SAND2019-4297C

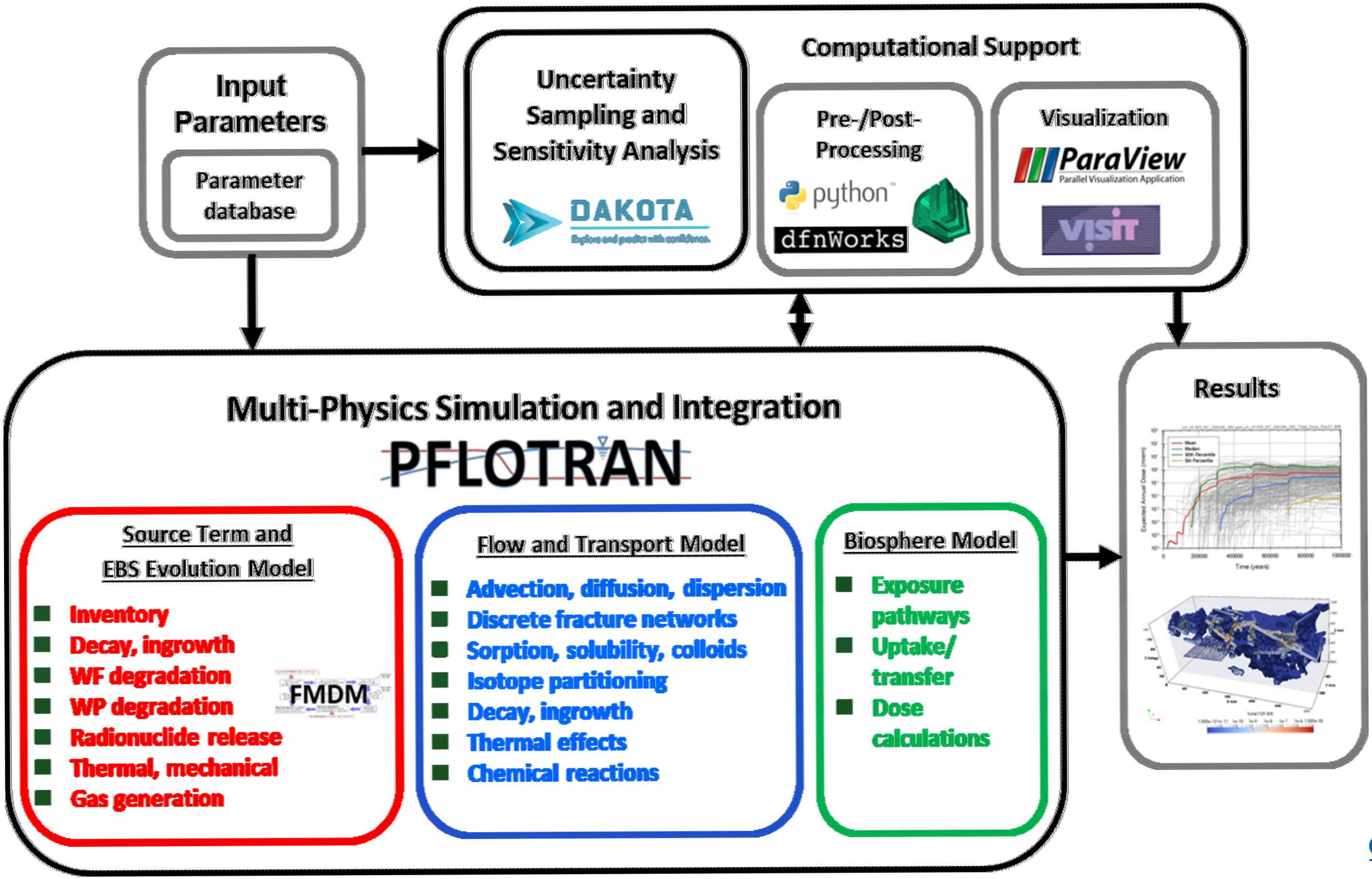
Methods of Sensitivity Analysis in *Geologic Disposal Safety Assessment (GDSA) Framework*

PRESENTED BY

Emily Stein, Laura Swiler, S. David Sevougian

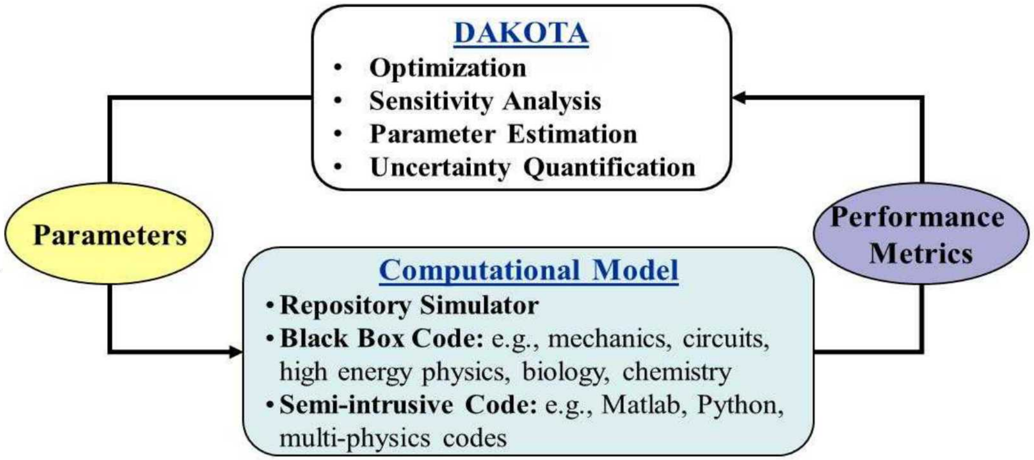
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

GDSA Framework



Dakota

- Flexible, extensible interface between simulation software and variety of system analysis methods
  - Uncertainty quantification (aleatory and epistemic)
  - Sensitivity/variance analysis
  - Deterministic/stochastic parameter estimation
  - Design optimization
- C++ Software Toolkit
- Open source GNU LGPL
- Supports parallel computation



DAKOTA
Explore and predict with confidence.

https://dakota.sandia.gov

Feedback to R&D

- Identify the model inputs for which a reduction of uncertainty would most reduce the uncertainty in the model output. [*Factor Prioritization*]
- Prioritize subsequent research.

Inform uncertainty analysis

- Identify model inputs that could be fixed or simplified without affecting model output. [*Factor Fixing*]
- Create a less computationally expensive and potentially more transparent analysis.

Understand system behavior

- Check that model behavior is realistic and robust.

e.g., Saltelli et al. 2008

Tried-and-true methods

- Propagation of aleatory and epistemic uncertainties
- Latin Hypercube Sampling (with controlled input variable correlation)
- Partial Correlation Coefficients (PCC)
  - The correlation between the residuals resulting from the linear regression of x_j with $x_{\sim j}$ and y with $x_{\sim j}$, where the notation $x_{\sim j}$ means all x except x_j.
- Standardized Regression Coefficients (SRC) via stepwise multiple linear regression
  - $SRC_j = \frac{\hat{s}_j}{\hat{s}} b_j$, where the b_j are determined by regression $\hat{y} = b_0 + \sum_{j=1}^{n_x} b_j x_j$
- Rank transformations (PRCC and SRRC)
  - Partial Rank Correlation Coefficients and Standardized Rank Regression Coefficients are calculated after replacing the raw values of x and y with rank values.

