



Understanding Model Inadequacy in TRISO Nuclear Fuel Fission Products Release Models: Empirical and Mechanistic Approaches

April 2025

Changing the World's Energy Future

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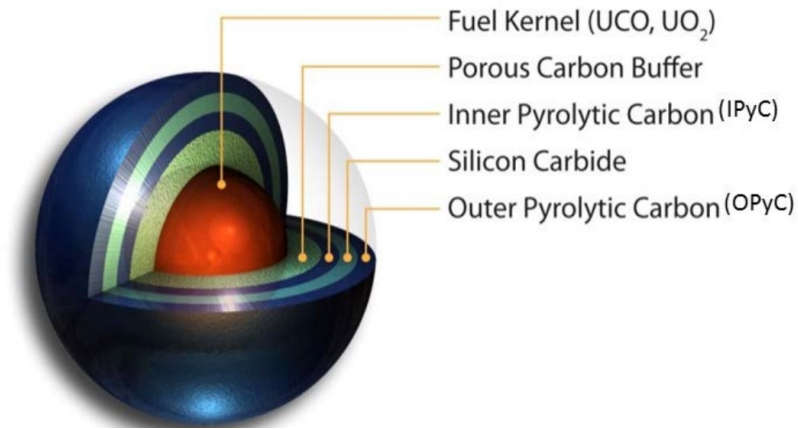
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Hirschhorn, Steve Novascone

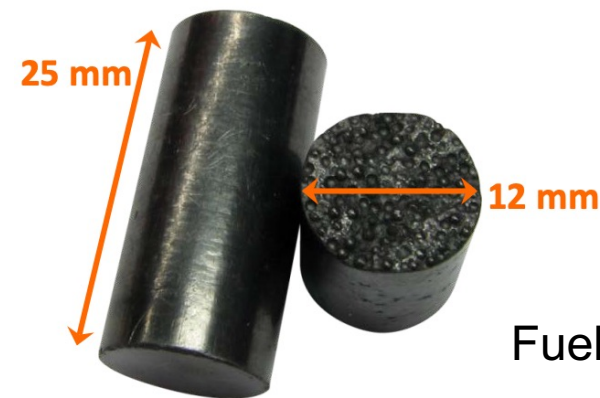
2025 MRS Spring Meeting & Exhibit

Tri-structural isotropic (TRISO) particle nuclear fuel

- TRISO stands for TRI-structural iSOtropic particle fuel
- Proposed for use in many advanced reactor concepts like micro-reactors owing to its robustness
- Interest from the DOE, DOD, and industries like Kairos Power, Xenergy
- Fuel kernel surrounded by several protective layers
- A fuel compact can have 1000s of tiny TRISO particles
- **Critical to model the fission products release for nuclear reactor safety**



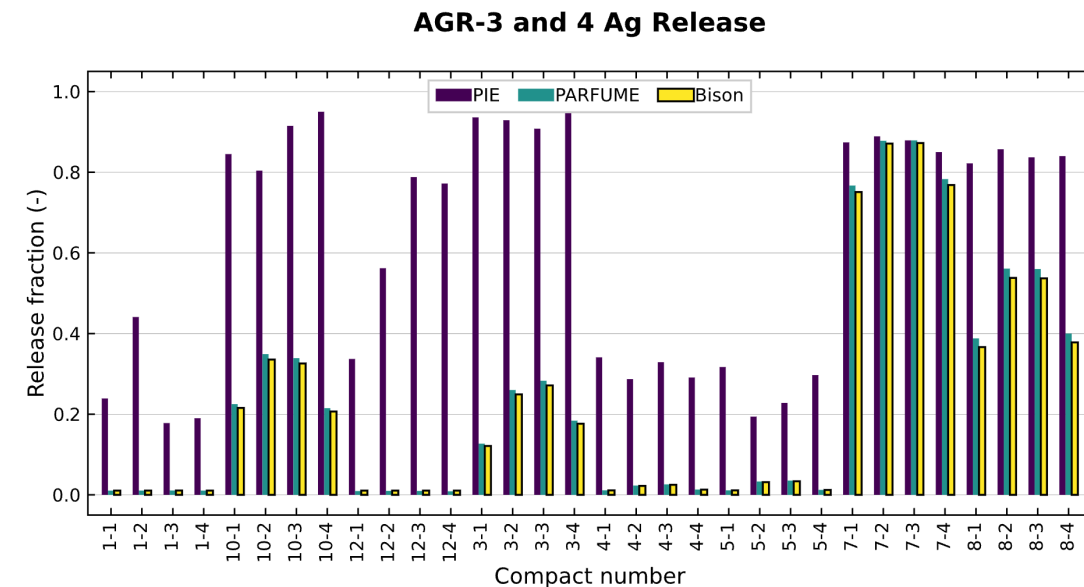
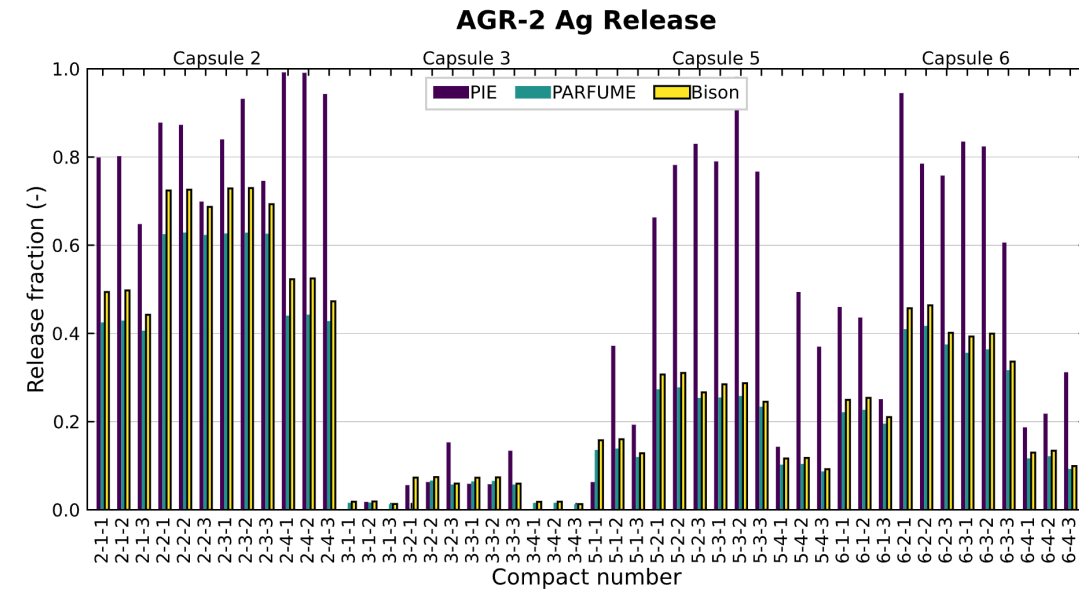
Single TRISO particle of radius
~400 μm (Davenport 2016)



