SAND2018-9077PE

Bayesian Calibration, Validation, and Rollup on Thermal Battery

1544 Department Meeting

Intern Presentations

08/08/2018

PRESENTED BY

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Manager: Angel Urbina, 01544

Advisor: Sankaran Mahadevan

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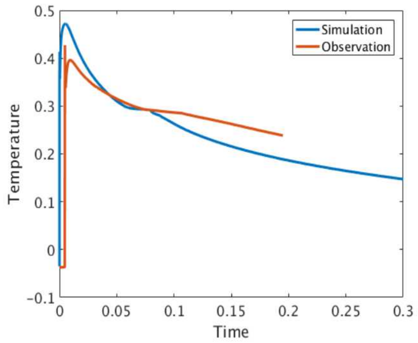
Outline

- Introduce thermal battery
- Calibration
  - Feature extraction
- Validation
  - Time dependent
- Roll-up
- Prediction of QOIs

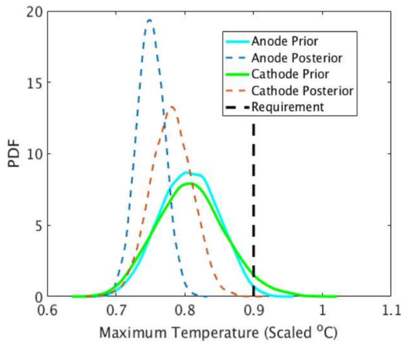
Intricacies:
Calibration with field data
Multi-level system

Objective:
Use experimental data to inform predictions

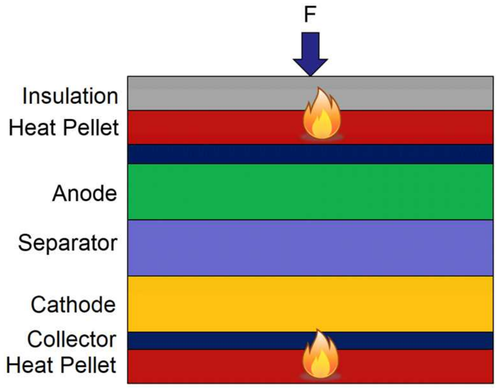
Experiment and Simulation

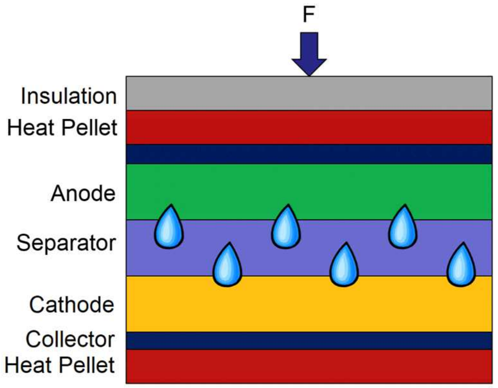


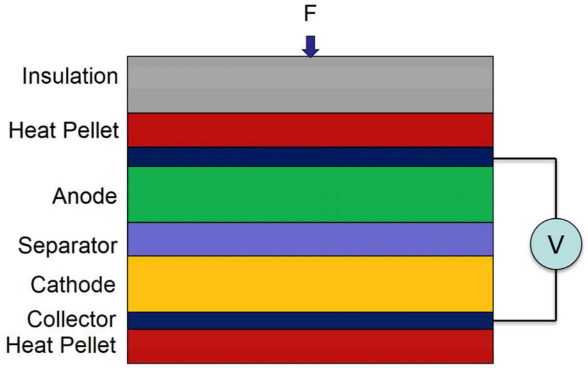
Predicted QOIs



1. Heat pellets produce heat
2. Heat travels via conduction to separator
3. Separator melts and deforms
4. Current begins to flow







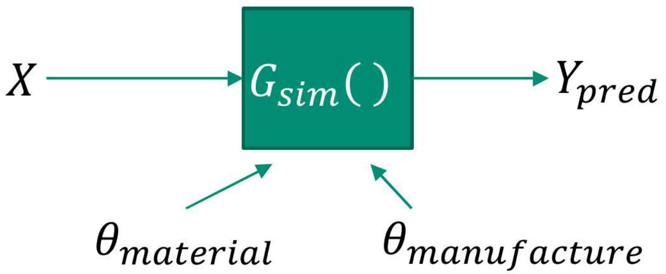
SAND2017-3397

Roberts, Harris, Piekos, Trembacki, Hetzler, Schroeder

Thermal Battery - UQ

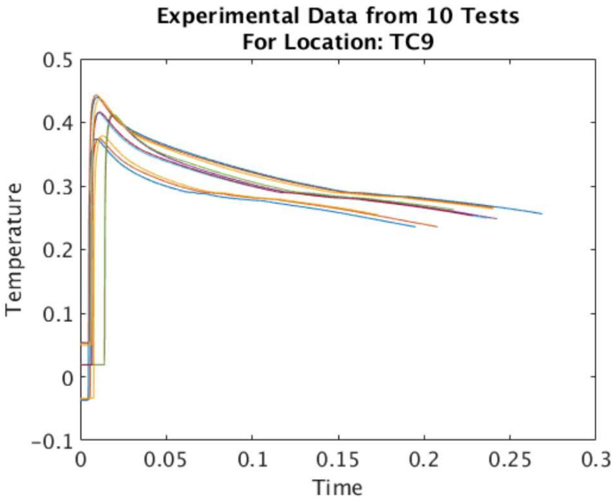
Uncertainty sources

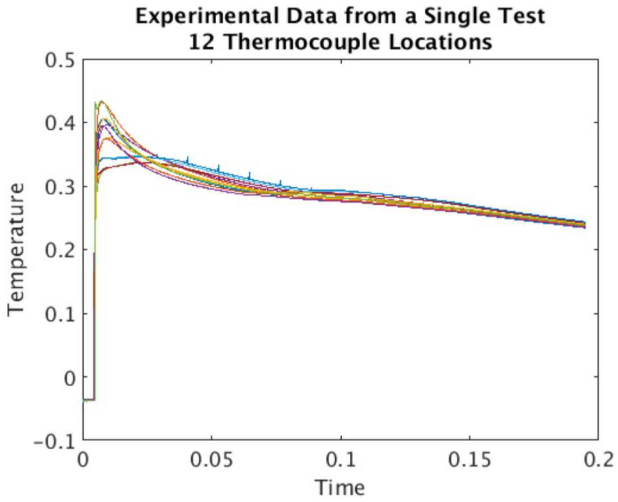
- Aleatory – irreducible, naturally varying
  - δ_{meas} – measurement noise
  - $\theta_{manufacture}$ – manufacturing parameters
- Epistemic – reducible, lack of knowledge
  - X – input conditions, controllable nominal value with epistemic uncertainty
  - $\theta_{material}$ – model parameter (calibration)
  - δ_{model} – model bias