Dakota in GDSA Framework

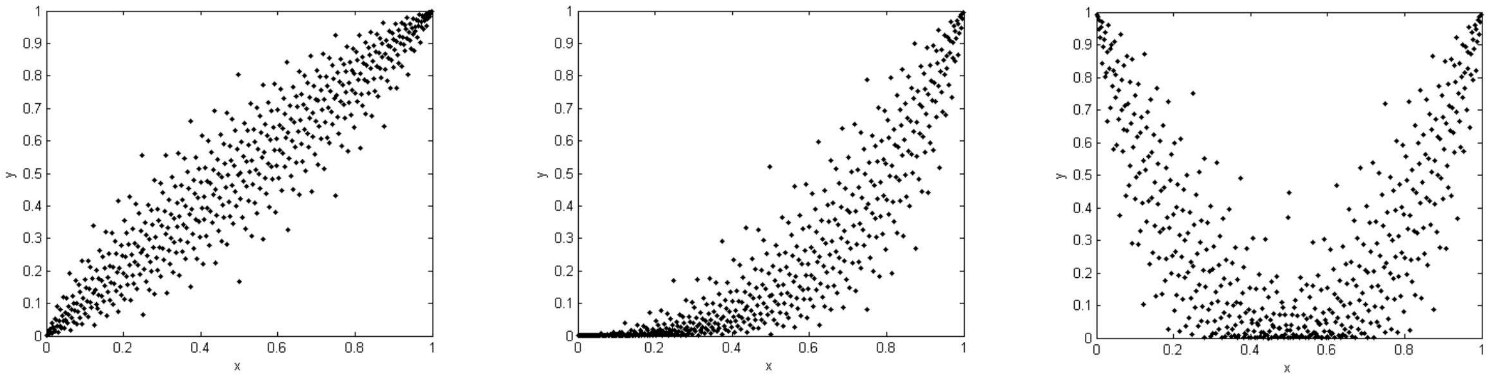
Adoption of new methods as standard of practice evolves

- Variance decomposition:
  - Fraction of variance in the output due to the variance in an input.
  - Main, higher-order, and total sensitivity indices
- Surrogate modeling techniques
- Importance sampling

Development Advantages

- Actively developed at Sandia National Laboratories
- Open source
- User-friendly post-processing
- Parallel architecture for high-performance computing

Variance Decomposition



Sensitivity Indices

- S_j – main effect of an input variable without variable interactions

$$S_j = \frac{V_{x_j}\left(E_{x_{\sim j}}(y|x_j = x_j{}^*)\right)}{V(y)}$$

- S_{ij} – effect of specific variable interactions
- S_T – total effect of an input variable including interactions

$$S_{T_1} = S_1 + S_{12} + S_{13} + S_{123}$$
$$S_{T_2} = S_2 + S_{12} + S_{23} + S_{123}$$
$$S_{T_3} = S_3 + S_{13} + S_{23} + S_{123}$$

- Model independent (theoretically)

The Challenge…

Computationally expensive

At least $m(d+2)$ evaluations of the model, where m is sample size (≥ 1000) and d is the number of uncertain inputs, to estimate the S_{ij} and S_T

Surrogate models

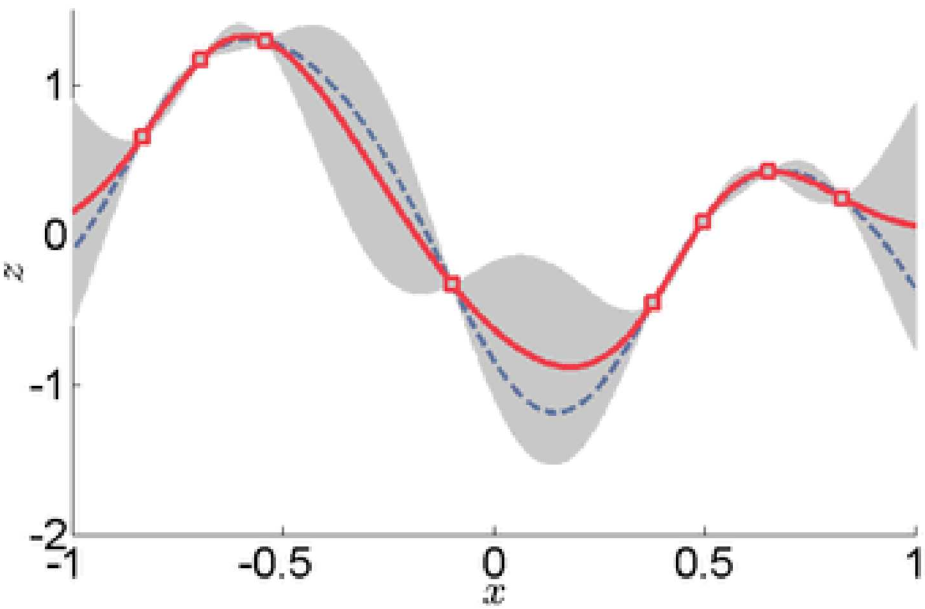
Given the large number of coupled processes and large number of epistemic uncertain inputs typically associated with repository PA, construction of appropriate surrogate models for calculation of sensitivity indices may be a challenge.

Using a probabilistic PA of a reference case deep geologic repository in shale as an example, we compare sensitivity indices

1. obtained from Polynomial Chaos Expansion and Gaussian Process surrogate models,
2. calculated from sample sizes of 50, 100, and 200 generated using incremental Latin hypercube sampling, and
3. using raw outputs (maximum I-129 concentrations) and log-transformed outputs.