Fuel compact with numerous TRISO particles (Demkowicz 2016)

Fission products modeling in BISON and comparison to experimental data

- The BISON fuel performance code models fission products (e.g., Ag, Cs, Sr) release from TRISO fuel.
- It models the thermo-mechanical phenomena which occur in the TRISO fuel and can take information from lower-length-scale simulations to inform the diffusion of fission products through the fuel layers.
- BISON uses inputs like temperature history and fluence to model fission product release. These inputs are provided from the Advanced Gas Reactor (AGR) program.
- The AGR program also has PIE data on the fractional fission product release. **A comparison of BISON predictions and AGR PIE for Ag shows significant uncertainties.**



Bayesian framework for computational models

$$f(\boldsymbol{\theta}, \sigma | \mathbf{x}, \mathbf{y}) \propto L(\mathbf{y} | \mathbf{x}, \hat{\mathbf{y}}, \boldsymbol{\theta}, \sigma) f(\boldsymbol{\theta}, \sigma)$$

$f(\boldsymbol{\theta}, \sigma)$: Prior of the uncertain model parameters

$L(\mathbf{y} | \mathbf{x}, \boldsymbol{\theta}, \sigma)$: Likelihood of observing the data given model inputs, parameters, and predictions

$f(\boldsymbol{\theta}, \sigma | \mathbf{x}, \mathbf{y})$: Posterior of the uncertain model parameters given model inputs and predictions

\mathbf{x} : Experimental configurations

$\boldsymbol{\theta}$: Model params to be inferred

σ : Sigma term to be inferred (model inadequacy + experimental noise)

$$y_k(\mathbf{x}) = \hat{y}_k(\mathbf{x}, \boldsymbol{\theta}) + \varepsilon$$

$$L(\mathbf{y} | \mathbf{x}, \boldsymbol{\theta}) \propto \frac{1}{\sqrt{\sigma}} \prod_{k=1}^K \exp\left(-\frac{(y_k(\mathbf{x}) - \hat{y}_k(\mathbf{x}, \boldsymbol{\theta}))^2}{2\sigma^2}\right)$$

Independent and Identically Distributed

Kennedy O'Hagan (KOH) Bayesian framework

Standard Bayesian

$$y_k(\mathbf{x}) = \hat{y}_k(\mathbf{x}, \boldsymbol{\theta}) + \varepsilon$$

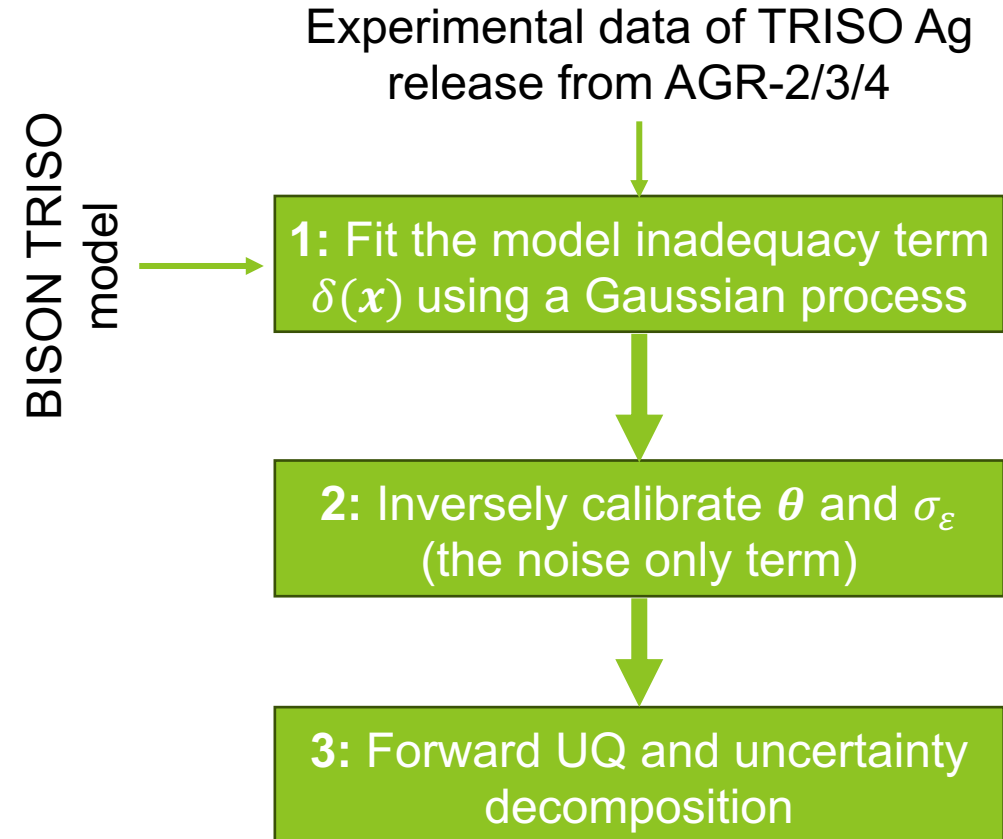
σ term accounts for both model inadequacy and experimental noise in a lumped fashion

