets.
  - Different measurement devices/techniques
  - Various working fluids
  - Fluid property evaluations
  - Untreated physics/insufficient scaling
  - Human error
- The biases between these datasets are, in general, not treated during the formulation and calibration of the empirical model.

Phenomenon	Model	Year
Single phase Pressure drop	Colebrook Equation	1938
Two-phase pressure drop	Beattie	1982
Single phase wall heat transfer	Dittus-Boelter (McAdams)	1985 (1954)
Nucleate boiling heat transfer	Rohsenow	1951
Film boiling heat transfer	Bromley	1948
Critical heat flux	Zuber	1958
Film boiling	Zuber/Berenson	1960
Interfacial heat transfer	Lee & Ryley	1968
Terminal Taylor bubble velocity	Griffith	1961

Motivation 2/2

- Code uncertainty is underestimated when biases between datasets are not considered.
- When uncertainties are untreated, it is equivalent to assuming they are zero; in these cases, there is no motivation to reduce uncertainties.
- The purpose of this work is twofold:
  - Quantify and understand these biases/uncertainties, and
  - Motivate researchers to revisit some of these problems using modern hardware, techniques, and data acquisition systems.

Background and Theory

Calibration: Bayesian Methods

- In general, calibration is a statistical method to infer unknown parameter values/distributions by observing state variables and corresponding data (physical or computational experiments).
- Bayesian methods allow for the incorporation of prior information from previous experiments or expert knowledge.
- Solves Bayes' formula, which formulates the desired posterior distribution in terms of the prior distribution and likelihood function.

$$\pi(\theta|y) = \frac{\mathcal{L}(y|\theta)\pi_o(\theta)}{\int_\Theta \mathcal{L}(y|\theta)\pi_o(\theta)d\theta}$$

- We employ sampling methods because (1) the denominator is difficult or impossible to integrate and (2) the product of the likelihood and prior cannot be easily sampled.
- Delayed Rejection Adaptive Metropolis (DRAM) is one such sampling method.[1,2]

1. H. Haario, M. E. Saksman, and J. Tamminen, "An Adaptive Metropolis Algorithm," Bernoulli, 7(2), pp. 223-242 (2001) doi: 10.2307/3318737.
2. A. Mira, "On Metropolis-Hastings Algorithm with Delayed Rejection," Metron, 59(3), pp. 231-241 (2001).

Statistical Model

- For calibration, fixed effects statistical models are generally used, where the experimental data is equal to some model with zero-mean Gaussian measurement noise.

$$y = f(x, \theta) + \varepsilon$$

- This work employs mixed-effects statistical models, where each parameter is a combination of global and random effects.

$$y = f(x, \theta + \beta) + \varepsilon$$

- Frequentist solution methods generally solve this problem through minimization of an approximated likelihood function.[1]
- Bayesian Calibration can be used to obtain estimates of the desired posteriors, using conditional probabilities and likelihood function from the literature.[2]
- Here, a hierarchical Metropolis-within-DRAM method is used.[3,4]
- The DRAM step estimates global parameters, and Metropolis estimates random parameters.

1. J. C. Pinheiro and D. M. Bates, "Approximations to the Log-Likelihood Function in Nonlinear Mixed-Effects Model," *J Comp Graphical Stat,* **4**(1) (1995).
2. J. C. Wakefield, et al., "Bayesian Analysis of Linear and Nonlinear Populations Models Using the Gibbs Sampler," *J Royal Stat Soc*, **43**(1) (1994).
3. K. L. Schmidt, Uncertainty Quantification for Mixed-Effects Models with Applications in Nuclear Engineering, PhD thesis, North Carolina State University (2016).
4. M. Laine, MCMC Toolbox for Matlab (2017), helios.fmi.fi/~lainema/mcmc/.

Methodology

1. Gather experimental data from the literature.
   - Some will be related to original dataset
   - This set of data can be expanded in future work
2. Formulate the statistical model.
   - Use initial frequentist optimization
   - Determine which parameters are fixed/global/random via information criteria minimization
3. Calibrate the statistical model to the experimental data.
   - Use the hierarchical Metropolis-within-DRAM algorithm
   - Burn-in determined based on rule-of-thumb (10^5 iterations)[1]
4. Examine the results.
   - Compare initial correlation, frequentist optimization, and Bayesian calibration.
   - Propagate chain through original model and construct 95% predictive intervals