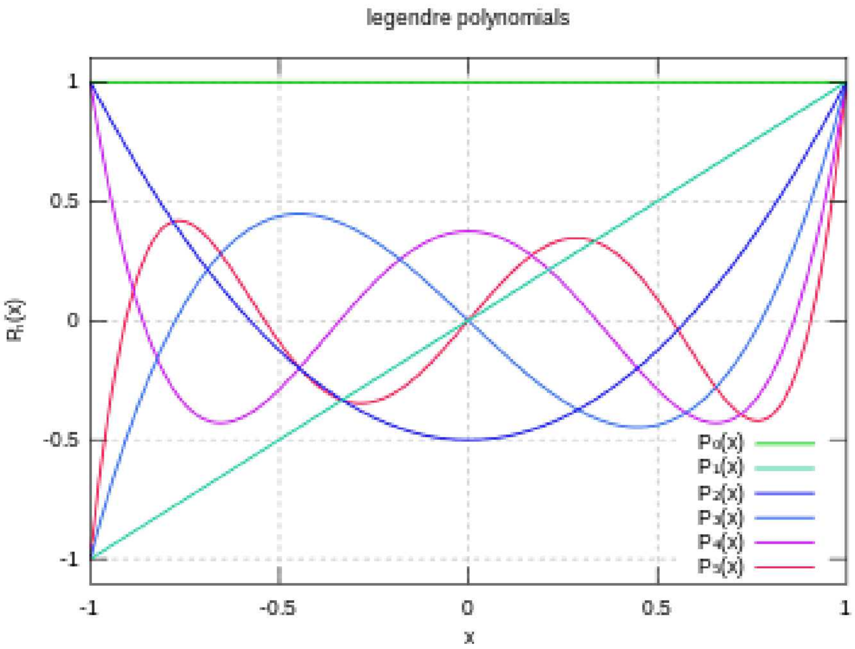
Gaussian Process

- Predicts the most likely value of output variable y at points on a response surface.
- Possible values for y at any point are part of a normal (Gaussian) distribution.
- The variance of that distribution is smaller close to the training points (zero at the training points) and larger further away.
- $m(d+2)$ evaluations gives S_j and S_T



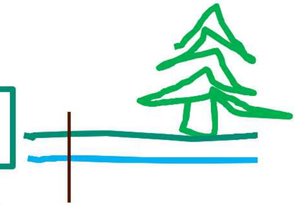
Polynomial Chaos Expansion

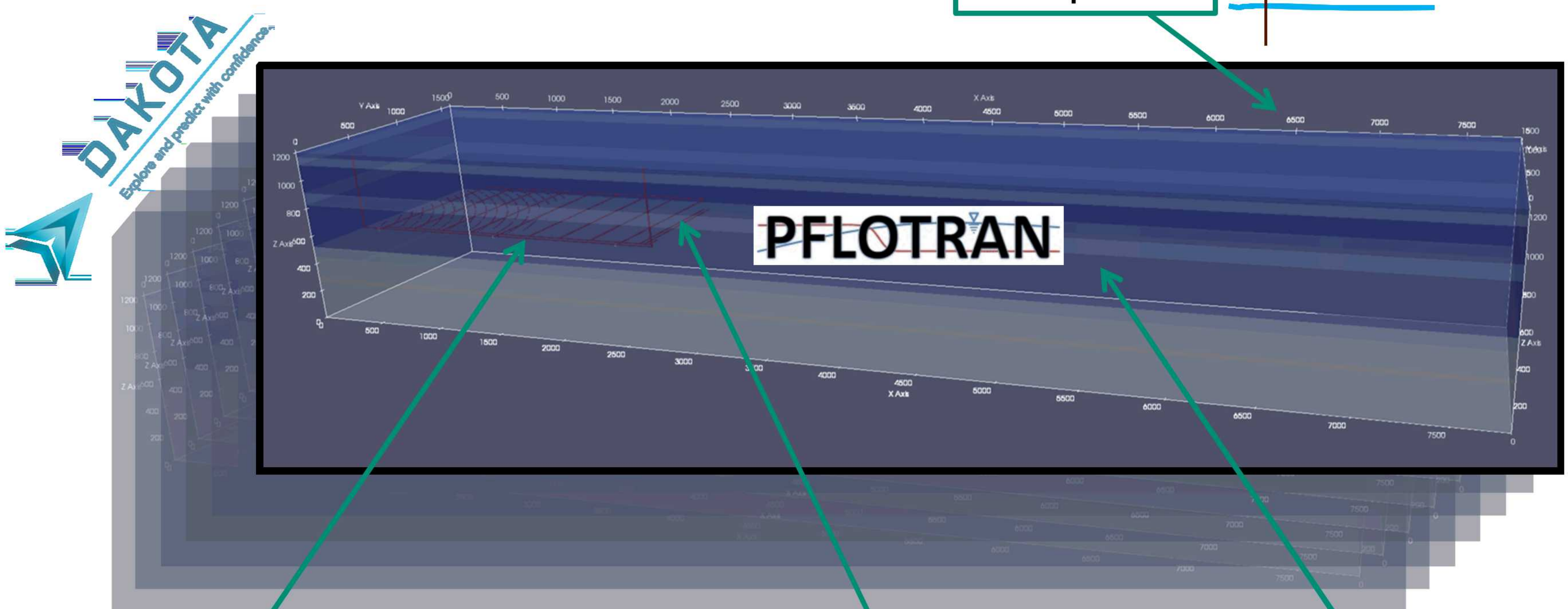
- Approximates values of the output variable using a series expansion comprised of orthogonal polynomials.
- Obtain S_j, S_{ij}, …, S_T from analytic functions of the coefficients.
- Number of terms: $P = \frac{(d+p)!}{d!p!}$, where p is the order of the polynomial.
- Use compressive sensing to fit the coefficients.