KOH Bayesian

$$y_k(\mathbf{x}) = \hat{y}_k(\mathbf{x}, \boldsymbol{\theta}) + \delta(\mathbf{x}) + \varepsilon$$

σ term accounts only for experimental noise.
Model the model inadequacy term $\delta(\mathbf{x})$

$\boldsymbol{\theta}$: Model parameters, σ : Total uncertainty (inadequacy + noise), σ_ε : Experimental noise uncertainty

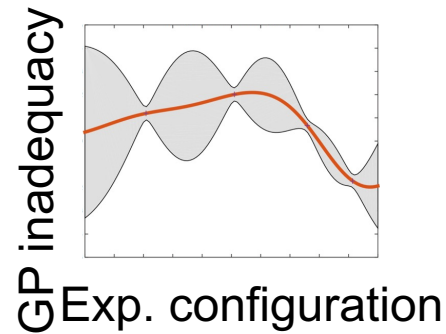


Kennedy O'Hagan (KOH) Bayesian framework

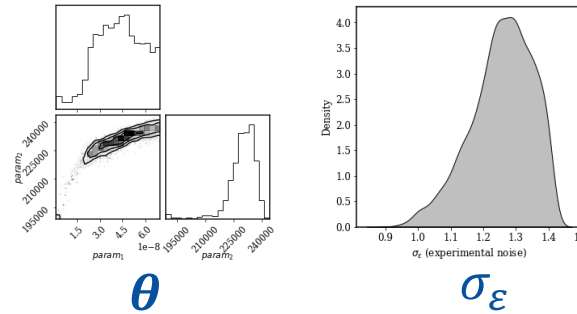
Best estimate of the model parameters θ

Standard Bayesian calibration or Deterministic optimization

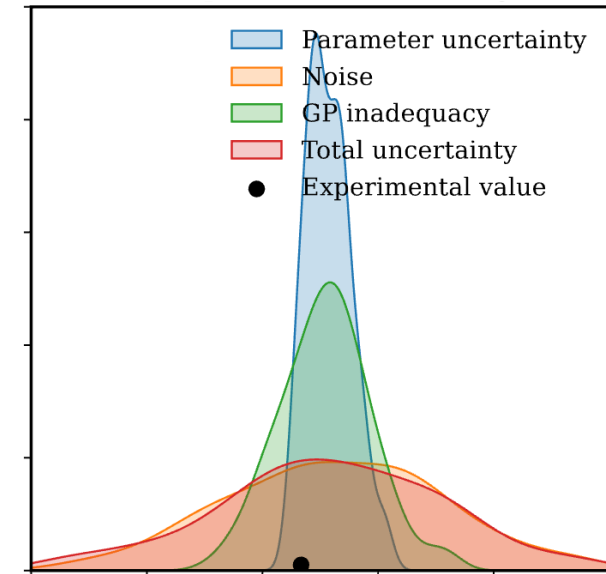
Module 1
GP inadequacy term hyper-parameters γ_δ



Module 2
Inverse UQ of $\{\theta, \sigma_\varepsilon\}$

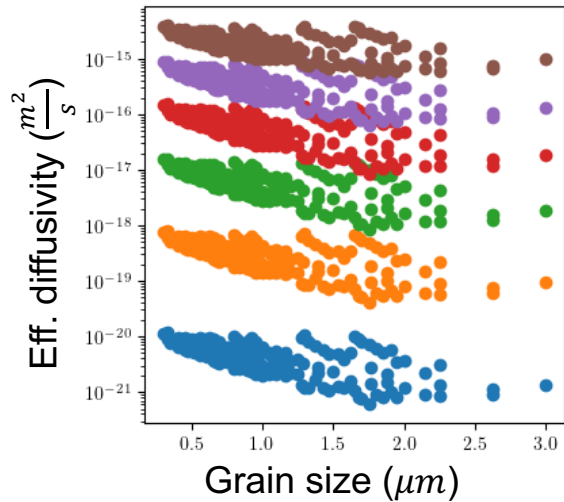


Module 3
Posterior predictive distribution



BISON models for TRISO fuel fission products release

Lower-length-scale data



MARMOT
(INL code)