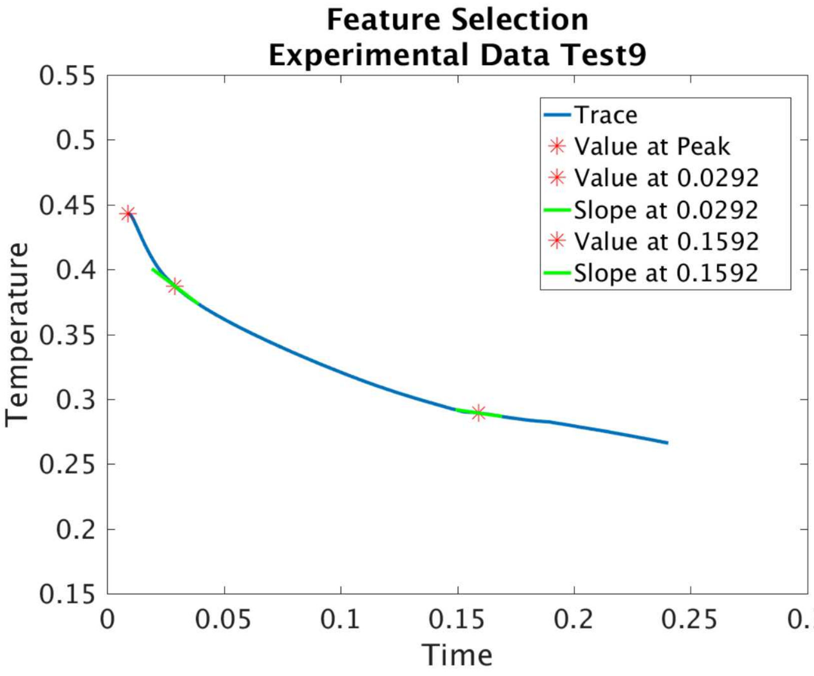


$$Y_{pred} = Y + \delta_{model}$$

$$Y_{obs} = Y + \delta_{meas}$$

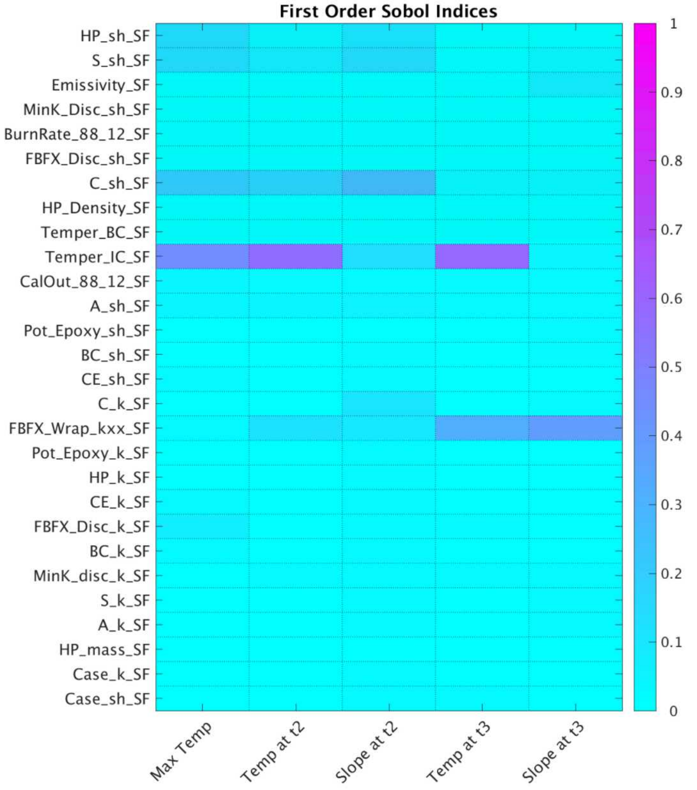




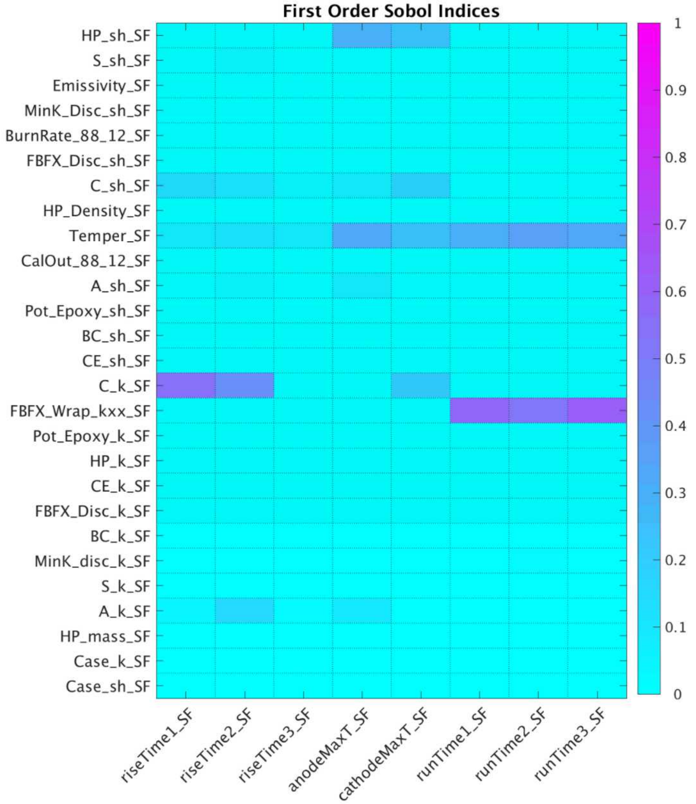


Sensitivity Analysis

Features



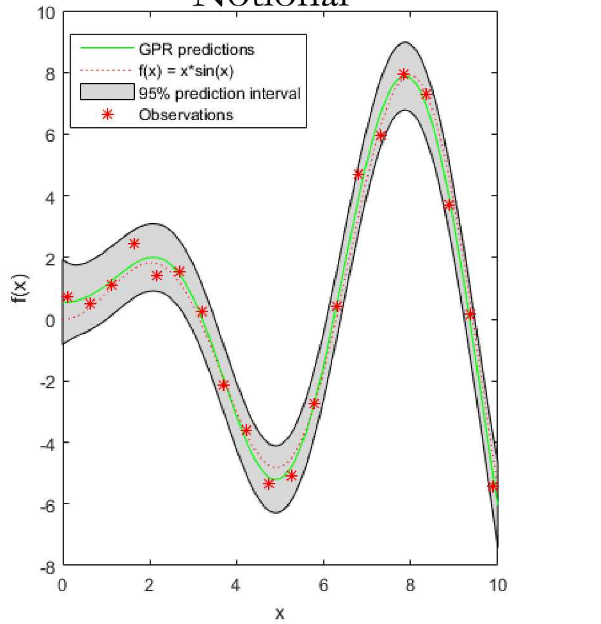
QOIs



Gaussian Process surrogate models

- Built for features and QOIs
- 5,000 training sites from LHS

Notional



MATLAB Gaussian Process Regression Models

Sensitive Parameters							Inputs	
HP_sh_SF	S_sh_SF	Emissivity_SF	C_sh_SF	C_k_SF	FBFX_Wrap_kxx_SF	A_k_SF	Temper_BC_SF	Temper_IC_SF

Calibration: Bayesian Implementation

Bayes' Theorem to find Posterior

- Find values of theta that are most probable given the data

$$P(\boldsymbol{\theta}|D) = \frac{P(D|\boldsymbol{\theta}) * P(\boldsymbol{\theta})}{P(D)}$$

$$P(\boldsymbol{\theta}|D) \propto P(D|\boldsymbol{\theta}) * P(\boldsymbol{\theta})$$

$$\propto P(D|\boldsymbol{\theta}) = L(\boldsymbol{\theta})$$

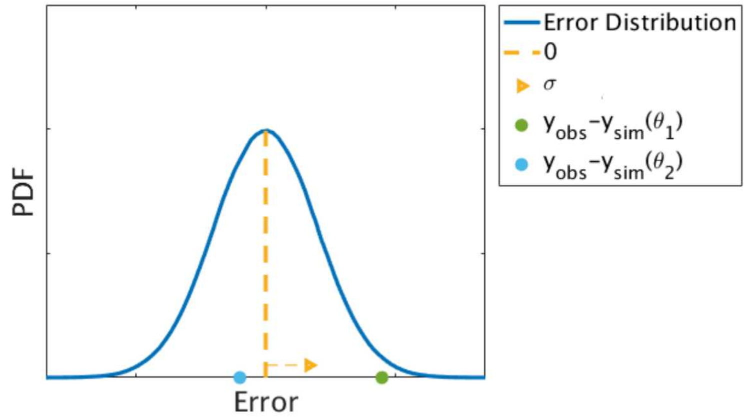
Assumptions

- Independence of 5 features
- Model bias is 0 mean with known variance

Solving for posterior

- Markov chain Monte Carlo (MCMC)
  - Samples from chain approach posterior distribution
- Particle filter (PF)
  - Particles weighted based on likelihood scores
  - Easily parallelizable
- Sample-based Bayesian methods require many model evaluations
  - Replace computationally expensive physics model with efficient surrogate model

Notional 1-D Likelihood



$$L(\boldsymbol{\theta}) = \prod_{i=1}^{N} \frac{1}{\sqrt{(2\pi)^k|\Sigma|}} exp\left(-\frac{1}{2}\left(\left(\boldsymbol{y}_{obs,i} - \boldsymbol{y}_{sim}(\boldsymbol{\theta})\right) - \boldsymbol{0}\right)^T \Sigma_y^{-1} \left(\left(\boldsymbol{y}_{obs,i} - \boldsymbol{y}_{sim}(\boldsymbol{\theta})\right) - \boldsymbol{0}\right)\right)$$

Current Implementation of PF				
7 calibration parameters	5 output variables	Samples: 10 million	Resampling algorithm 20 iterations	40 cores ~30hrs

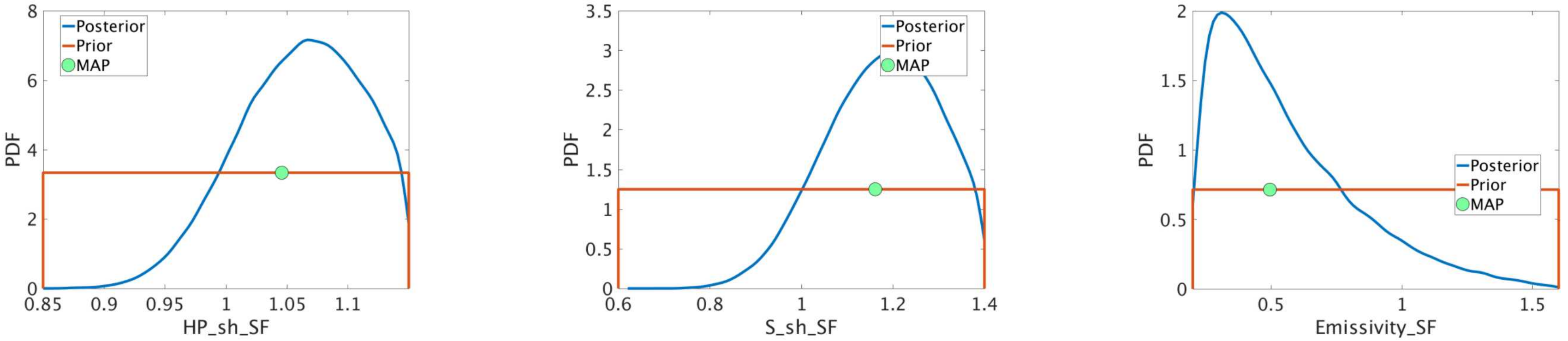
PF resampling algorithm

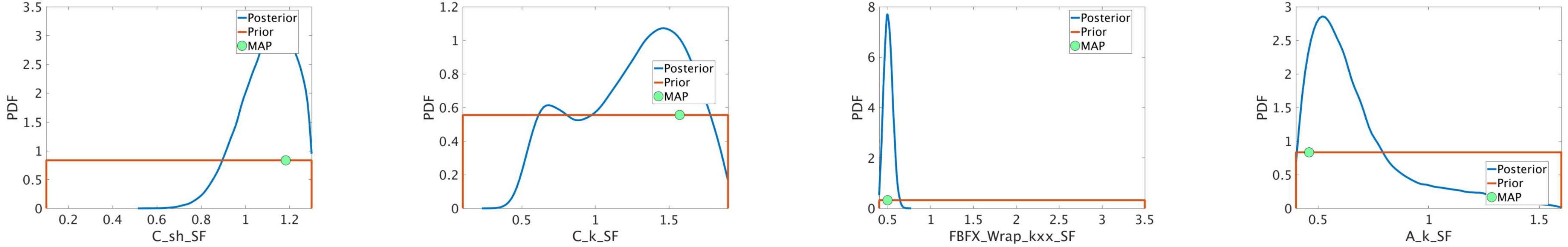
- Relationship to genetic algorithm
  - Selection – keep best performing parents
  - Crossover – keep combinations of best performing parents
  - Mutation – make random changes to some of the parents