1. R. C. Smith. *Uncertainty Quantification, Theory, Implementation, and Applications*. SIAM (2014)

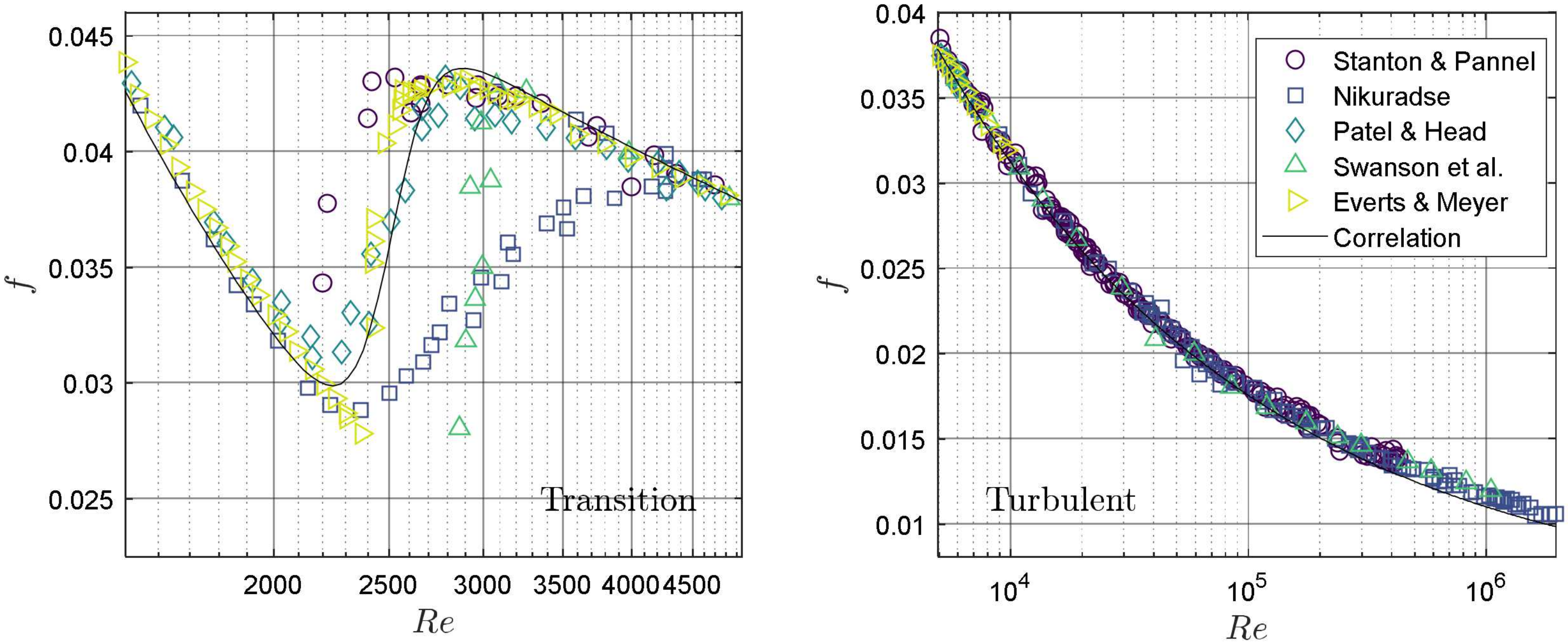
Results

Friction Factor 1/3

- Single phase friction in smooth tubes (Colebrook equation/Moody chart)
- Here, a new correlation is used which represents the transition region using a logistic function.

$$f = (1 - S) f_{laminar} + S f_{turbulent}$$

$$f = \left[1 - \frac{1}{1 + e^{-q_1(Re - q_2)}}\right] \frac{64}{Re} + \frac{q_3 + q_4 Re^{-q_5}}{1 + e^{-q_1(Re - q_2)}}$$



Friction Factor 2/3

- Through minimization of the information criteria, only q_1 and q_2 require random effects.

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

Global	Random	AIC	BIC
	q_1, q_2, q_3, q_4, q_5	-5297.7	-5302.0
q_5	q_1, q_2, q_3, q_4	-5299.7	-5303.6
q_4, q_5	q_1, q_2, q_3	-5301.7	-5305.2
q_3, q_4, q_5	q_1, q_2	-5303.7	-5306.8
q_2, q_3, q_4, q_5	q_1	-4770.1	-4772.8
q_1, q_2, q_3, q_4, q_5		-4515.4	-4517.8

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q_3, q_4, q_5	q_1, q_2	-5303.7	-5306.8
q_2, q_3, q_4, q_5	q_1	-4770.1	-4772.8
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$q_3, q_4,$	q_1, q_2, q_5	-5301.7	-5305.2

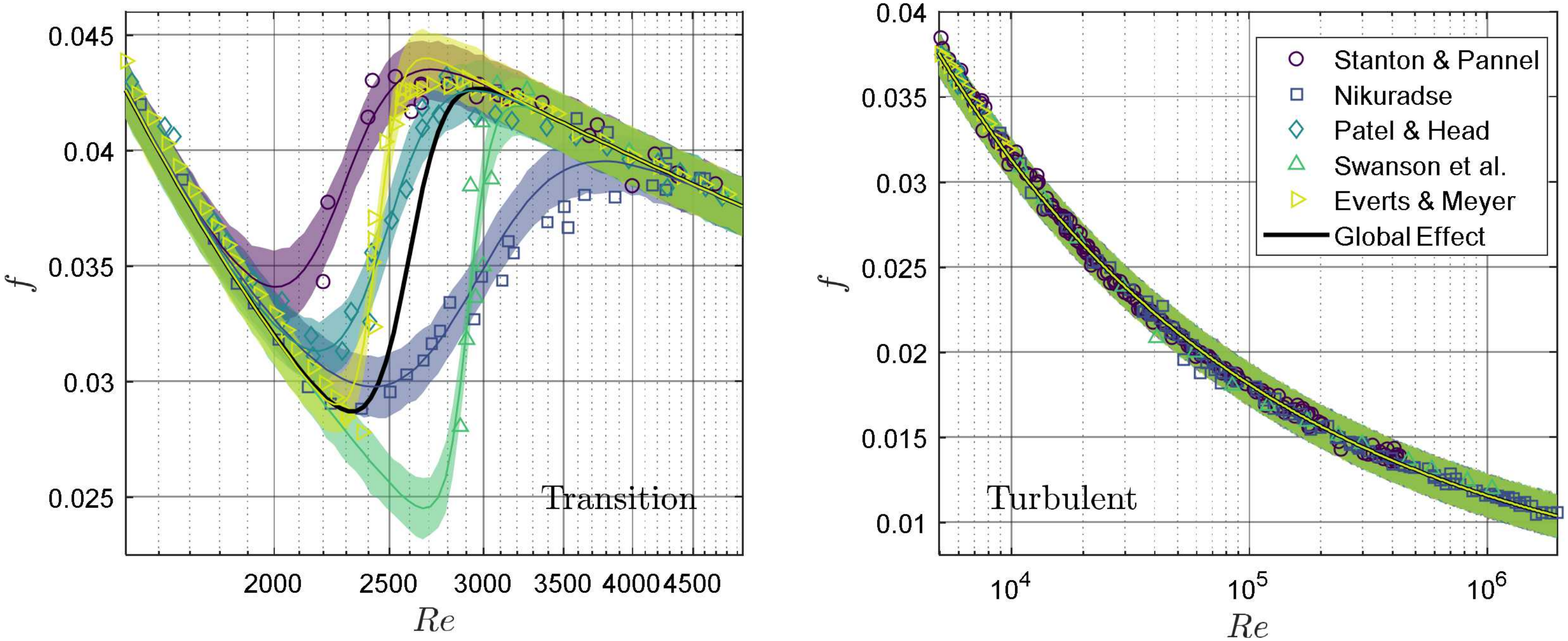
- Through minimization of the information criteria, only q_1 and q_2 require random effects.