Arrhenius equation
(diffusion coeff:
model params)

Find the best
equation
(parametric)

Fit a Gaussian
process
(non-parametric)

TRISO fuel Silver release

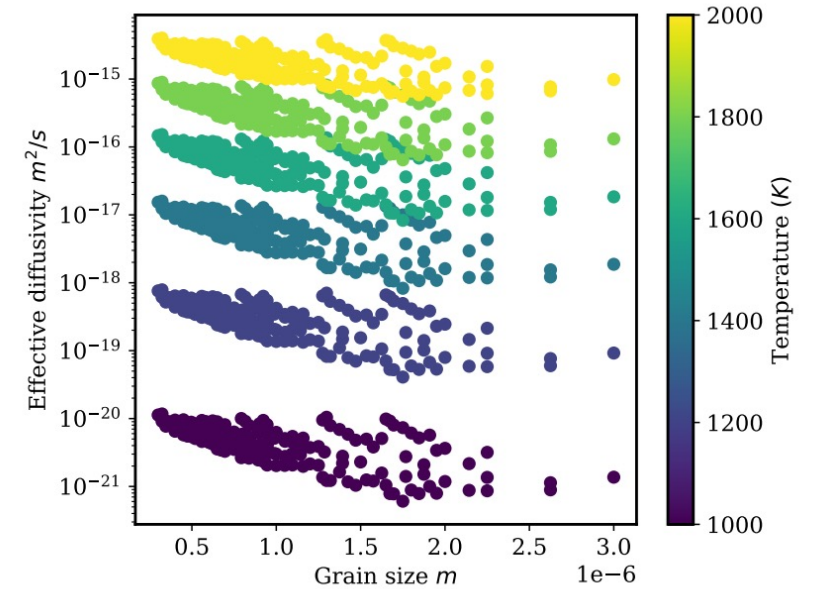
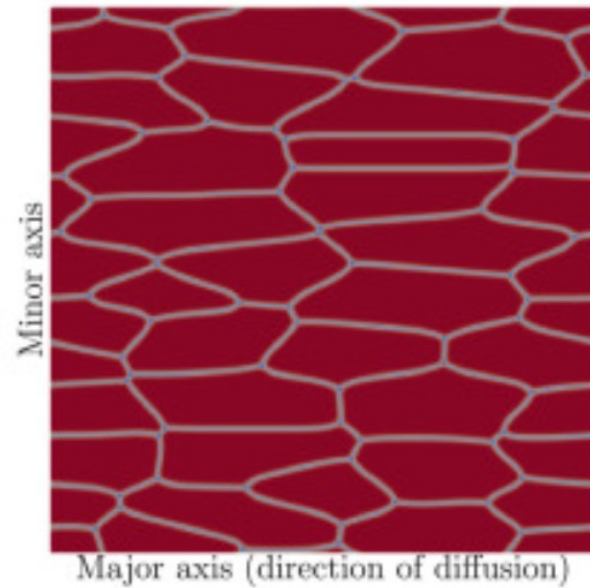
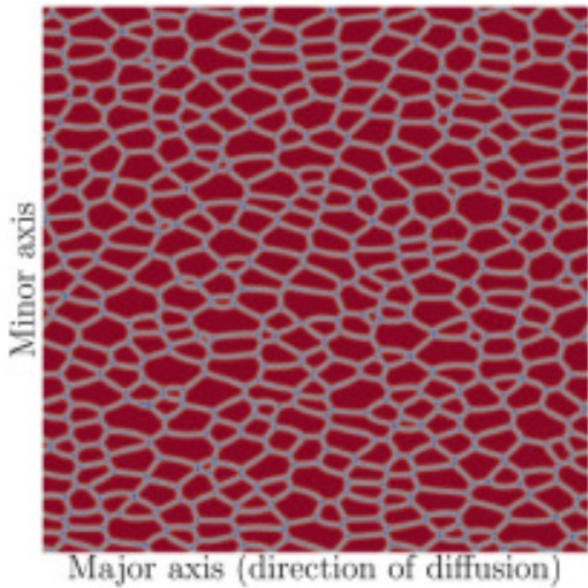
OPyC
SiC
IPyC
Buffer
Kernel