Components of a Reference Case

Biosphere

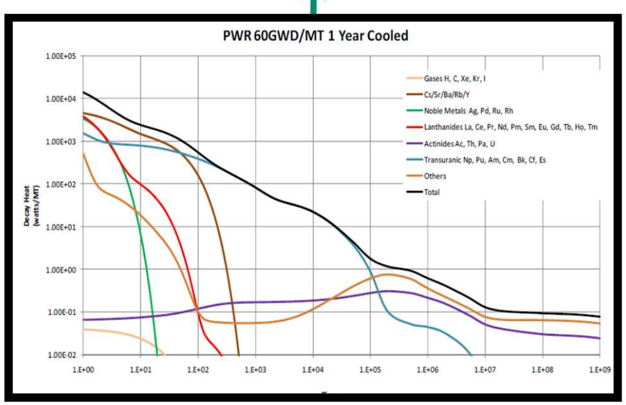


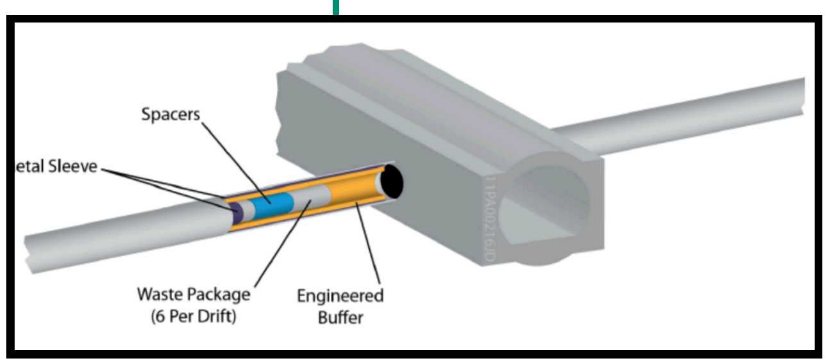


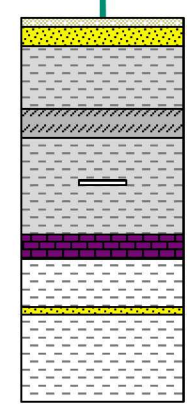
Waste Source Term

Engineered Barrier System

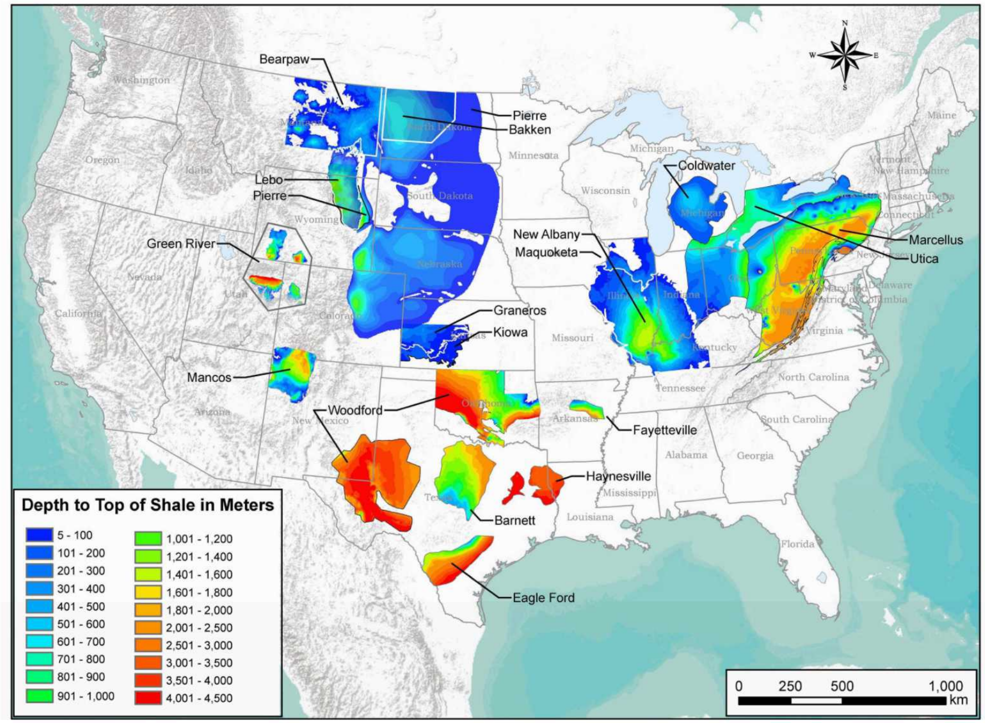
Natural Barrier System

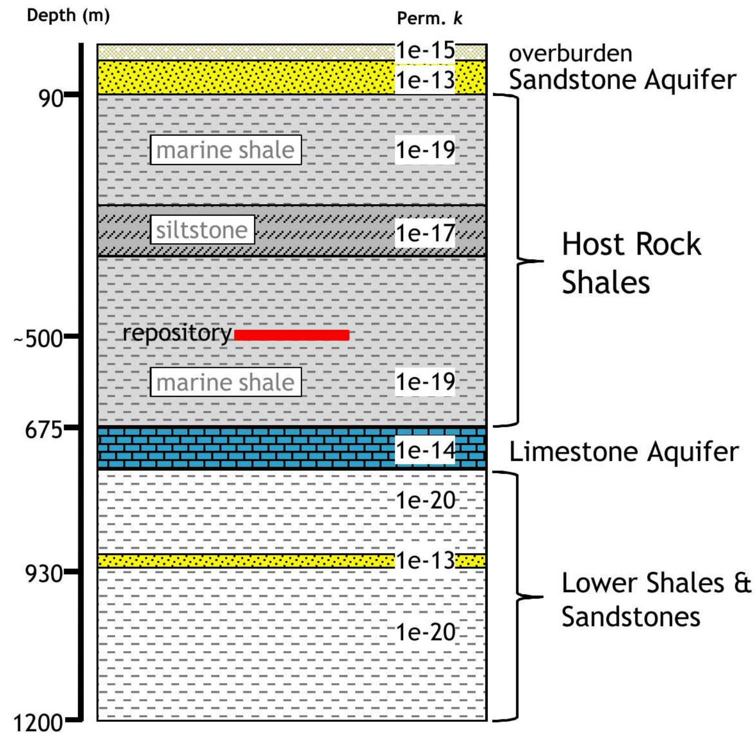






Shale Reference Case – Natural Barrier System





Low permeability ◆ High sorption ◆ Self-healing

Perry and Kelley 2017

Shale Reference Case – Engineered Barrier System

12-PWR waste package

In-drift axial emplacement

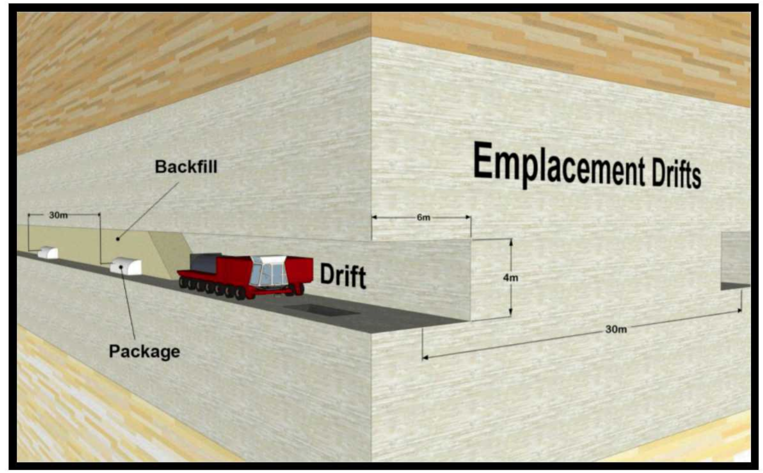
30-m drift spacing

20-m center-to-center WP spacing

Bentonite/sand buffer

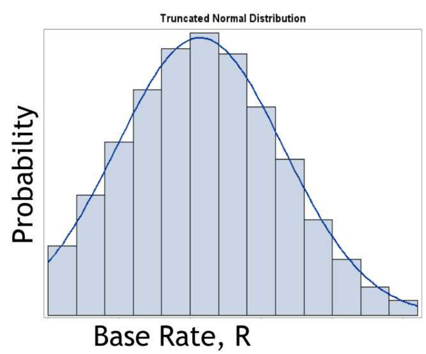
WP degradation

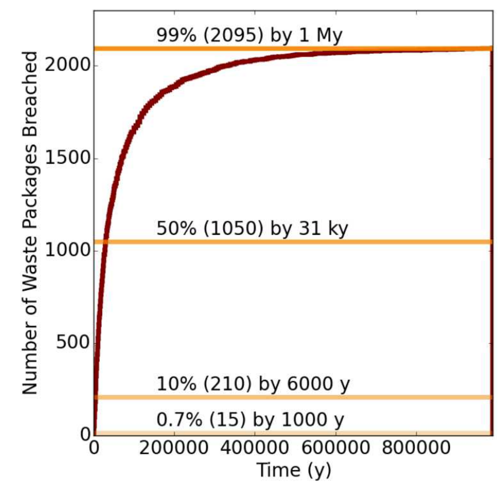
- Temperature-dependent
- Log-normal distribution
- 50% breached by 31 ky