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

		Frequentist Optimization					**Bayesian Calibration (mean results)**				
		Stanton	Nikuradse	Patel	Swanson	Everts	Stanton	Nikuradse	Patel	Swanson	Everts
θ_1	0.01	0.01022					0.01042				
β_{1l}		-0.00269	-0.00667	-0.00289	0.00480	0.00745	-0.00285	-0.00685	-0.00299	0.00472	0.00776
θ_2	2500	2582					2584				
β_{2l}		-331.5	272.4	-124.3	325.8	-142.4	-334.7	270.7	-126.1	324.3	-143.9
θ_3	0.005	0.005169					0.005156				
θ_4	0.5	0.4354					0.4336				
θ_5	0.32	0.3054					0.3048				
σ^2		5.996e-7					5.940e-7				
Σ		$\begin{bmatrix} 2.844e-5 & 0 \\ 0 & 6.552e4 \end{bmatrix}$					$\begin{bmatrix} 4.663e-5 & 0 \\ 0 & 1.017e4 \end{bmatrix}$				

Friction Factor 3/3

- Through propagation of the Bayesian chains through the original model, uncertainty bounds can be found for each individual experiment.
- Here, the 95% prediction intervals are shown, and they capture the appropriate percentage of the data.
- Only the parameters which determine the transition region have random effects, so the laminar and turbulent regions do not have laboratory-dependent uncertainty.

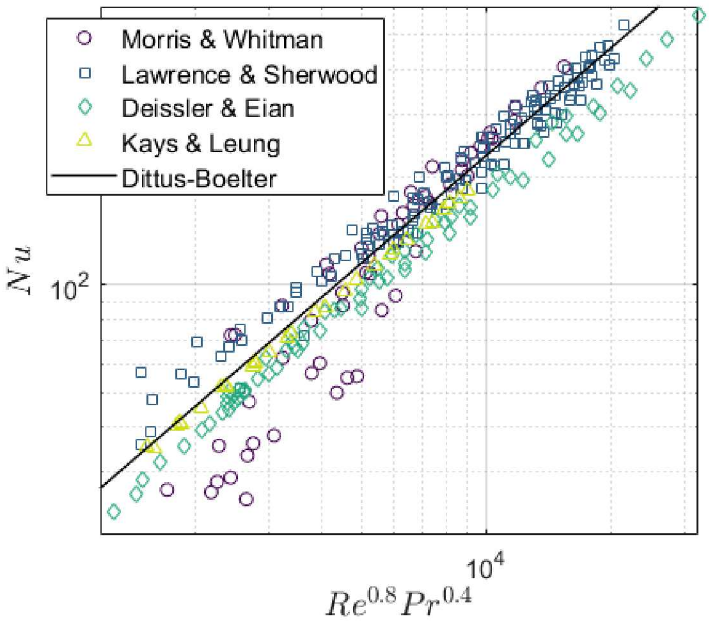


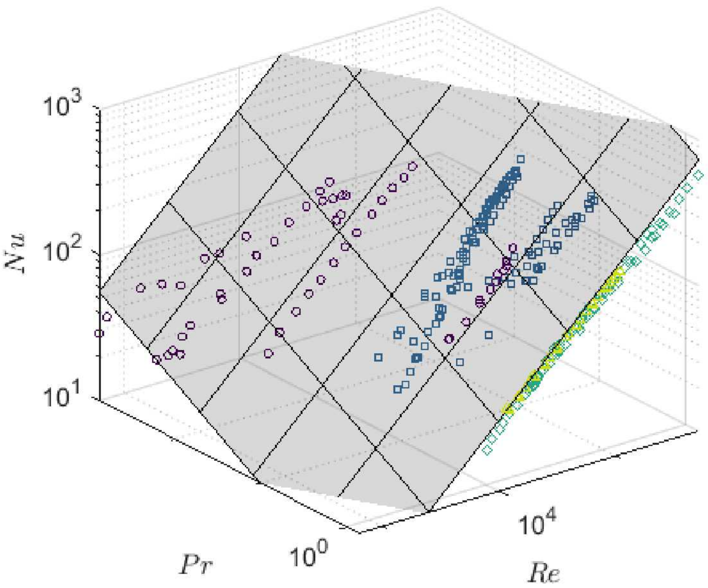
Heat Transfer Coefficient 1/3

- Single phase forced convection heat transfer in smooth tubes
- Represented by the Dittus-Bolter equation, which was created for analysis of automobile radiators