Calibration: Posteriors

Particle filter shows convergence

- Negligible improvement in likelihood score from iteration 1 to 20

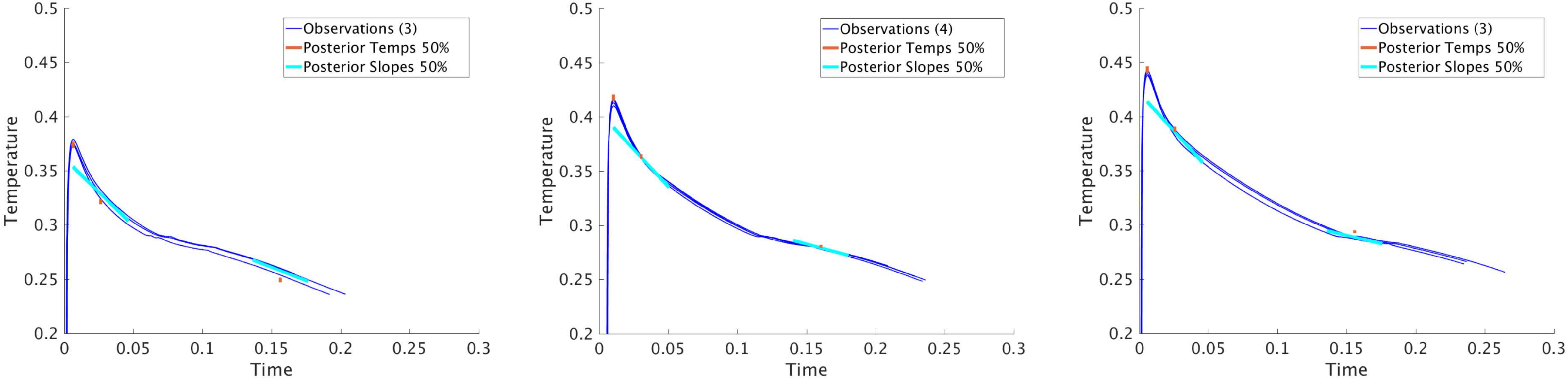




MAP Values							
Error Terms	HP_sh_SF	S_sh_SF	Emissivity_SF	C_sh_SF	C_k_SF	FBFX_Wrap_kxx_SF	A_k_SF
Known	1.046	1.161	0.495	1.183	1.572	0.498	0.459
Prior Nominal	1	1	1	1	1	1	1

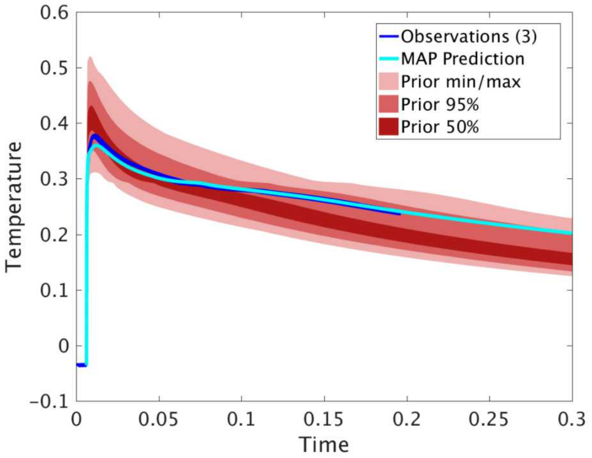
Calibration: Calibration Fit in Feature Space

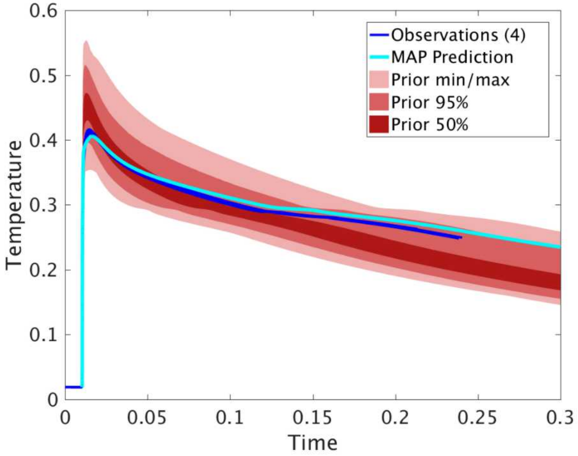
Calibrated features align well with the experiments used for calibration

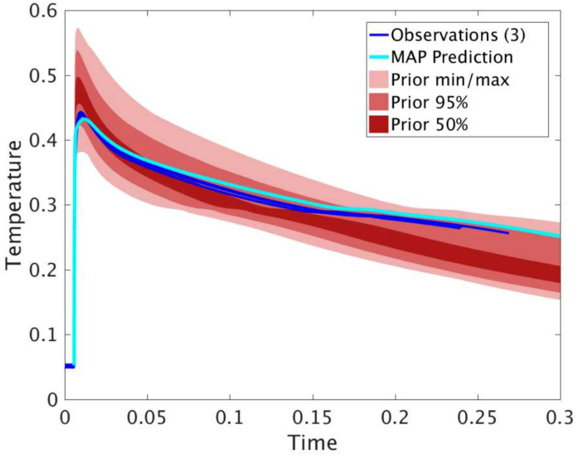


Calibration: Calibration Fit in Trace Space

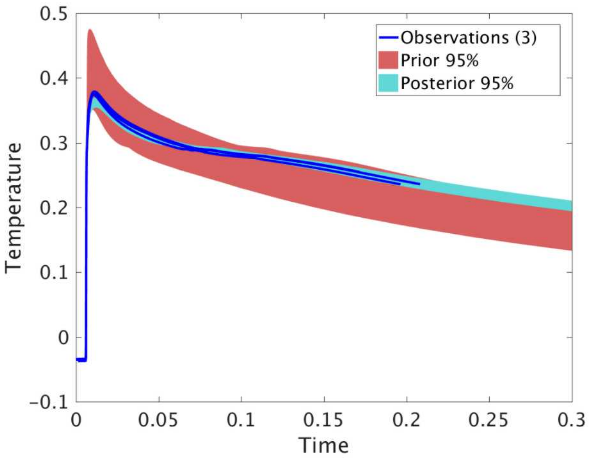
Accuracy

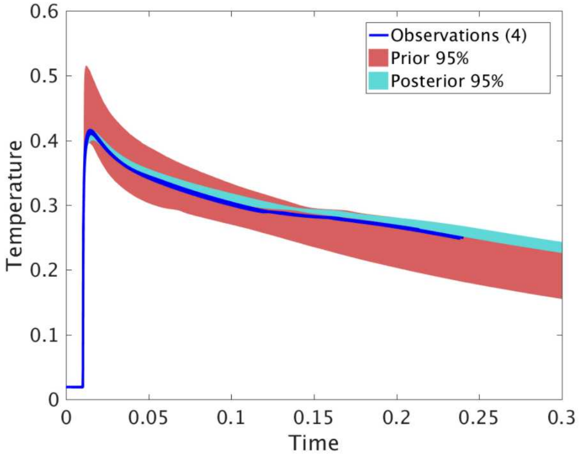


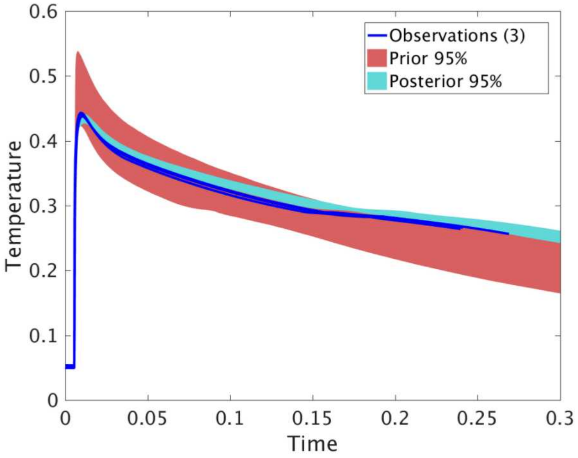




Precision







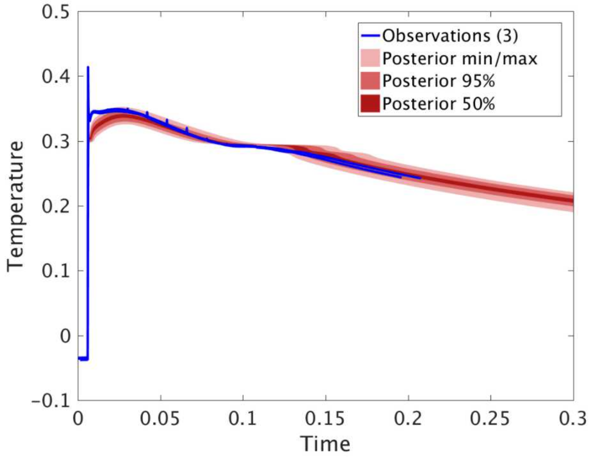
Validation: Metric

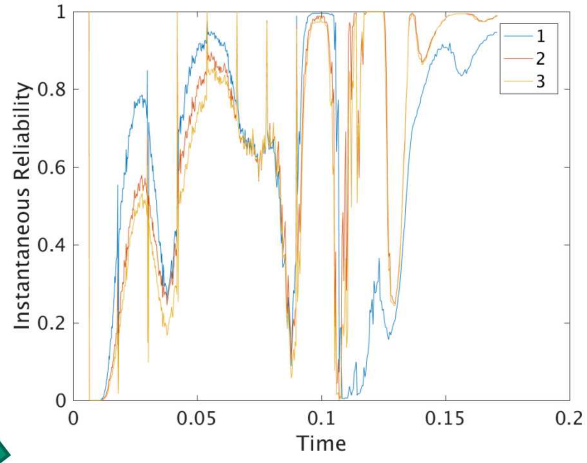
Validation metrics

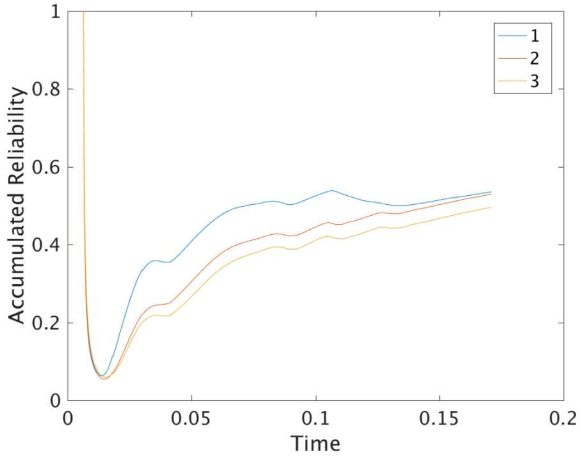
- Can be difficult to boil validation down to a single metric value
  - Especially for time-dependent outputs
- Accumulated model reliability metric [1,2]
  - $r(t) = \frac{1}{N_t} \sum_{q=1}^{N_t} \left[\frac{1}{M} \sum_{k=1}^{M} I_k(t_q) \right]$
  - $I_k(t_q) = \begin{cases} 1, if \ \left| Y_e(t_q) - Y_m^{(k)}(t_q) \right| \leq \varepsilon(t_q) \\ 0, otherwise \end{cases}$