R_{eff} = canister degradation rate

$$R_{eff} = R \cdot e^{C\left[\frac{1}{60^{\circ}\mathrm{C}} - \frac{1}{T(x,t)}\right]}$$

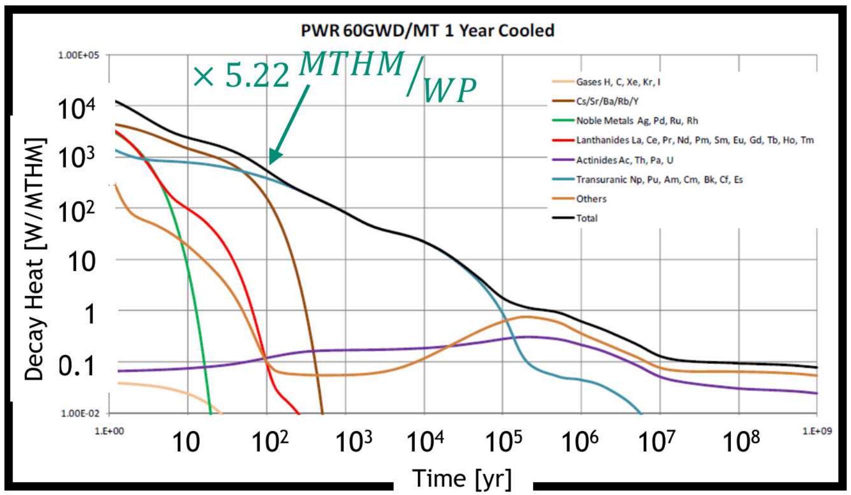




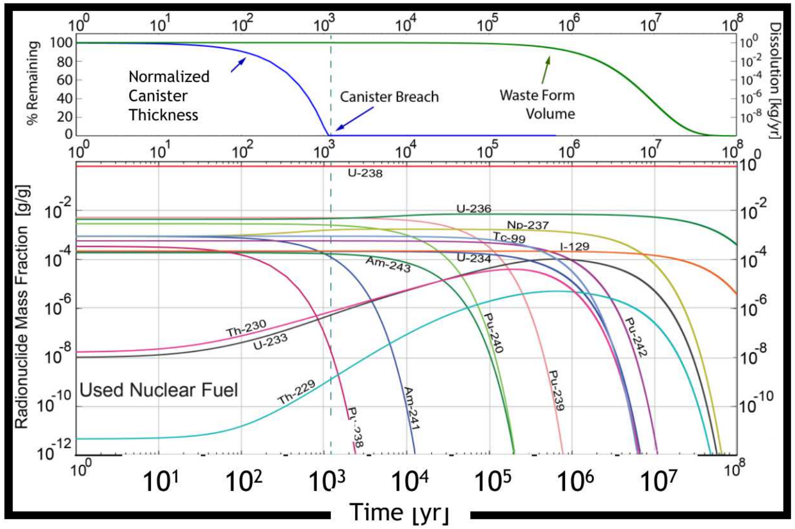
Shale Reference Case – Waste Package Source Terms