$$Nu = q_1 Re^{q_2} Pr^{q_3}$$

- Data is shown in both two and three dimensions





Heat Transfer Coefficient 2/3

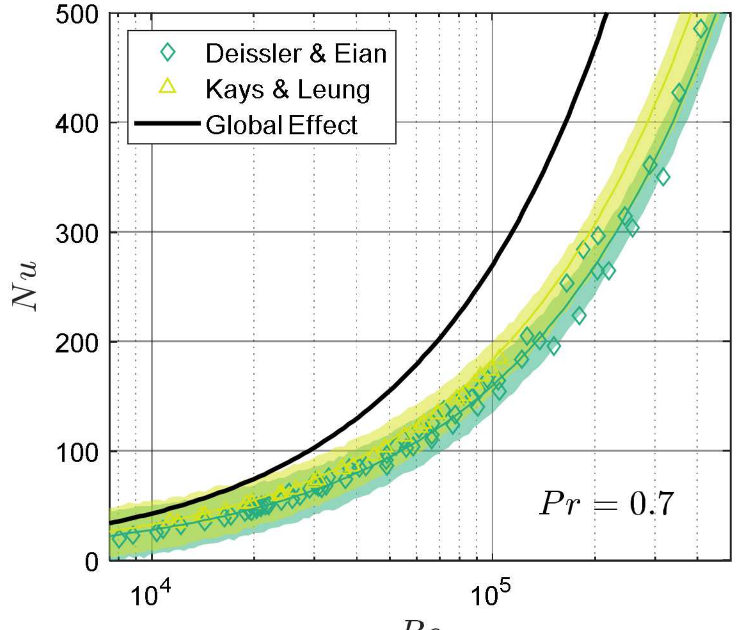
- Through minimizing AIC and BIC, all three parameters require random effects to fit the data.

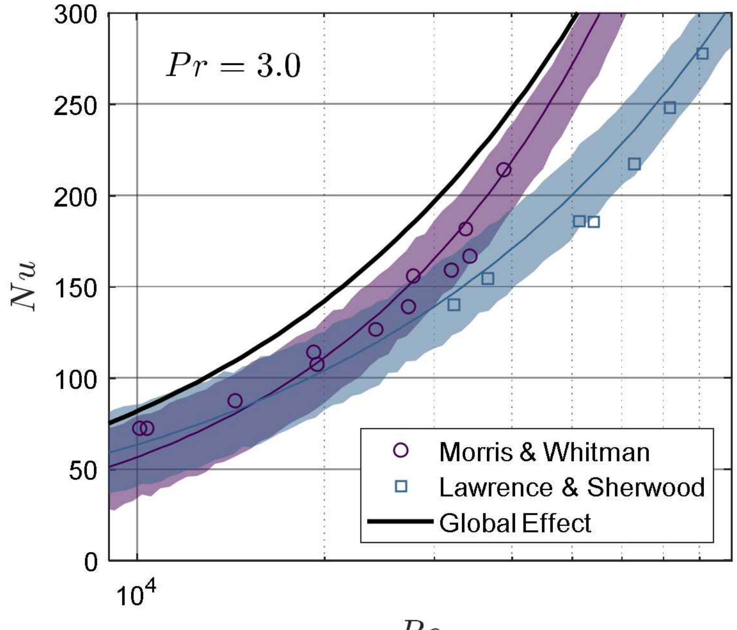
$$Nu = (\theta_1 + \beta_{1l})Re^{(\theta_2+\beta_{2l})}Pr^{(\theta_3+\beta_{3l})}$$

		Frequentist Optimization				Bayesian Calibration (mean results)			
		Morris	Lawrence	Deissler	Kays	Morris	Lawrence	Deissler	Kays
θ_1	0.023	0.0285				0.03234			
β_{1l}		-0.0244	0.0211	8.58e-4	0.00247	-0.0277	0.0203	-7.89e-4	0.00770
θ_2	0.8	0.8064				0.7978			
β_{2l}		0.176	-0.0877	-0.0470	-0.0410	0.176	-0.0842	-0.0428	-0.0524
θ_3	0.4	0.4431				0.4433			
β_{3l}		-0.0326	0.0327	-3.07e-5	-1.06e-3	-0.0379	0.0315	0.0191	-0.0128
σ^2		183.3				184.07			
Σ		$\begin{bmatrix} 3.065e-4 & 0 & 0 \\ 0 & 1.105e-2 & 0 \\ 0 & 0 & 1.187e-3 \end{bmatrix}$				$\begin{bmatrix} 5.570e-4 & 0 & 0 \\ 0 & 1.827e-2 & 0 \\ 0 & 0 & 3.469e-3 \end{bmatrix}$			

Heat Transfer Coefficient 3/3

- Again, the chains are propagated through the original model.
- It is difficult to plot three dimensional prediction intervals, so they are plotted for fixed Prandtl number.
- The appropriate fraction of data is within the prediction intervals.
- The global effect, which only uses the fixed parameters, is significantly different than any of the laboratory results.