Threshold, $\varepsilon(t_q)$

- $\pm 3 * Max(\epsilon_{measurement})$







<u>Validation Test Plotted</u>

IC: Low

Location: Cathode Center cell 5

[1] Ao, Hu, Mahadevan 2017
[2] Neal, Hu, Mahadevan, Zumberge 2018 (under review)

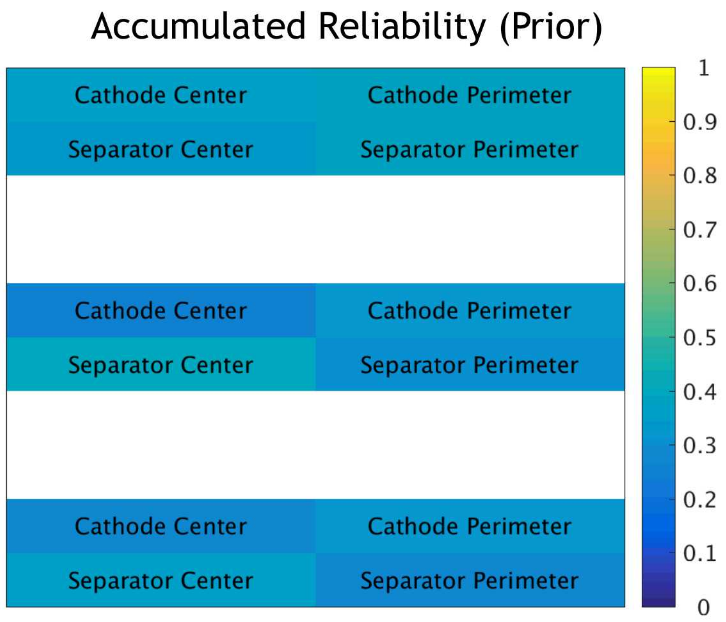
Validation: Results

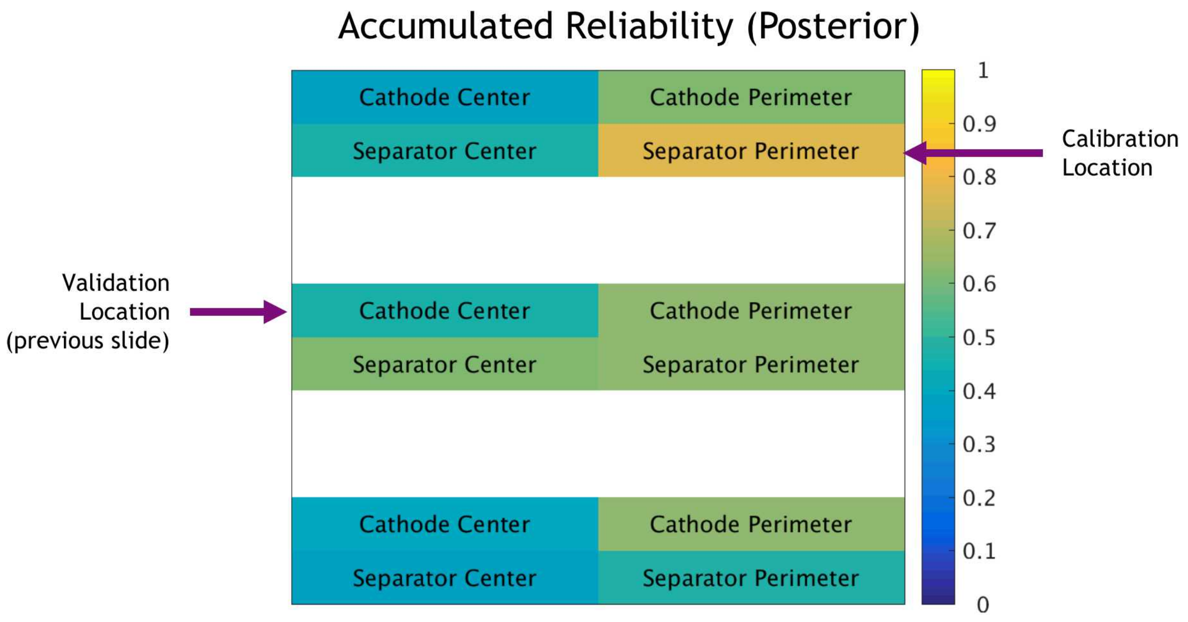
Posterior shows higher reliability than prior

Variability over initial temperatures

Variability over space

Accumulated Reliability			
Temperature	Low	Med	High
Prior	0.374	0.294	0.321
Posterior	0.763	0.431	0.422

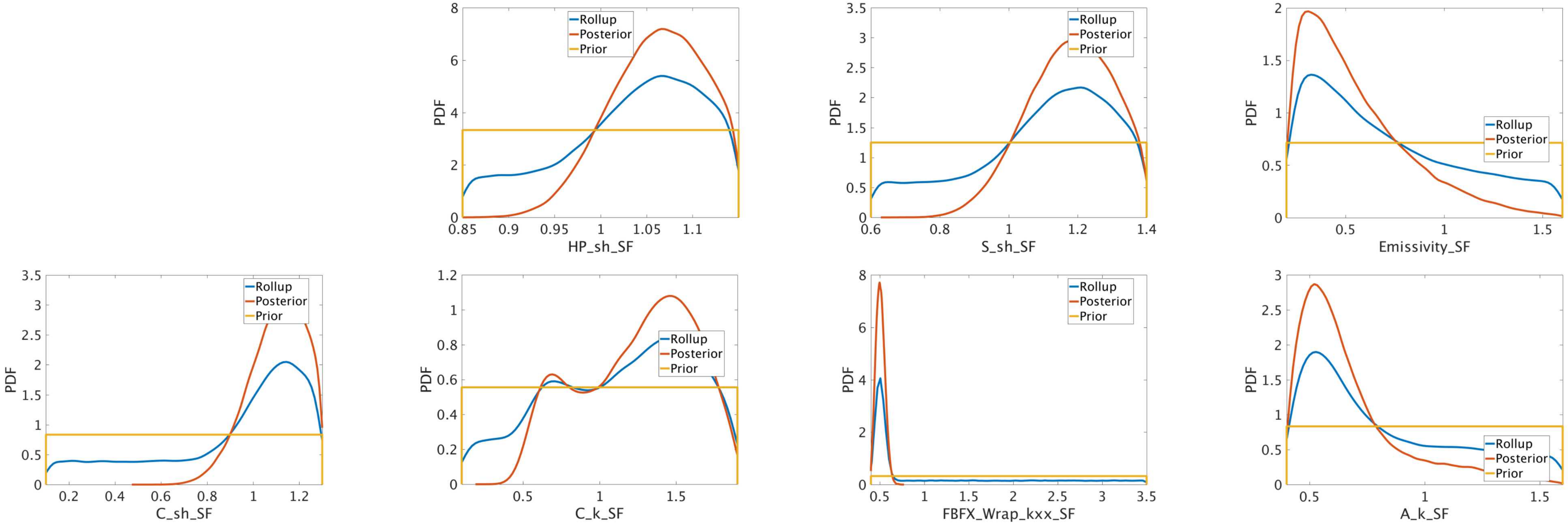




Rollup: Combining Calibration and Validation

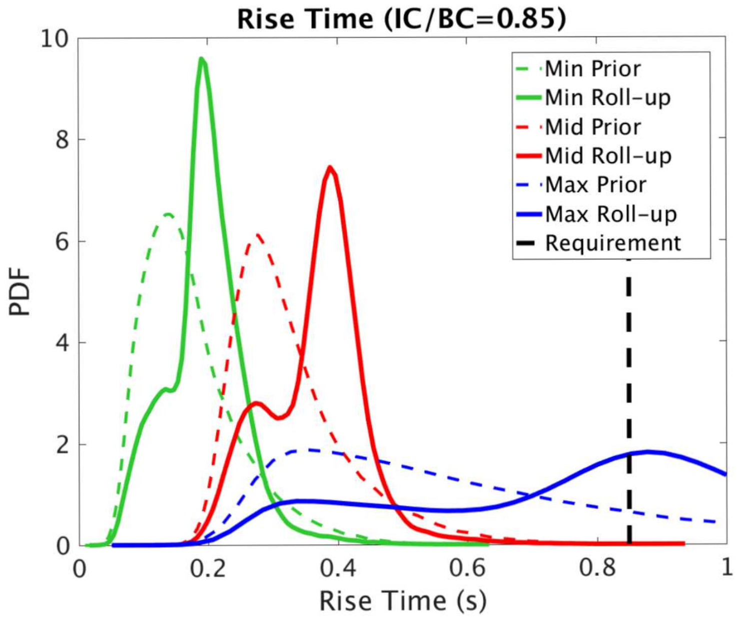
Weighted combination of posterior and prior; weights obtained from validation

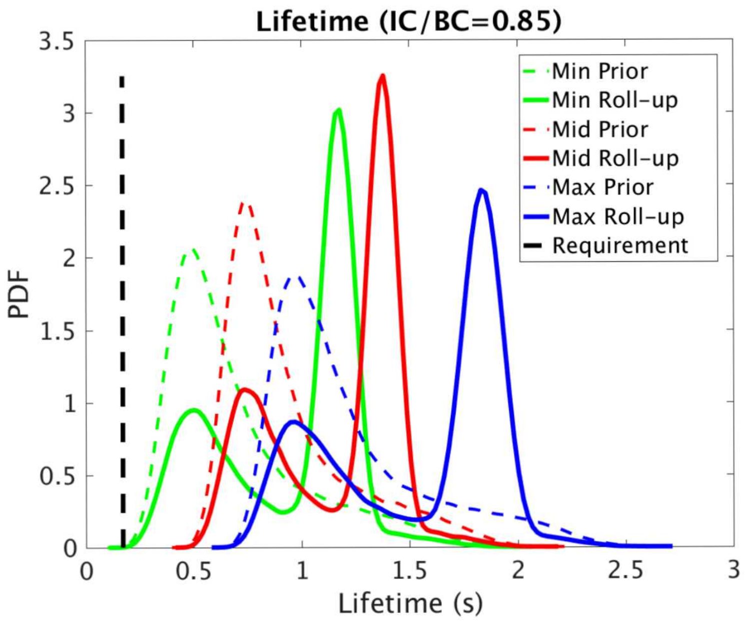
- $f(\boldsymbol{\theta}|D^C, D^V) = P(G)f(\boldsymbol{\theta}|D^C) + P(G')f(\boldsymbol{\theta})$
- D^C – calibration data, D^V – validation data, G – event that model is reliable