SiC layer
diffusivity

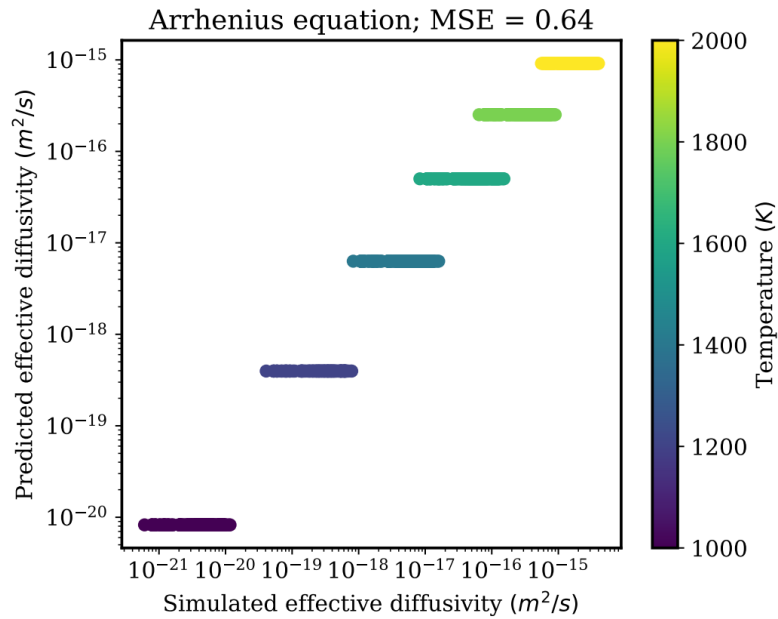
BISON fuel performance code

Lower-length-scale simulations

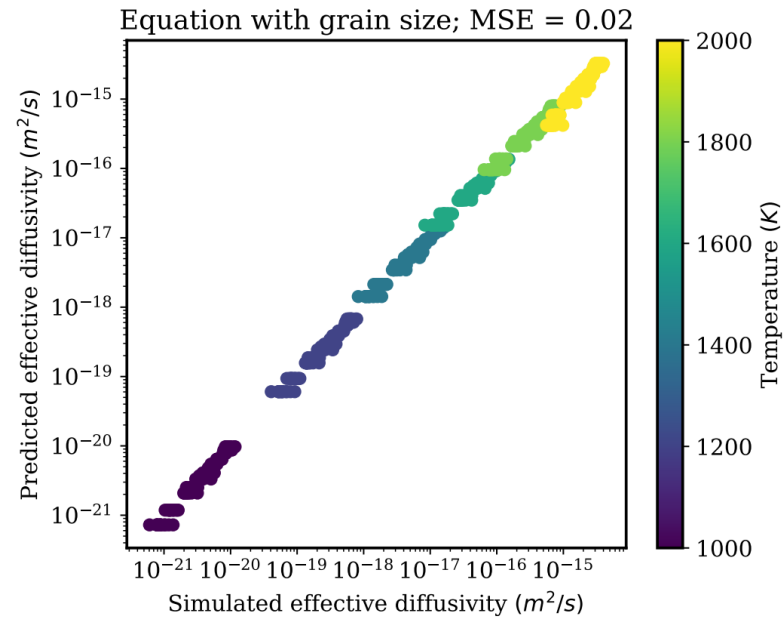


Simon et al. 2022

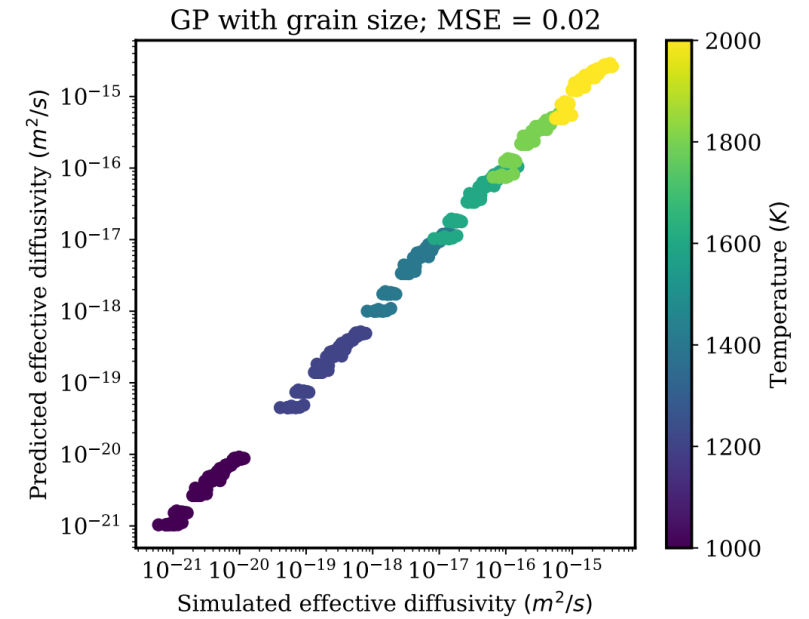
Lower-length-scale data fits



Arrhenius eqn.