Assumptions ➤ Source Terms

- 60 GWD/MT burn-up
- 4.73 wt% ^{235}U enrichment
- 100 yrs Out of Reactor



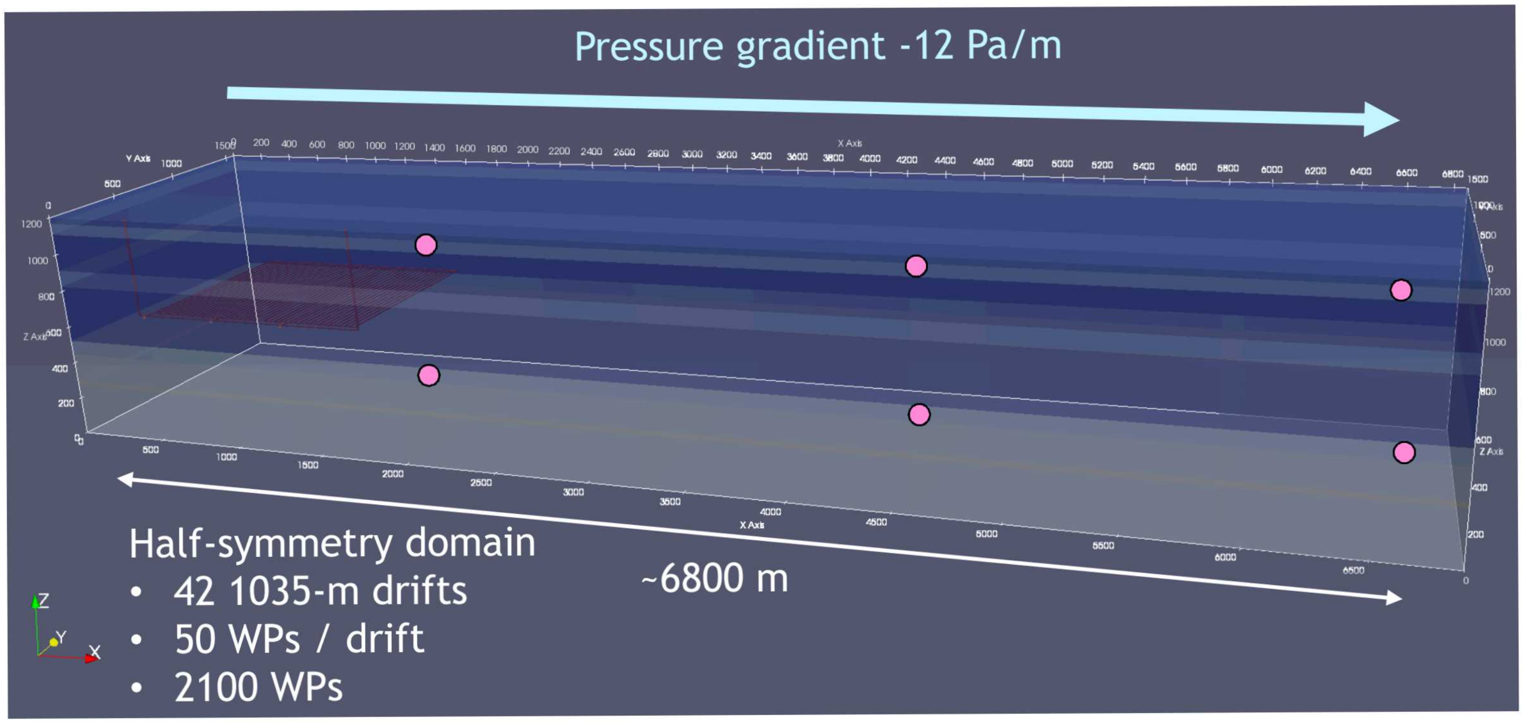
Initial WP heat = 3084 W



18 Radionuclides

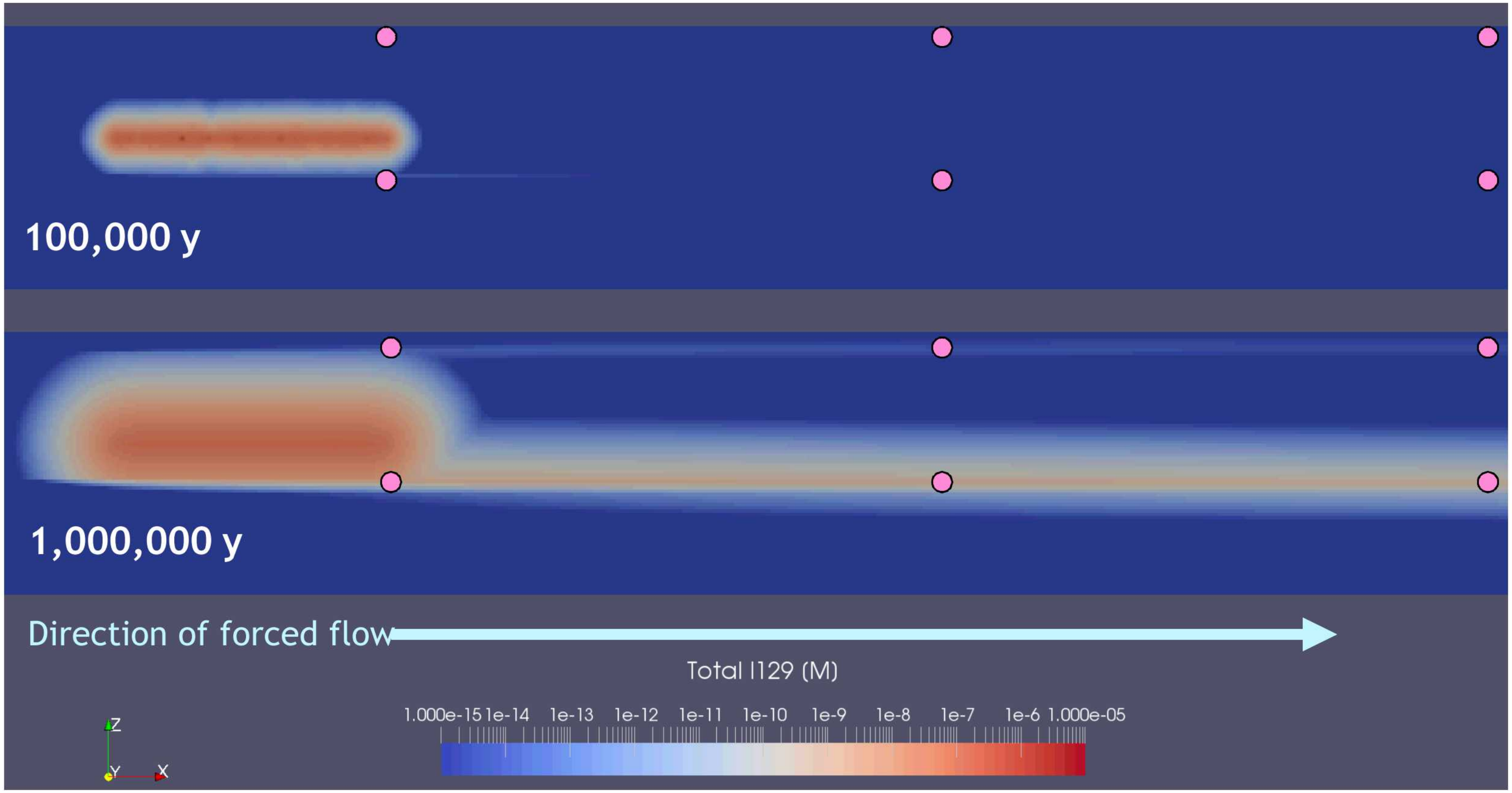
^{241}Am, ^{243}Am, ^{238}Pu, ^{240}Pu, ^{242}Pu, ^{237}Np, ^{233}U, ^{234}U, ^{236}U, ^{238}U, ^{229}Th, ^{230}Th, ^{226}Ra, ^{99}Tc, ★ ^{129}I, ^{135}Cs, ^{36}Cl