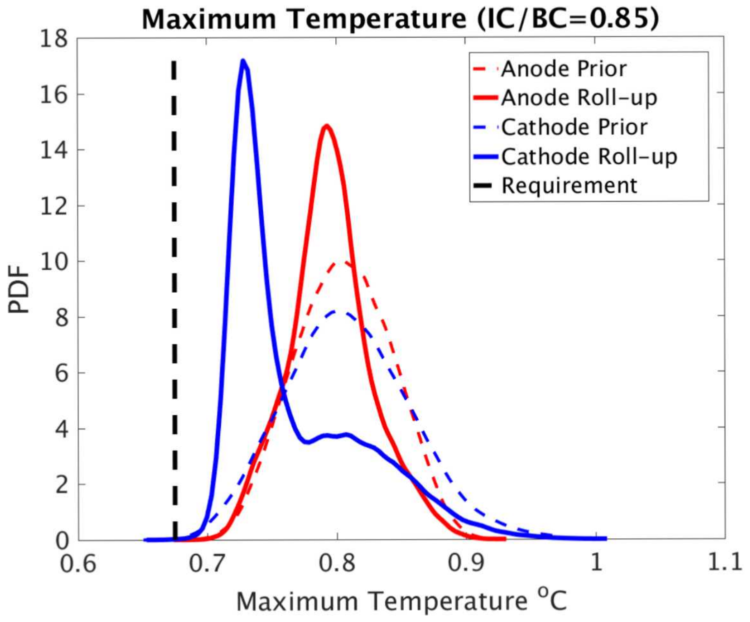


Prediction Battery: QOIs

Reduced uncertainty in propagating roll-up parameter distributions







Conclusions & Future Work

Conclusions
- Calibration using feature extraction was successful
- Selection of bias tolerance has large impact in rollup
- QOI predictions are bimodal due to weighting of prior & posterior

On going work
- Present at IMAC XXXVII
- Submit to MVUQ best paper competition

Future work
- Explore other methods of Bayesian calibration with field data
  - More information could possibly be extracted from experimental data
- Consider non-zero mean and correlated model bias in calibration

Thank you

Questions?

kneal@sandia.gov

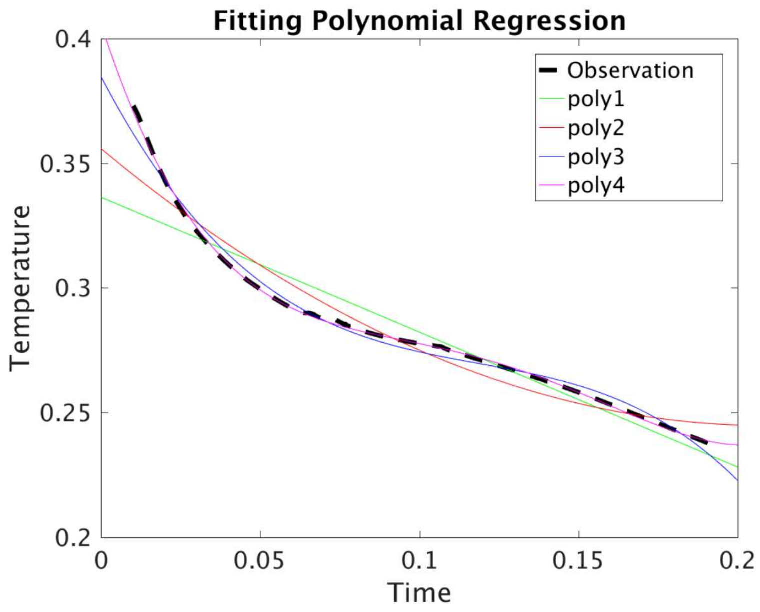
Backup Slides

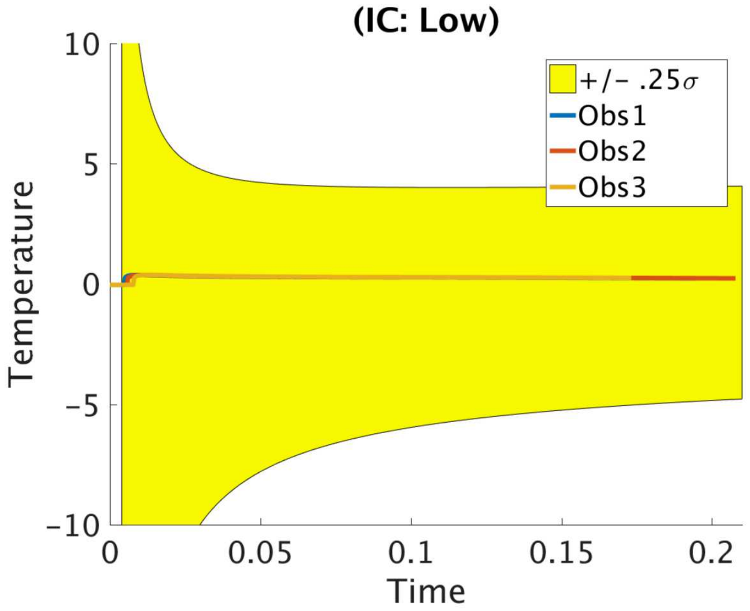
Last Year

Fit a mathematical function to the temperature trace

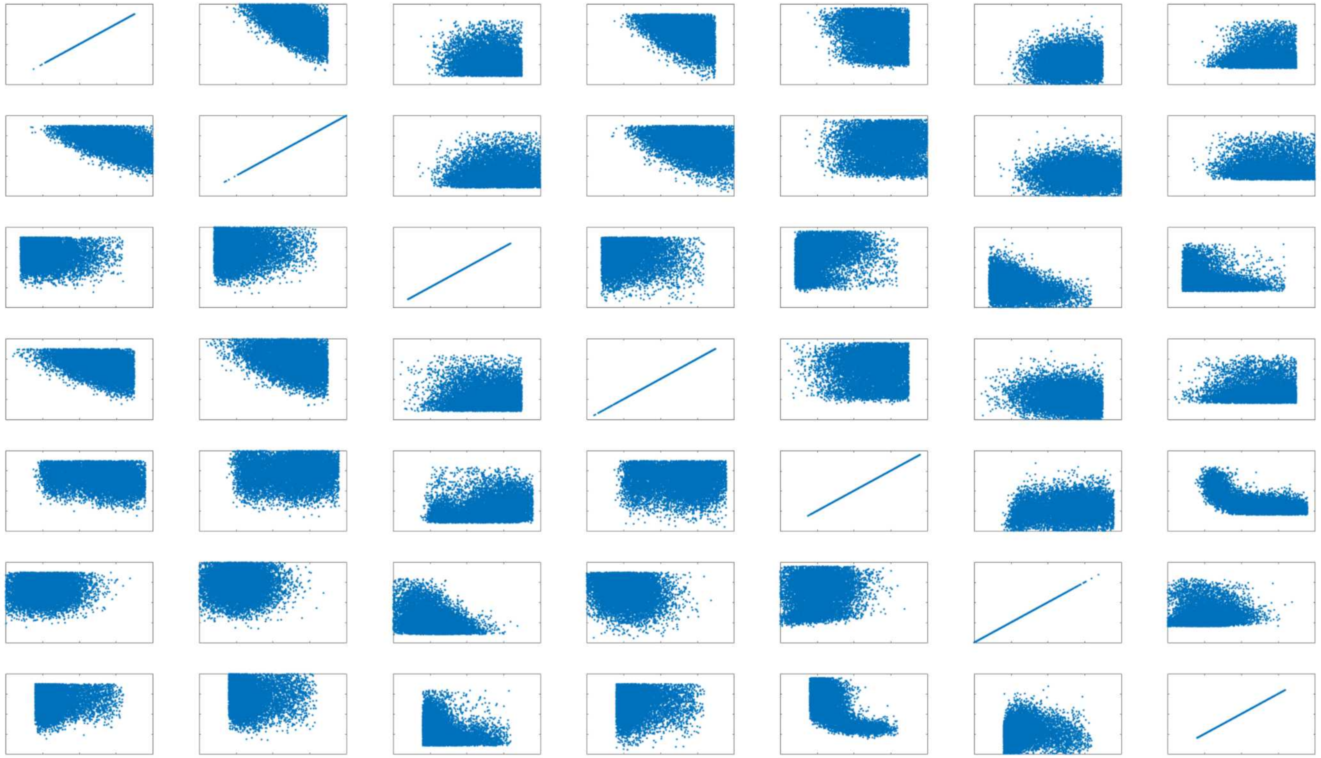
Performed calibration in coefficient space