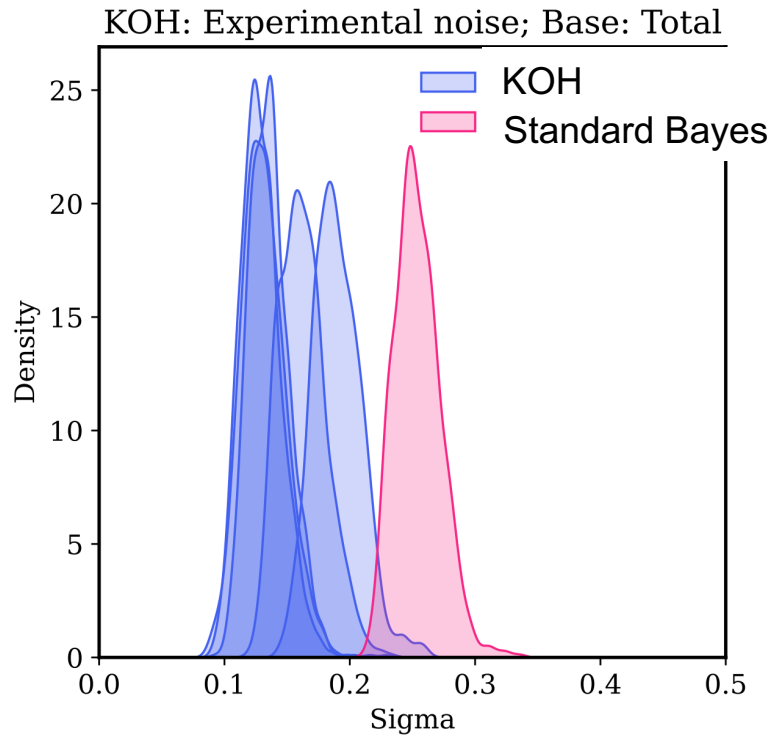


Parametric fit

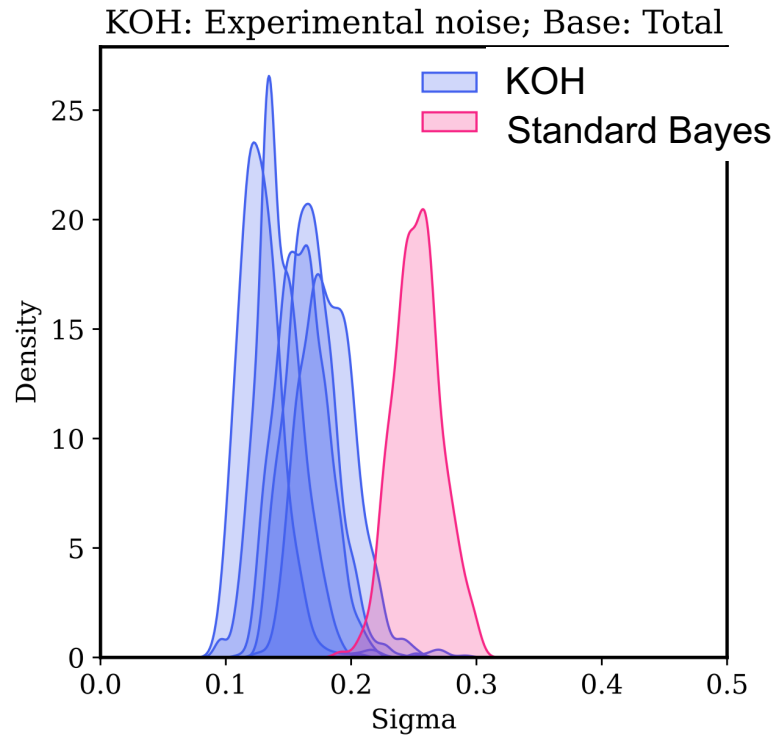


**Non-parametric fit
(GP)**

Inverse analysis with AGR-2/3/4 silver release data



Arrhenius eqn.



**Non-parametric fit
(GP)**

Inverse analysis with AGR-2/3/4 silver release data

	Arrhenius	LLS-informed GP
KOH repetition 1	$\sigma_\varepsilon = 0.129$	$\sigma_\varepsilon = 0.167$
KOH repetition 2	$\sigma_\varepsilon = 0.189$	$\sigma_\varepsilon = 0.181$
KOH repetition 3	$\sigma_\varepsilon = 0.162$	$\sigma_\varepsilon = 0.160$
KOH repetition 4	$\sigma_\varepsilon = 0.131$	$\sigma_\varepsilon = 0.129$
KOH repetition 5	$\sigma_\varepsilon = 0.135$	$\sigma_\varepsilon = 0.142$
KOH mean	$\sigma_\varepsilon = 0.149$	$\sigma_\varepsilon = 0.155$
Standard Bayesian	$\sigma = 0.254$	$\sigma = 0.253$

σ_ε represents the experimental noise uncertainty.

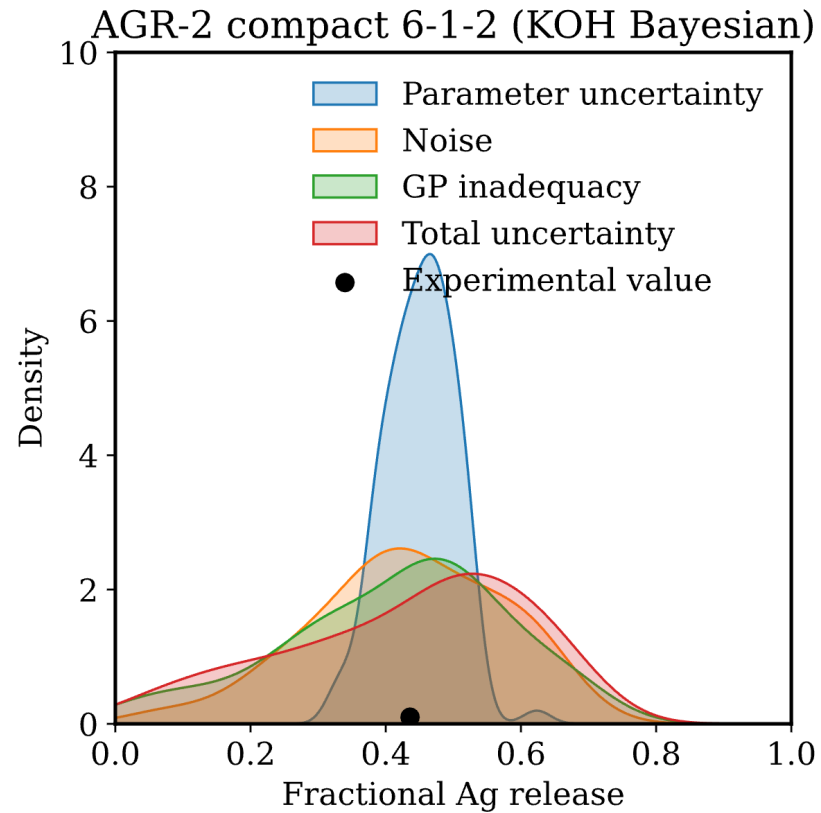
σ represents both the model inadequacy and experimental noise uncertainties.