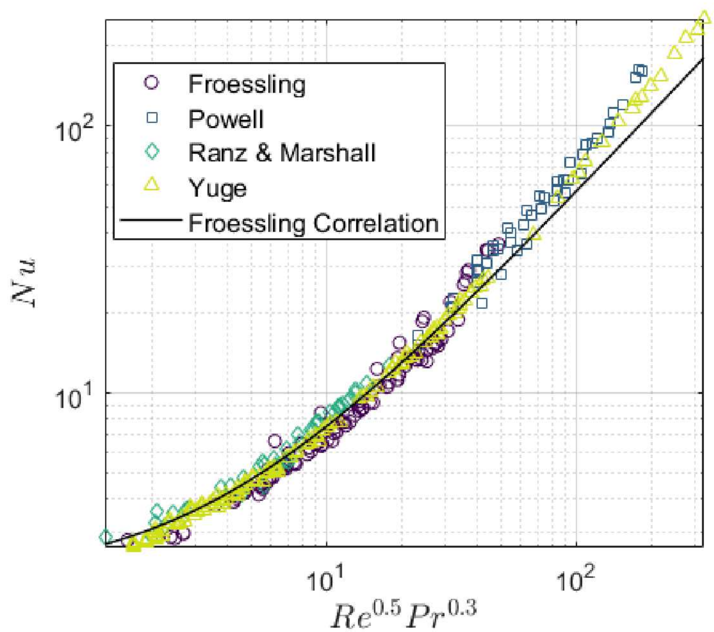


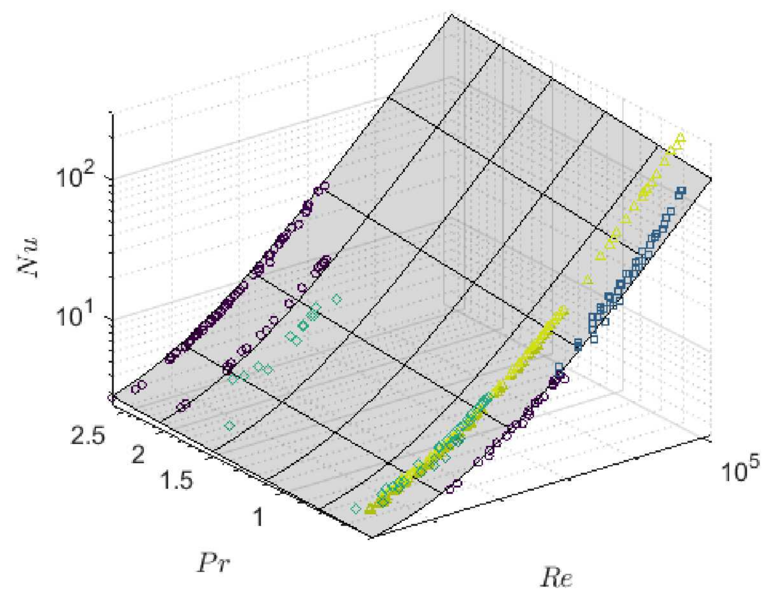
Mass Transfer Coefficient 1/3

- Mass or heat transfer from a solid sphere to the surrounding medium.
- Used to approximate interfacial transfer for bubbles/droplets.

$$Nu = 2.0 + \theta_1 Re^{\theta_2} Pr^{\theta_3}$$

- Originally proposed by Froessling (1938), but θ_1 has been adjusted by various authors; most recently, Ranz & Marshall (1952) and Lee & Ryley (1968).





Mass Transfer Coefficient 2/3

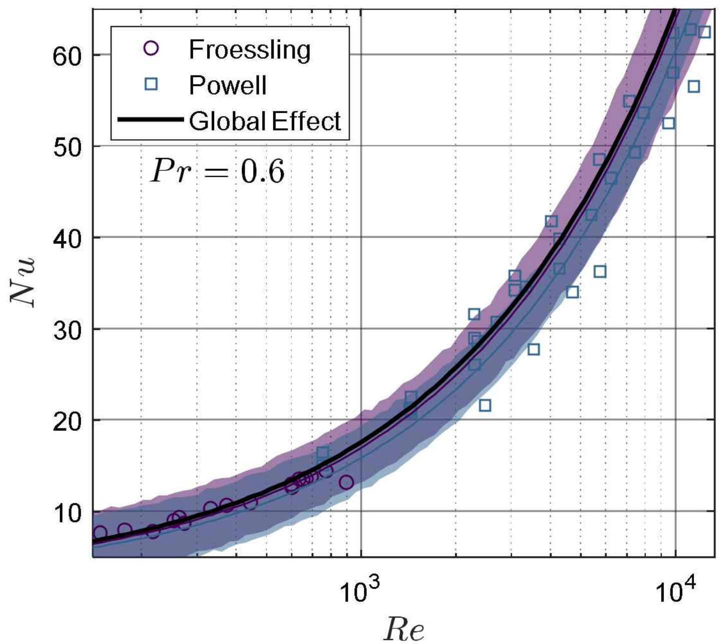
- The statistical model is formulated such that q_1 and q_2 have random effects.