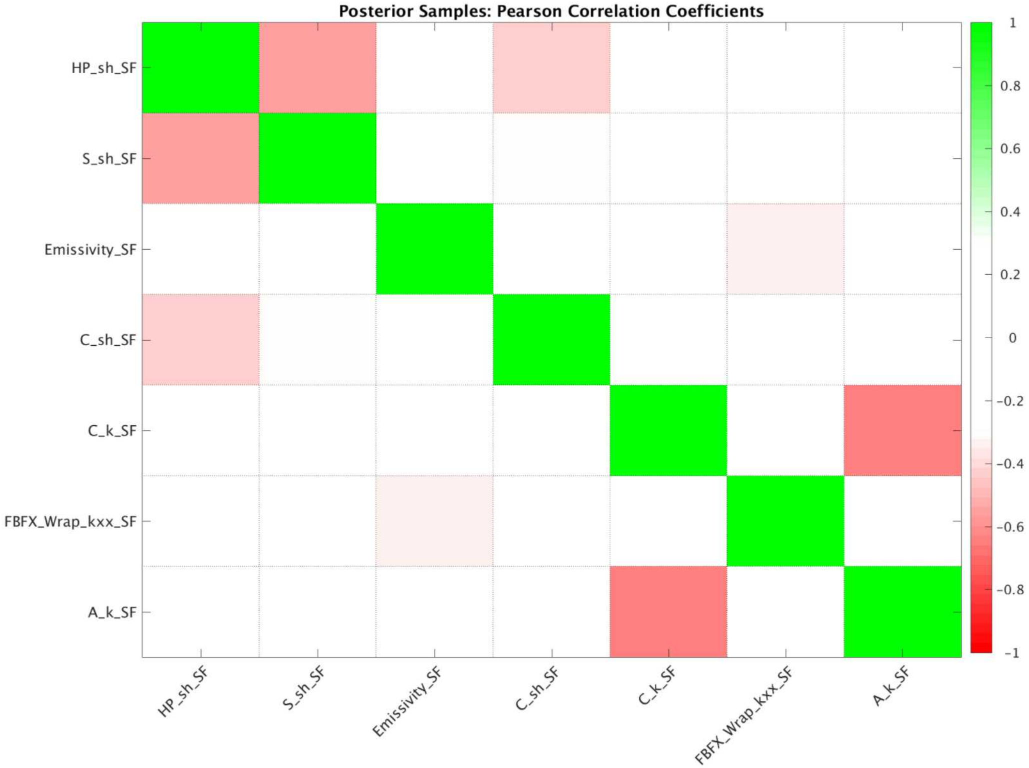
Large calibration fit uncertainty



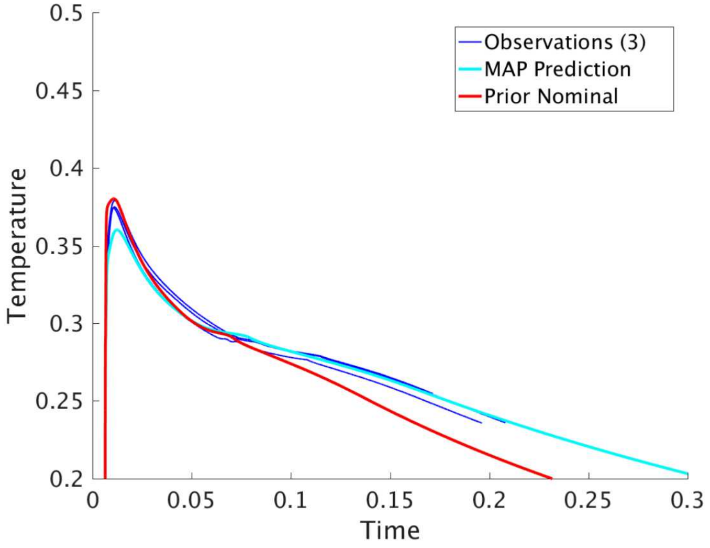


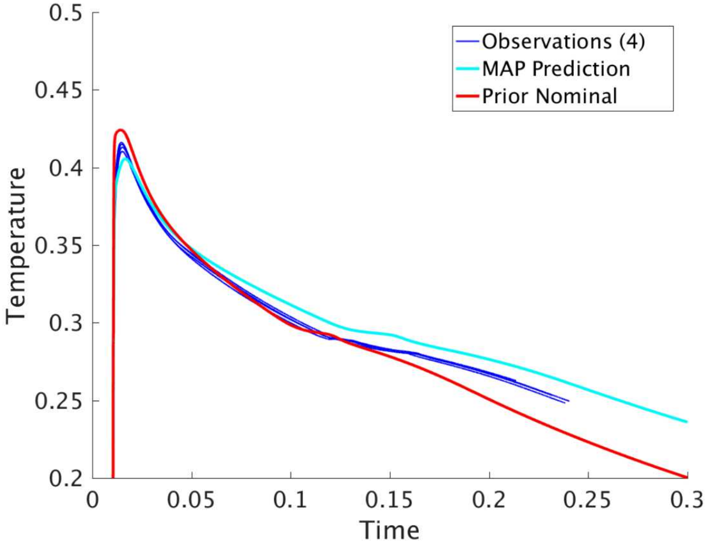
Calibration: Correlation of Posterior Samples

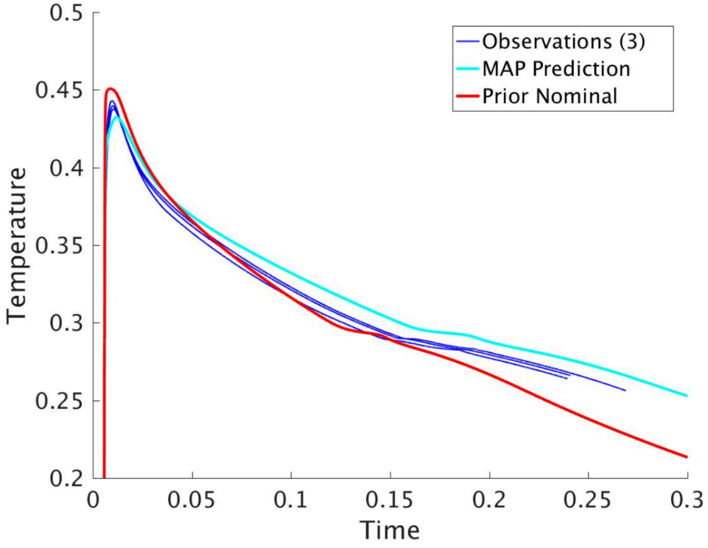




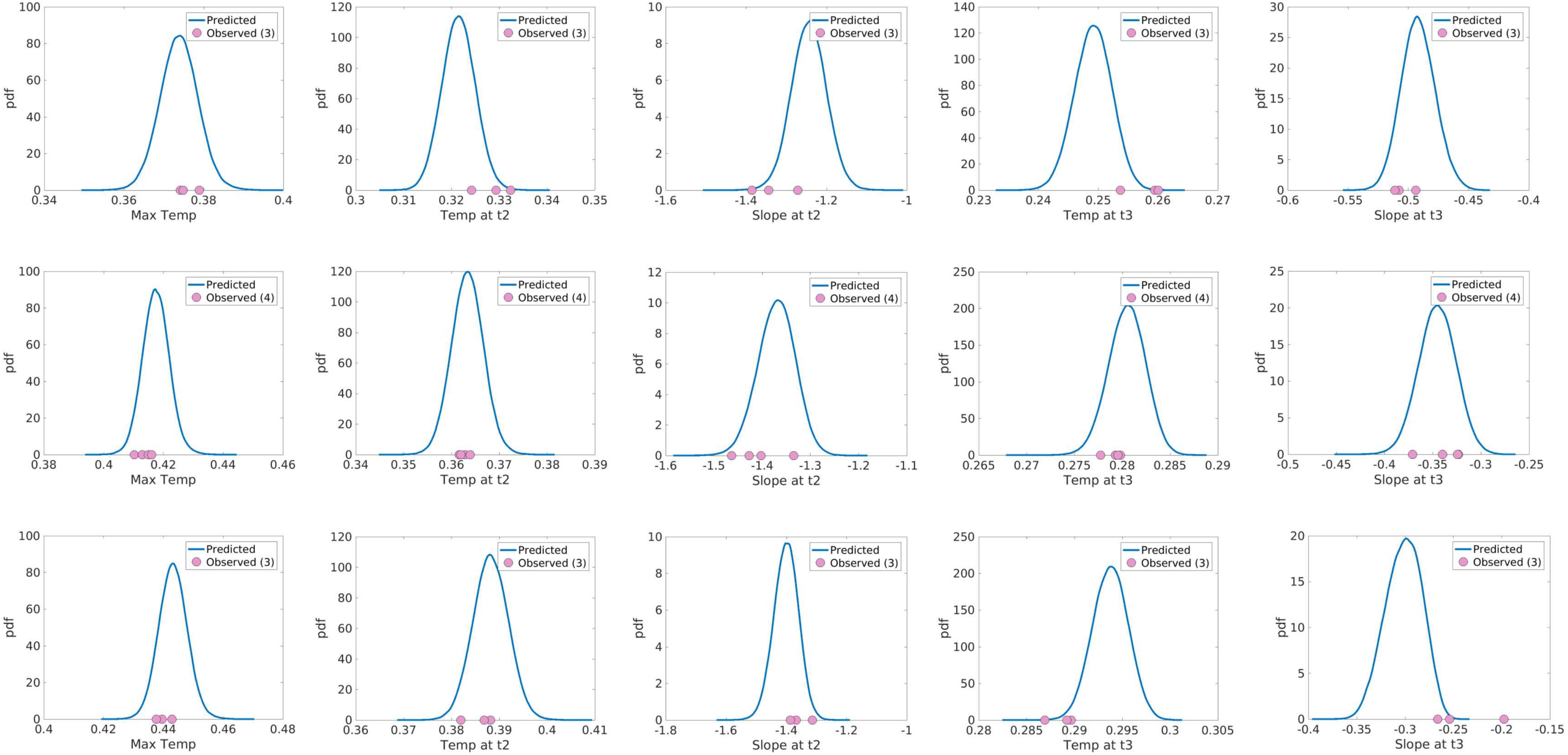
Calibration: Comparing Traces of MAP and Prior Nominal