- Arrhenius and LLS models similar inadequacy level
- Model inadequacy most dominant source of uncertainty, followed by experimental noise

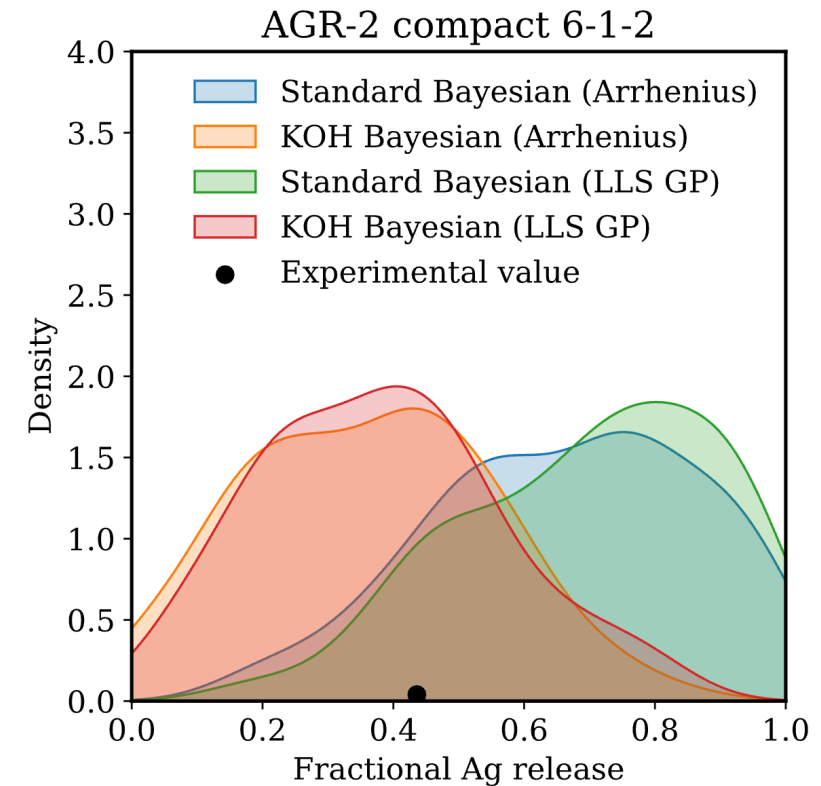
Component	%
Model inadequacy	55
Experimental noise	40
Model parameters	5