Model Domain



~7 million hexes ◆ 512 cores ◆ ~3 hours

^{129}I Concentration – Deterministic

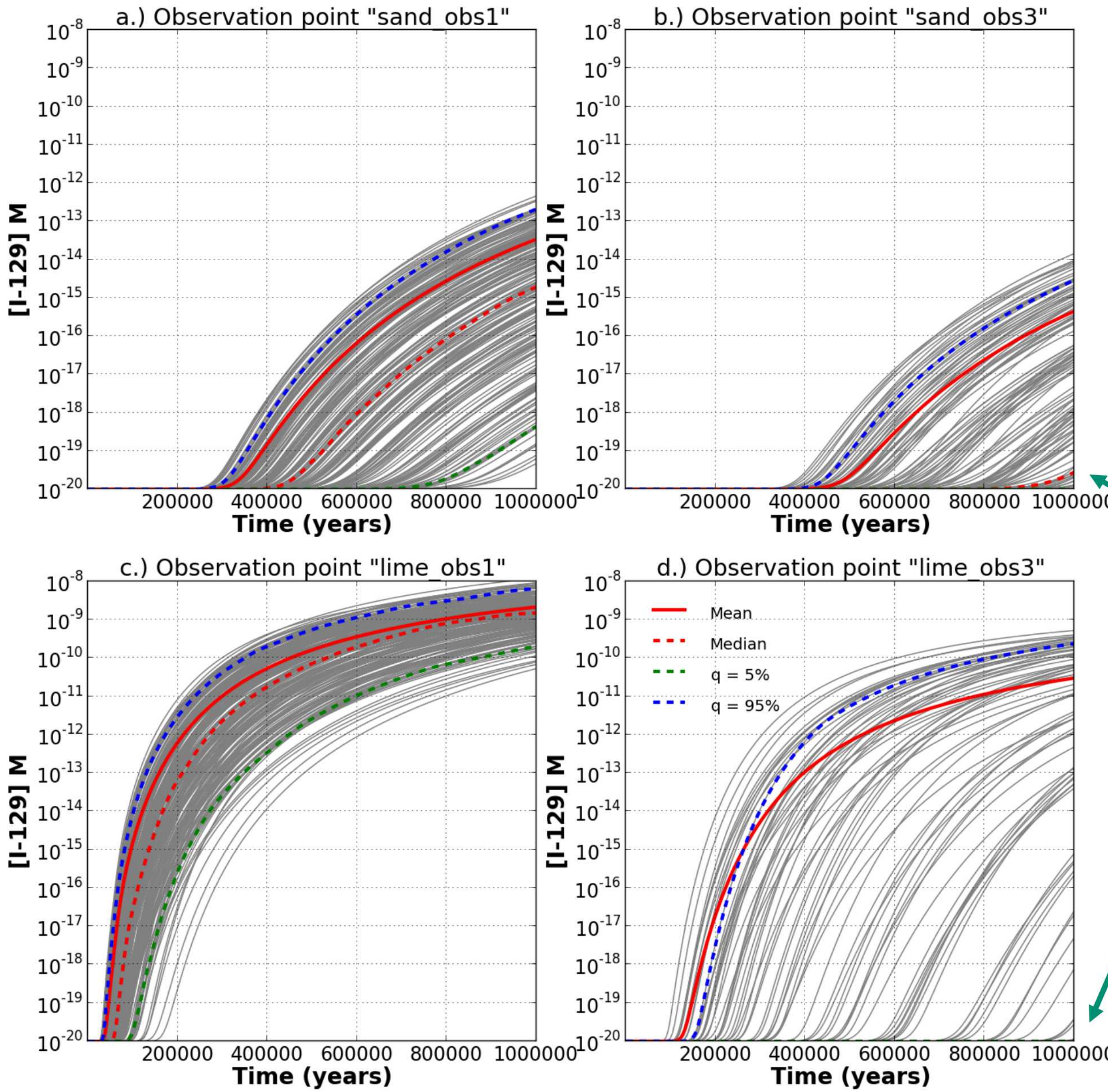


Sampled Parameters

Parameter	Description	Range	Units	Distribution
rateSNF	SNF Dissolution Rate	10^{-8} - 10^{-6}	yr^{-1}	log uniform
rateWP	Mean Waste Package Degradation Rate	$10^{-5.5}$ - $10^{-4.5}$	yr^{-1}	log uniform
kSand	Upper Sandstone k	10^{-15} - 10^{-13}	m^2	log uniform
kLime	Limestone k	10^{-17} - 10^{-14}	m^2	log uniform
kLSand	Lower Sandstone k	10^{-14} - 10^{-12}	m^2	log uniform
kBuffer	Buffer k	10^{-20} - 10^{-16}	m^2	log uniform
kDRZ	DRZ k	10^{-18} - 10^{-16}	m^2	log uniform
pShale	Host Rock (Shale) ϕ	0.1 – 0.25	-	uniform
bNpKd	Np K_d Buffer	0.1 – 702	m^3kg^{-1}	log uniform
sNpKd	Np K_d Shale	0.047 – 20	m^3kg^{-1}	log uniform

DAKOTA
Explore and predict with confidence.

200 Realizations – [I-129] at 4 observation points

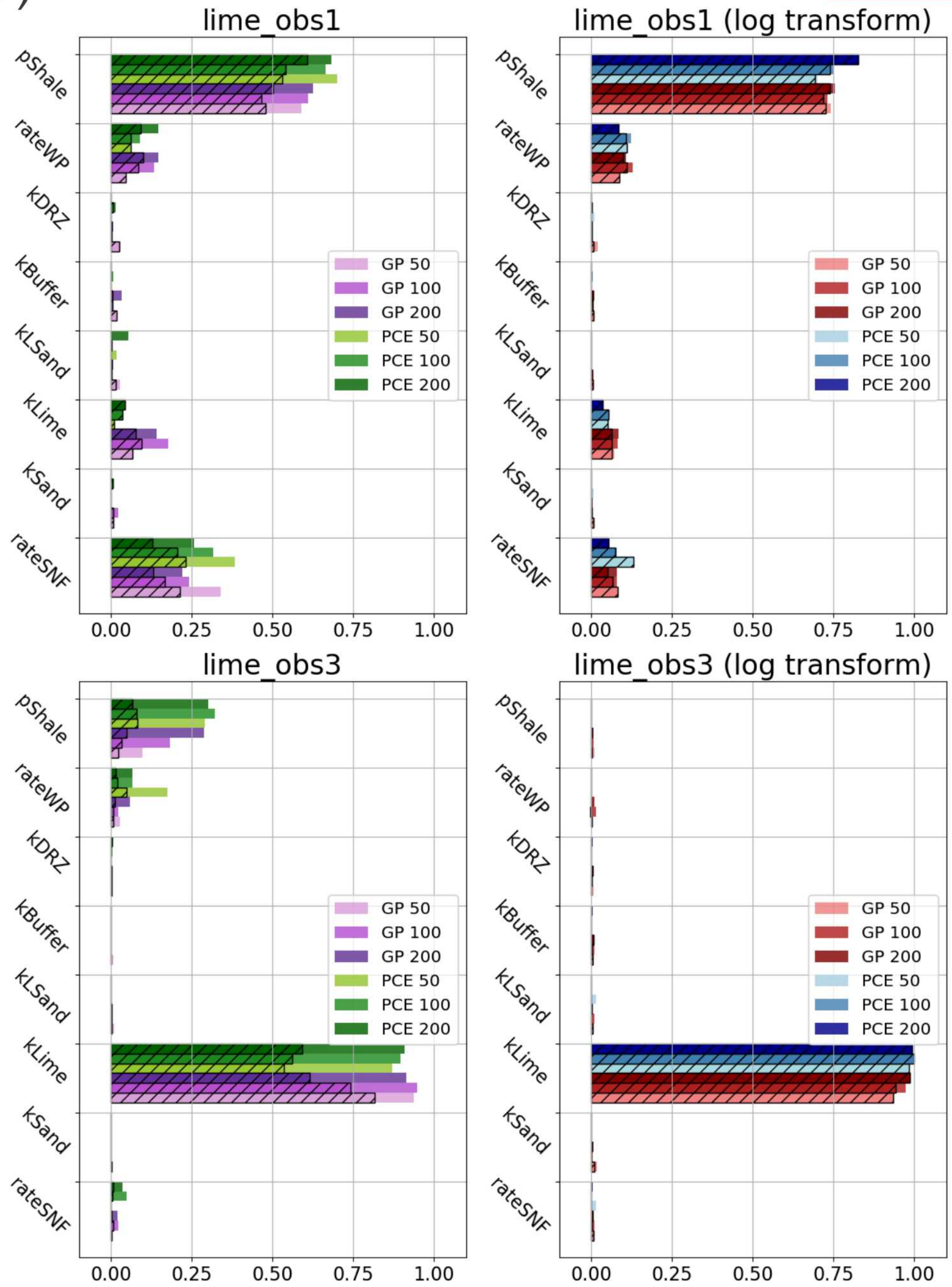


Median and 5th percentile.

High-Level Analysis (Lower Aquifer)

Regardless of method and sample size:

- Max [I-129] is sensitive to the porosity of the shale host rock (pShale).
- Further from the repository, max [I-129] is sensitive to the permeability of the aquifer.
- $S_T \sim 0$ for kDRZ, kBuffer indicates values of these variables could be fixed without changing variance of the output.