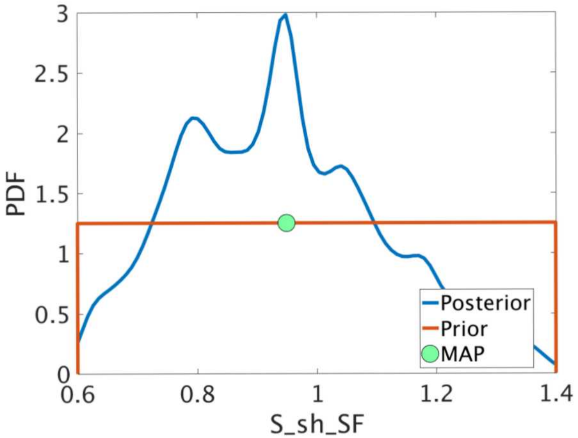


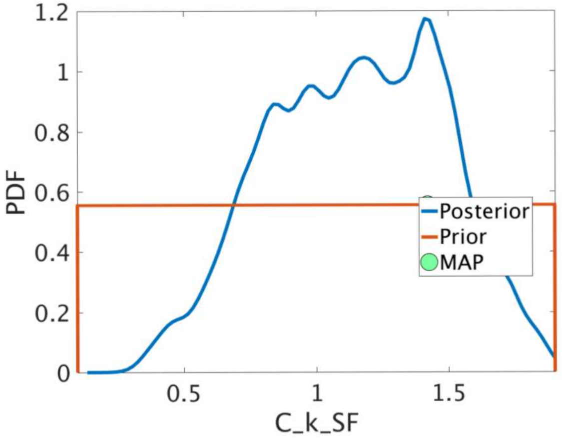
Calibration: Checking Feature Space

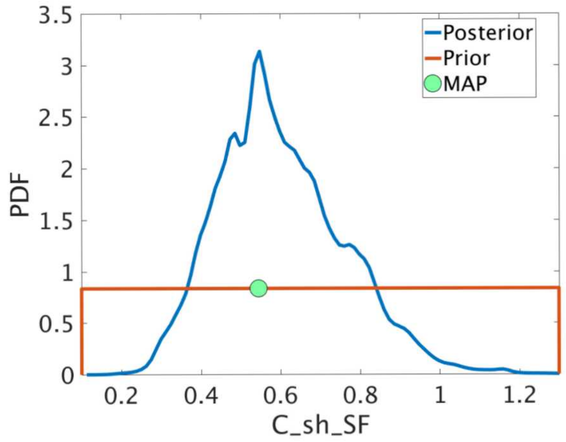


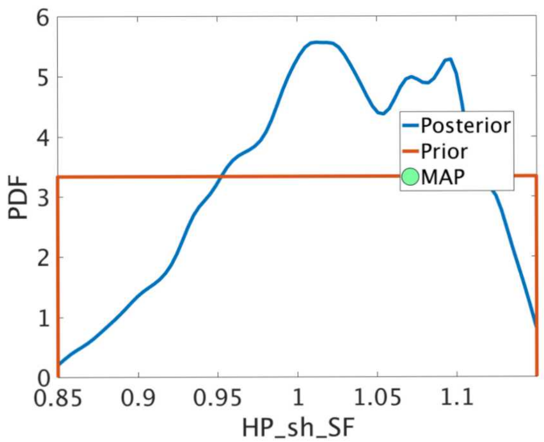
Calibration with Model Error Calibrated

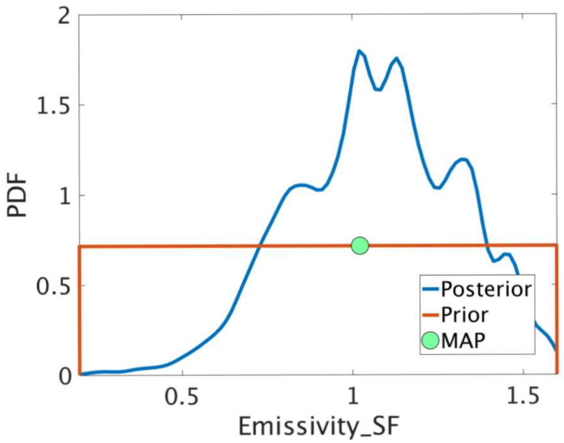
Calibration: Posterior Model Parameters

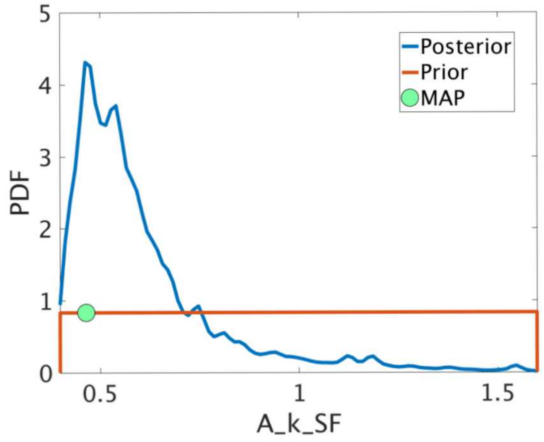


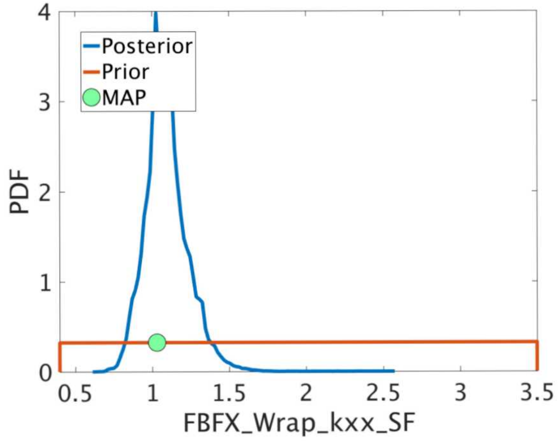




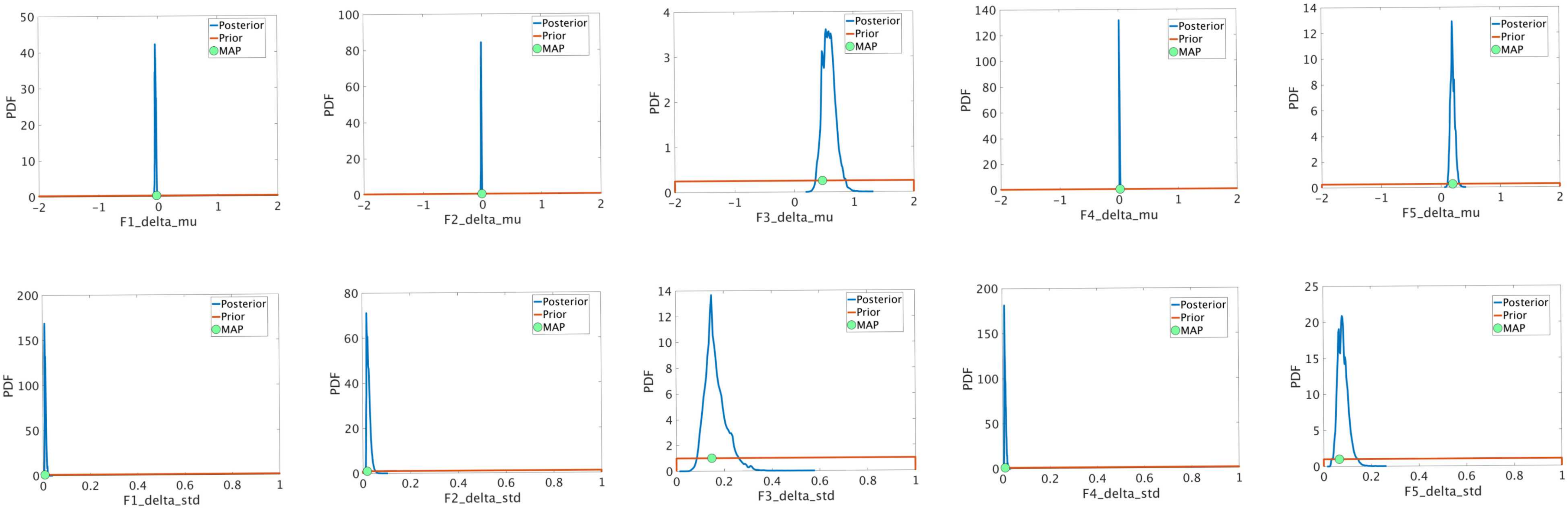








Calibration: Posterior Error Terms

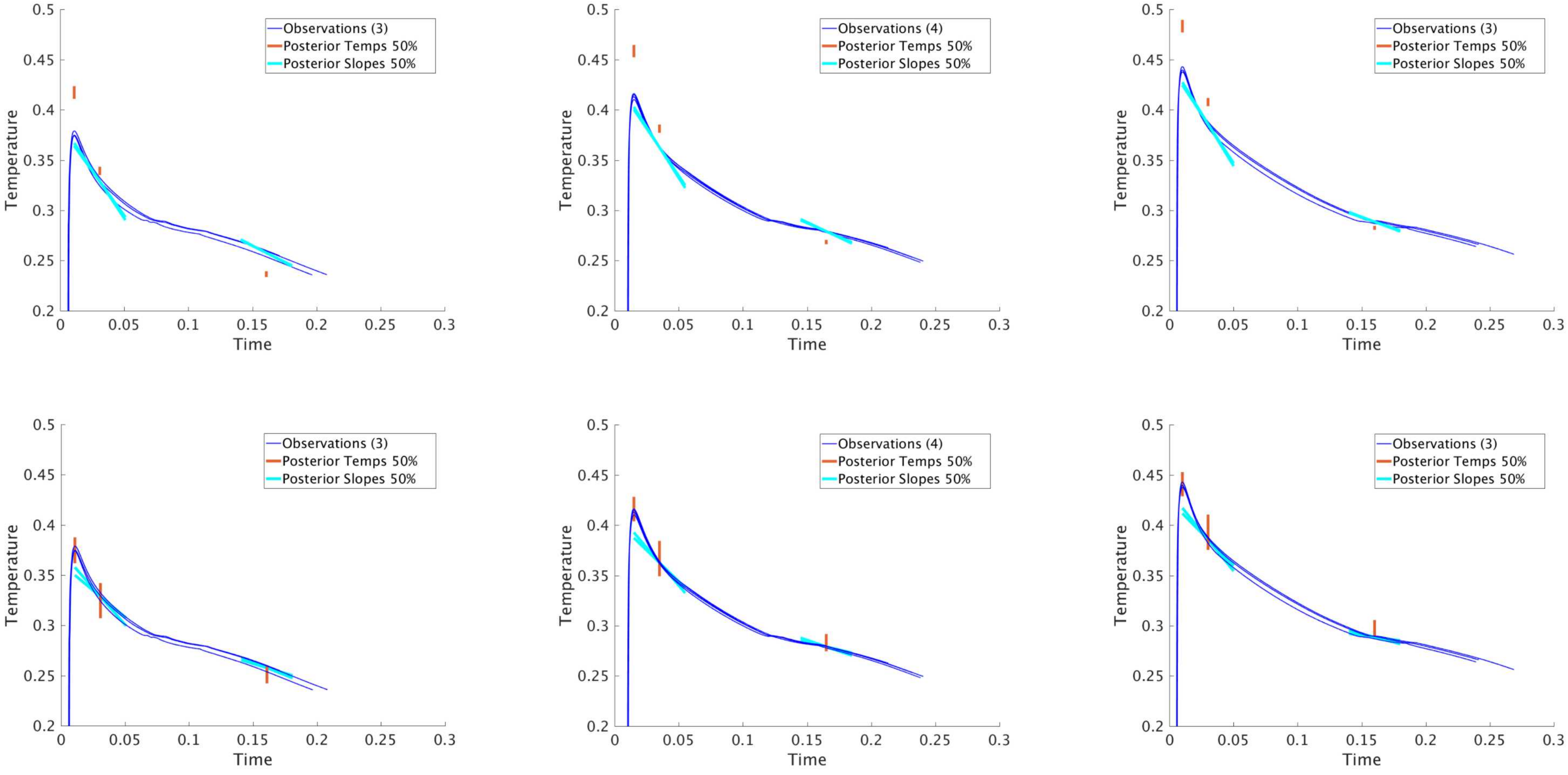


Calibration: Calibration Fit of Features

Without Error

With Error

Can’t propagate error to traces



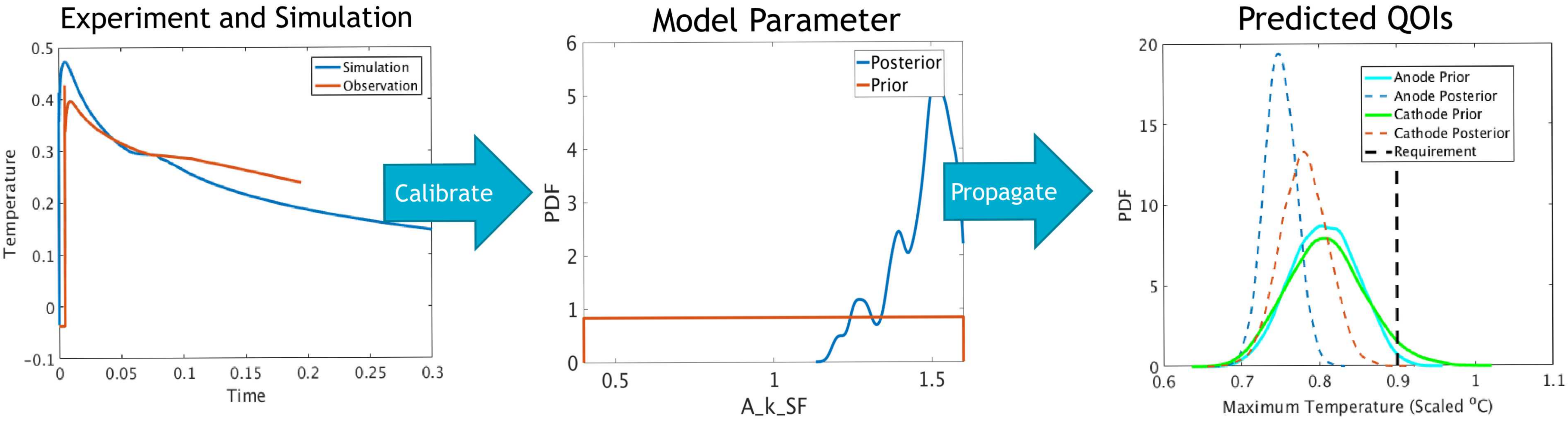
MCMC Workshop
Bayesian Calibration with Field Data

Outline

- Introduction to Bayesian calibration
- Field outputs
- Thermal battery current work

Objective: use experiment data to calibrate model parameters

→ thereby reducing uncertainty in predictions



Bayesian Calibration

Posterior Likelihood Prior

$$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B)}$$

Data

Bayes' Theorem

- Use observations to update beliefs

Posterior

- Find values of theta that are most probable given the data

$$P(\boldsymbol{\theta}|D) = \frac{P(D|\boldsymbol{\theta}) * P(\boldsymbol{\theta})}{P(D)}$$

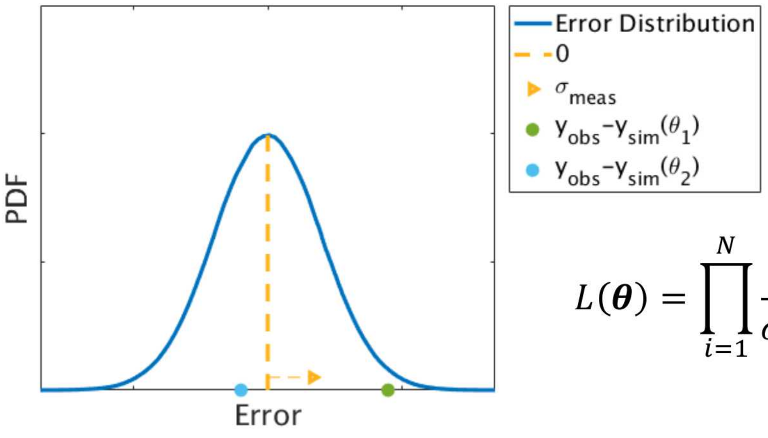
$$P(\boldsymbol{\theta}|D) \propto P(D|\boldsymbol{\theta}) * P(\boldsymbol{\theta})$$

$$\propto P(D|\boldsymbol{\theta}) = L(\boldsymbol{\theta})$$

Uncertainty sources

- Aleatory – irreducible, naturally varying
  - Measurement noise
- Epistemic – reducible, lack of knowledge
  - Model parameter uncertainty (calibration)
  - Model bias

Notional 1-D Likelihood



Likelihood (case 1):

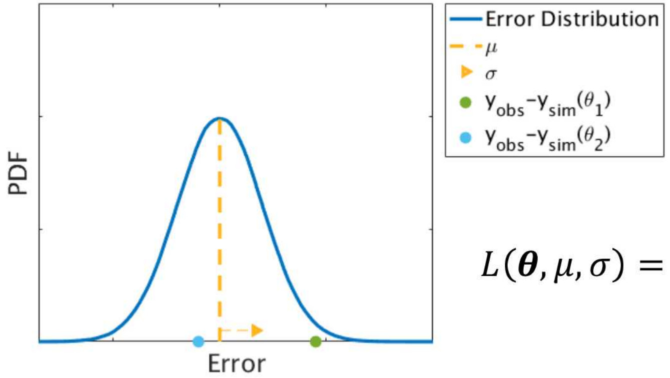
- $Y_{obs} = Y_{sim} + \epsilon_{meas}$
- Measurement noise: i.i.d. with $N(0, \sigma^2)$

$$L(\boldsymbol{\theta}) = \prod_{i=1}^{N} \frac{1}{\sigma\sqrt{2\pi}} exp\left(-\frac{1}{2\sigma^2}\left(\left(y_{obs,i} - y_{sim}(\boldsymbol{\theta})\right) - 0\right)^2\right)$$

Bayesian Calibration Cont'd

Likelihood (case 2):

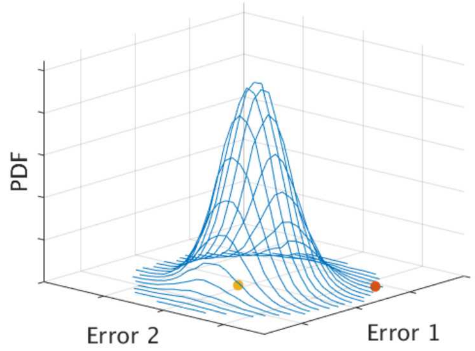
- $Y_{obs} = Y_{sim} + \epsilon_{meas} + \delta_{model}$
- Model error can take on different forms
- Kennedy O'Hagan Framework