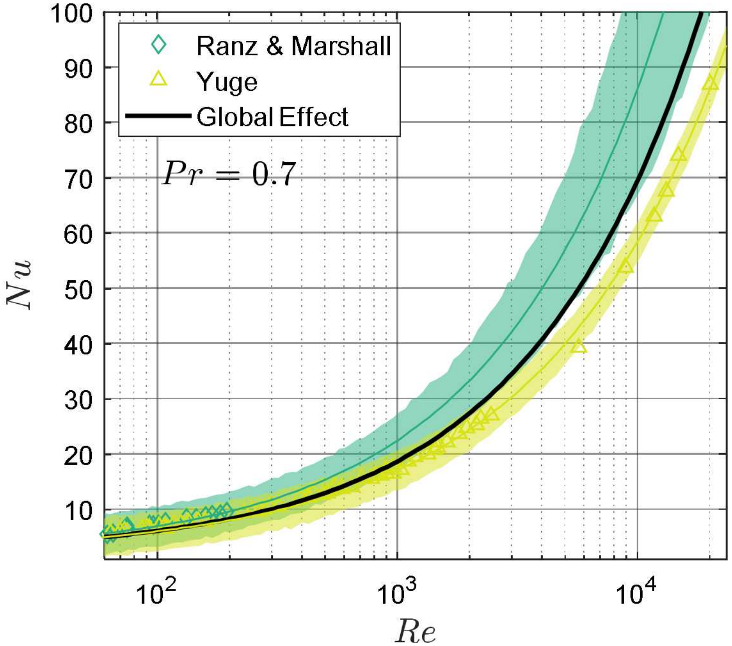
$$Nu = 2 + (\theta_1 + \beta_{1l})Re^{(\theta_2+\beta_{2l})}Pr^{\theta_3}$$

		Frequentist Optimization				**Bayesian Calibration (mean results)**			
		Froessling	Powell	Ranz	Yuge	Froessling	Powell	Ranz	Yuge
θ_1	0.55	0.2920				0.2957			
β_{1l}		-0.0275	-0.0625	0.0442	0.0458	-0.0310	-0.0653	0.0510	0.0439
θ_2	0.5	0.6080				0.6066			
β_{2l}		0.00853	0.0176	0.00930	-0.0355	0.0101	0.0189	0.00659	-0.0344
θ_3	0.33	0.4414				0.4436			
σ^2		4.621				4.672			
Σ		$\begin{bmatrix} 2.705e-3 & 0 \\ 0 & 6.002e-4 \end{bmatrix}$				$\begin{bmatrix} 5.972e-3 & 0 \\ 0 & 1.246e-3 \end{bmatrix}$			

Mass Transfer Coefficient 3/3

- Bayesian chains are propagated through the original model.
- Observational error should be laboratory-dependent, ε_l.
  - For Froessling and Ranz, all data is captured in the interval (error overestimated)
  - For Powell, half the data is captured (error underestimated)





Conclusion

- Some simple empirical relations have been examined using the legacy data from which they were derived (in some cases, this data is supplemented with other sources).
- Many possible sources of experimental bias, some hypotheses are supported by mixed effects results.
  - Transition to turbulence can be impacted by entry geometry, development, pump vibrations, and even working fluid.
  - Variety of working fluids in heat transfer experiments.
  - Choice of diffusion coefficients in the mass transfer experiments, which were very uncertain at the time.
- Biases between experiments have been quantified, which allows an accurate quantification of experimental uncertainty.
- Through reexamination and repeated experiments, it may be possible to reduce these uncertainties.

Future Work

- There are some possible improvements to the calibration method.
  - Random effects drawn from a non-normal distribution (e.g., Johnson distribution)
  - Dependent hyperparameters (Σ is currently diagonal).[1]
  - Nonlinear or laboratory-dependent observational error, ε.
  - Incorporation of more sophisticated parameter-selection algorithm.[1]
  - Use of empirical convergence criterion. [2]
- Incorporation of more recent data, which often includes more physics (pipe roughness, natural circulation, geometry, etc.).
- Application to other nuclear correlations used in nuclear codes, with specific focus on severe accident analysis.
- Use of results to quantify and exclude "poor" data.

1. K. L. Schmidt, Uncertainty Quantification for Mixed-Effects Models with Applications in Nuclear Engineering, PhD thesis, North Carolina State University (2016).
2. S. Brooks and A. Gelman, "General Methods for Monitoring Convergence of Iterative Simulations," *J Comput Graph Stat*, **7** (1998).
3. J. C. Wakefield, et al., "Bayesian Analysis of Linear and Nonlinear Populations Models Using the Gibbs Sampler," *J Royal Stat Soc*, **43**(1) (1994).

- Thanks to the following individuals for their assistance with mixed-effects Bayesian Calibration:

  North Carolina State University Paul R. Miles, Kathleen L. Schmidt, Ralph Smith

AIC and BIC

- Penalized-likelihood criteria that are often used to choose best predictor during regression analysis. Model with minimized value represents the best fit.
- Measure of fit + penalty for complexity
- Akaike information criterion (AIC)