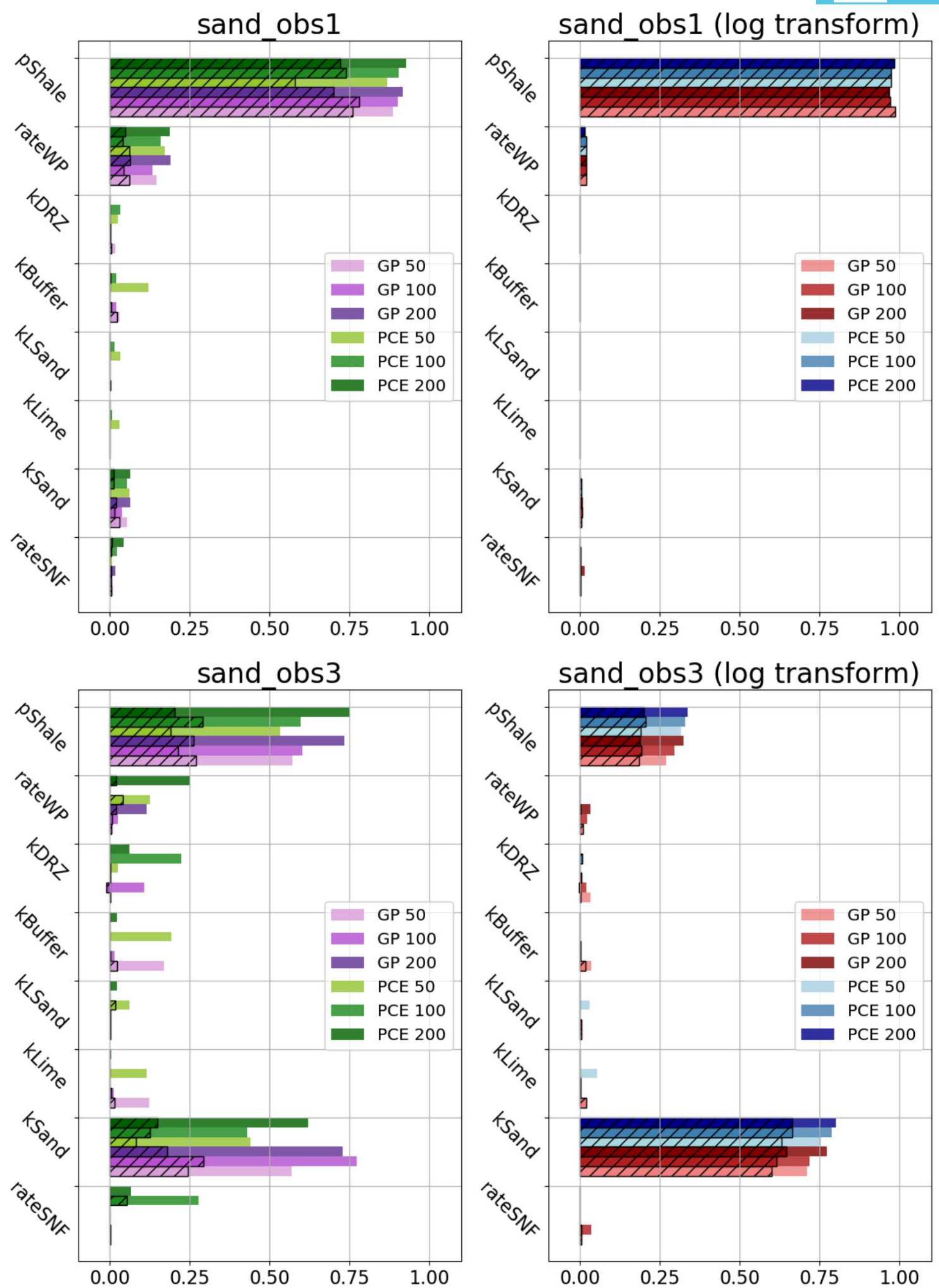
A Closer Look (Upper Aquifer)

Using the log-transform

- S_j and S_T of more influential input variables are (generally) larger
- S_j and S_T of less influential input variables are (generally) smaller
- $\sum S_j$ accounts for a larger fraction of the variance in the output
- Consistent S_j and S_T
- Sample size of 50 may be large enough to reliably estimate sensitivity indices.

Using raw [I-129]

- Greater sensitivity to waste package degradation rate (rateWP).
- Inconsistent S_j and S_T
- Sample size of 200 may not be large enough to reliably estimate sensitivity indices.



Conclusions

- Using log-transformed concentration results in larger sensitivity indices for more influential input variables, smaller sensitivity indices for less influential input variables, and more consistent estimates of sensitivity indices between methods (PCE and GP) and between analyses repeated with samples of different sizes.
- However, sensitivity indices calculated using raw concentrations identify sensitivity to input variables and variable interactions that the log-transformed results do not, perhaps because sensitivity indices calculated using raw concentrations discriminate amongst influences contributing to variance at the upper end of the concentration range.

QUESTIONS?

Thanks to the DOE NE-8 Spent Fuel and Waste Science and Technology campaign for supporting development of GDSA Framework.

References

1. A. SALTELLI et al., *Global Sensitivity Analysis. The Primer.* John Wiley & Sons, Ltd., England (2008).
2. B. M. ADAMS et al., *Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.8 User's Manual.* SAND2014-4253. Sandia National Laboratories, Albuquerque, NM (2018).
3. A. SALTELLI et al., 2010. "Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index". *Computer Physics Communications*, 181(2), 259-270 (2008).
4. B. SUDRET, "Global sensitivity analysis using polynomial chaos expansions". *Reliability Engineering & System Safety*, 93(7), 964-979 (2008).
5. V. G. WEIRS et al., "Sensitivity analysis techniques applied to a system of hyperbolic conservation laws". *Reliability Engineering & System Safety*, 107, 157-170 (2012).
6. L. LE GRATIET, L., S. MARELLI and B. SUDRET, "Metamodel-Based Sensitivity Analysis: Polynomial Chaos Expansions and Gaussian Processes," in R. Ghanem et al. (Eds.), *Handbook of Uncertainty Quantification* (pp. 1289-1325), Springer International Publishing, Switzerland (2017).
7. D. BECKER et al., Proceedings of the International High Level Waste Conference, Knoxville, TN, April 14-18 (2019).
8. P. E. MARINER et al., *Advances in Geologic Disposal System Modeling and Shale Reference Cases.* SFWD-SFWST-2017-000044 / SAND2017-10304R. Sandia National Laboratories, Albuquerque, NM (2017).
9. P. C. LICHTNER et al., PFLOTRAN User Manual, http://www.documentation.pflotran.org, 2018.
10. J. C. HELTON and F. J. DAVIS, "Latin hypercube sampling and the propagation of uncertainty in analyses of complex systems". *Reliability Engineering & System Safety,* 81(1), 23-69 (2003).
11. C. J. SALLABERRY, J.C. HELTON, and S. A. HORA, "Extension of Latin Hypercube Samples with correlated variables." *Reliability Engineering & System Safety,* 93(7), 1047-1059 (2008).