On an average considering AGR-2/3/4

Forward analysis

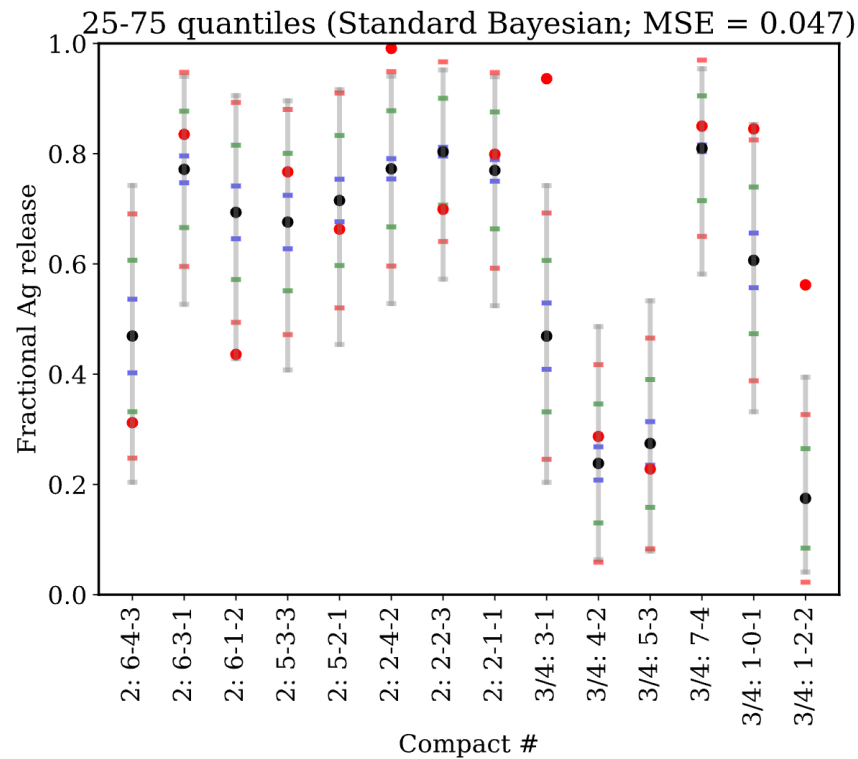


Components of uncertainty via the KOH framework

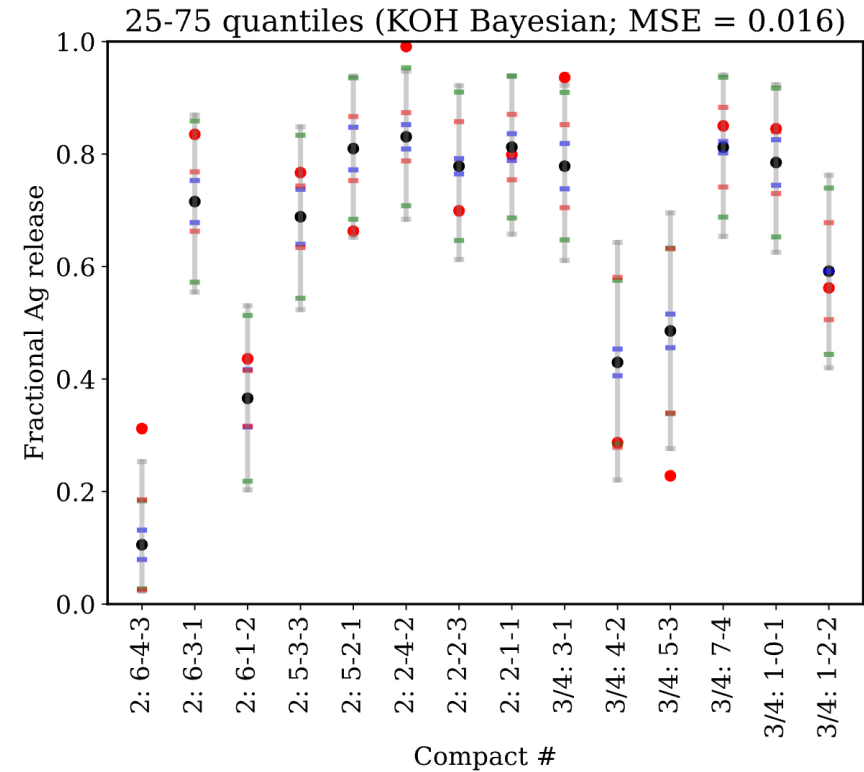


Accounting for model inadequacy via KOH improves the predictive capability of BISON

Forward analysis



(a)

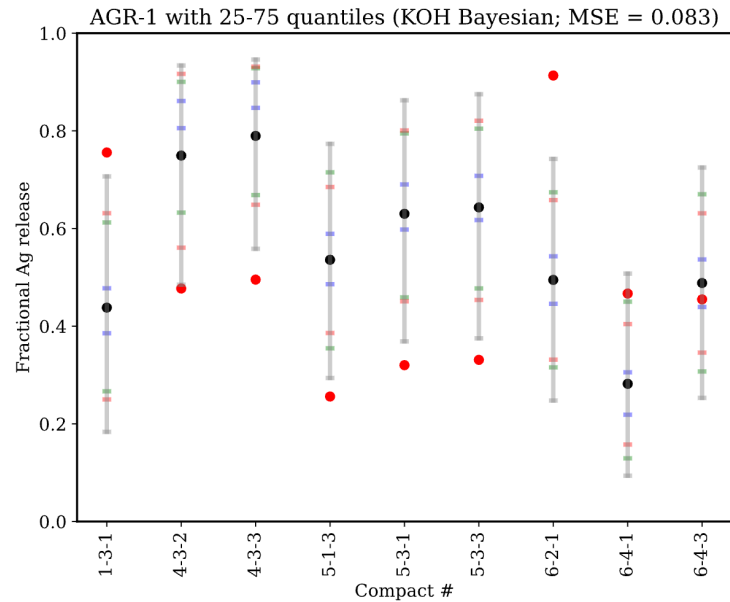


(b)

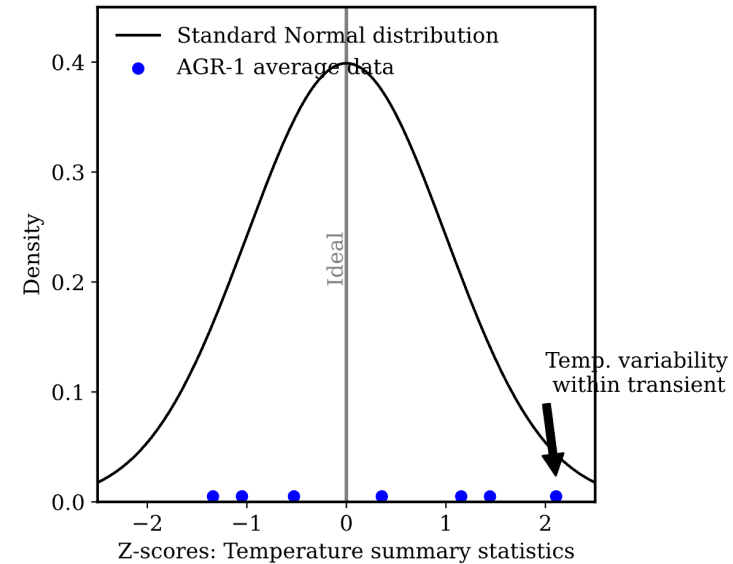


Accounting for model inadequacy via KOH improves the predictive capability of BISON

Forward analysis: Blind prediction on AGR-1



(a)



(b)

● Experimental value ● Median prediction
| Total | Parametric | Experimental | Model/GP inadequacy

The temperature inputs for AGR-1 are sometime two standard deviations away compared to AGR-2/3/4. This results in larger predictive confidence bands.



Summary and future work



Thank you!
(Som.Dhulipala@inl.gov)

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