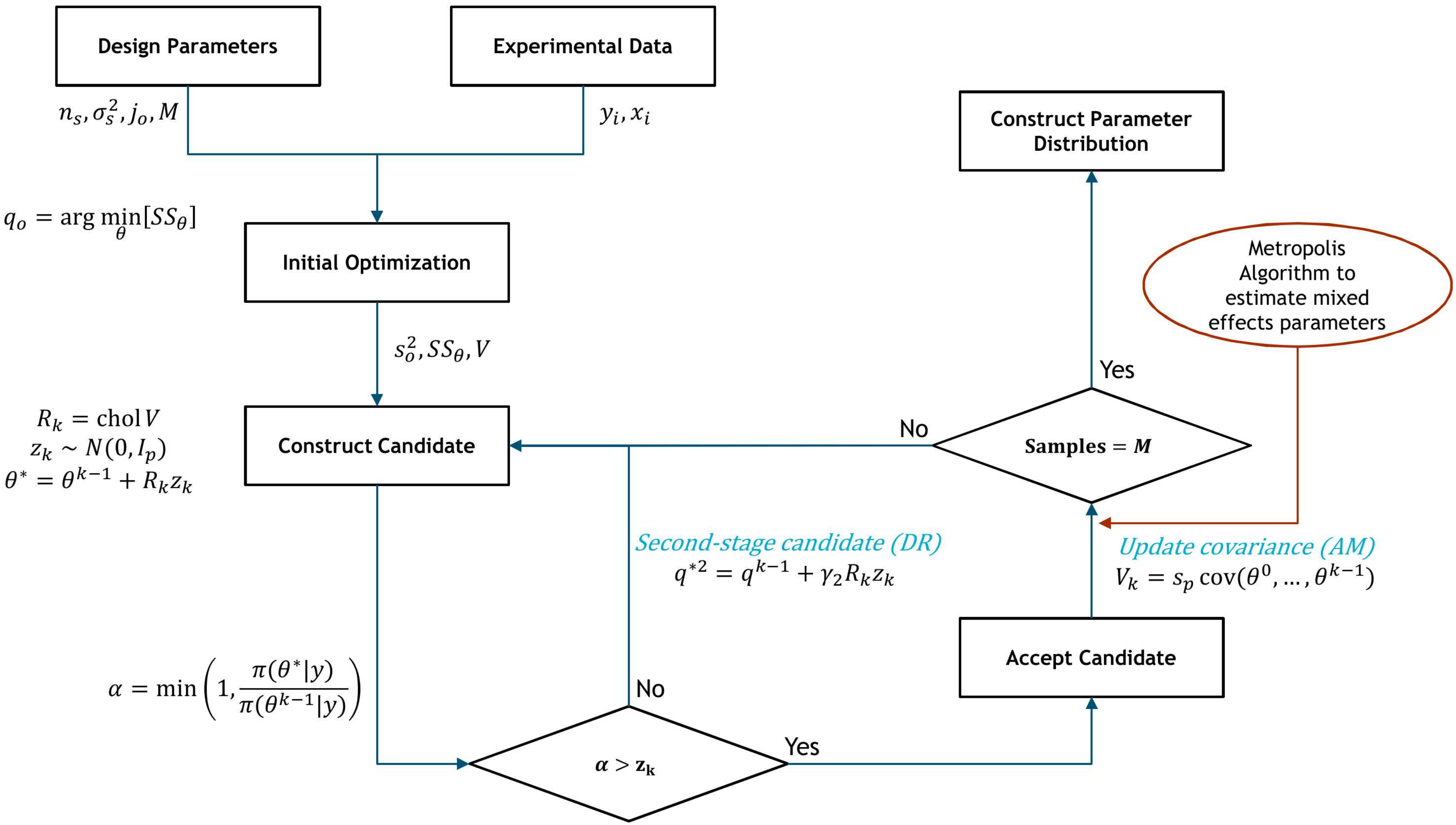
$$AIC = -2 \ln \mathcal{L} + 2p$$

- Bayesian information criterion (BIC)