  - Treat model error as a Gaussian random process with unknown mean and covariance



$$L(\boldsymbol{\theta}, \mu, \sigma) = \prod_{i=1}^{N} \frac{1}{\sigma\sqrt{2\pi}} exp\left(-\frac{1}{2\sigma^2}\left((y_{obs,i} - y_{sim}(\boldsymbol{\theta})) - \mu\right)^2\right)$$

Likelihood (case 3):

- Multiple output quantities
- Covariance matrix of errors needed



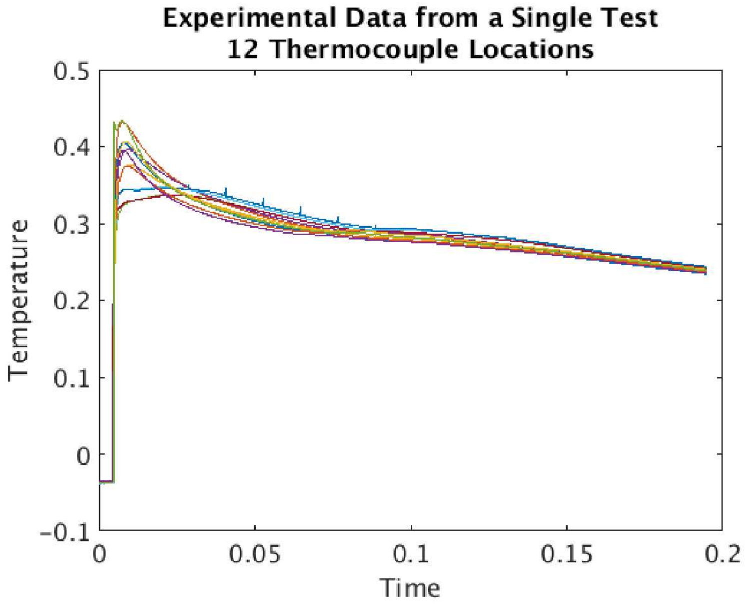
$$L(\boldsymbol{\theta}, \boldsymbol{\mu}, \boldsymbol{\sigma}) = \prod_{i=1}^{N} \frac{1}{\sqrt{(2\pi)^k|\Sigma|}} exp\left(-\frac{1}{2}\left(\left(\boldsymbol{y}_{obs,i} - \boldsymbol{y}_{sim}(\boldsymbol{\theta})\right) - \boldsymbol{\mu}\right)^T \Sigma_y^{-1} \left(\left(\boldsymbol{y}_{obs,i} - \boldsymbol{y}_{sim}(\boldsymbol{\theta})\right) - \boldsymbol{\mu}\right)\right)$$

Solving for posterior

- Markov chain Monte Carlo (MCMC)
  - Samples from chain approach posterior distribution
- Particle filter (PF)
  - Particles weighted based on likelihood scores
  - Easily parallelizable
- Sample-based Bayesian methods require many model evaluations
  - Replace computationally expensive physics model with efficient surrogate model

Current Implementation of PF				
17 calibration parameters	5 output variables	Samples: 10 million	Resampling algorithm 10 iterations	50 cores ~11hrs

Field Quantities



Spatially and temporally varying outputs

- High dimensional output space

2 main challenges

Building surrogate models

- Gaussian process, polynomial chaos, ANN, etc.
- Inputs are RVs and outputs are random processes/fields
  - Include time/space as an input
  - Build separate surrogate for each location
  - Decomposition / dimension reduction technique

Constructing likelihood function

- High dimensional joint pdf
- Need correlation for error covariance matrix

Current Efforts on Thermal Battery

Feature Extraction
- 3 temperature values and 2 slopes

Decompose the trace
- Through a mathematical function/coefficients or through PCA eigenvectors/eigenvalues

Dakota
- Stepwise parameter identification then discrepancy estimation

DAKOTA
Explore and predict with confidence.

Estimate model bias state
- Then covariance matrix is known
- Combined parameter identification and state estimation is a challenge