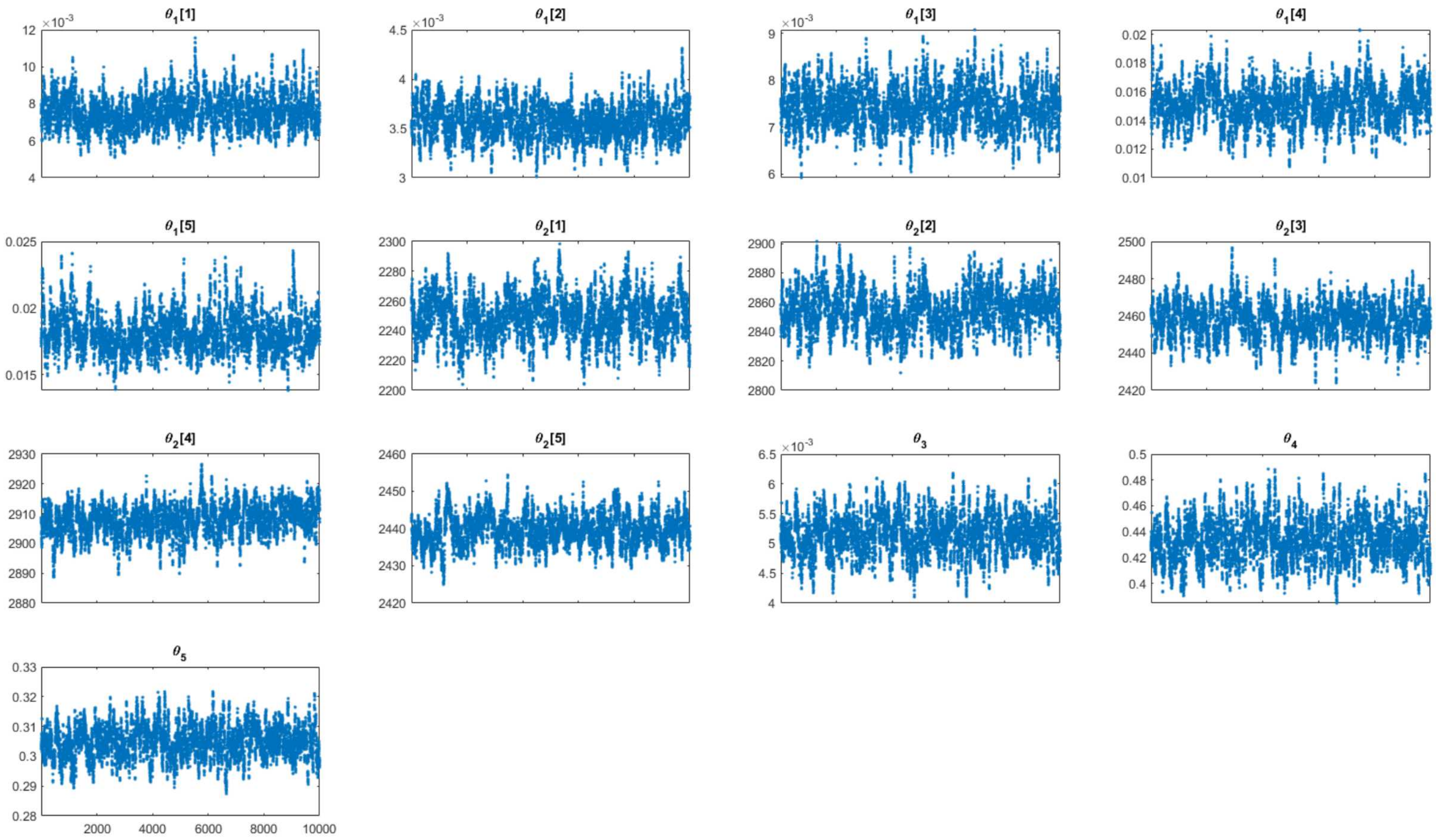
$$BIC = -2 \ln \mathcal{L} + p \ln N$$

$\mathcal{L}$: Likelihood
p: number of parameters
N: number of data points

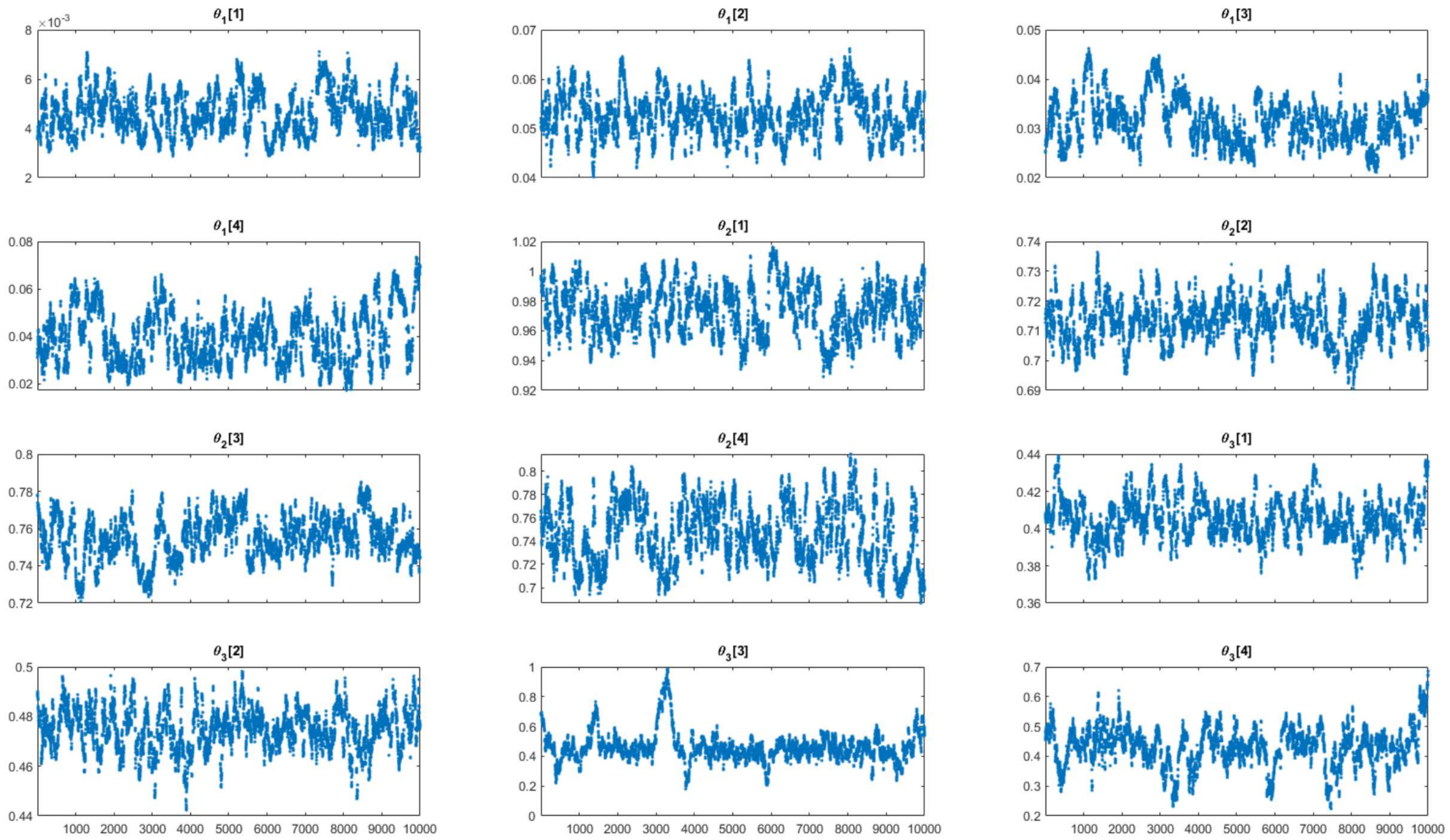
Metropolis-within-DRAM Algorithm



Friction Factor Chains



Heat Transfer Coefficient Chains



Mass Transfer