

Surrogate Modeling of Spatially Heterogeneous Source Terms for Probabilistic Assessment of Repository Performance



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How Can We Include the *Spatial Heterogeneity* of Numerous Complex Sources?

- Thousands of sources over a large area
- Slow source term process model
- Hundreds of realizations

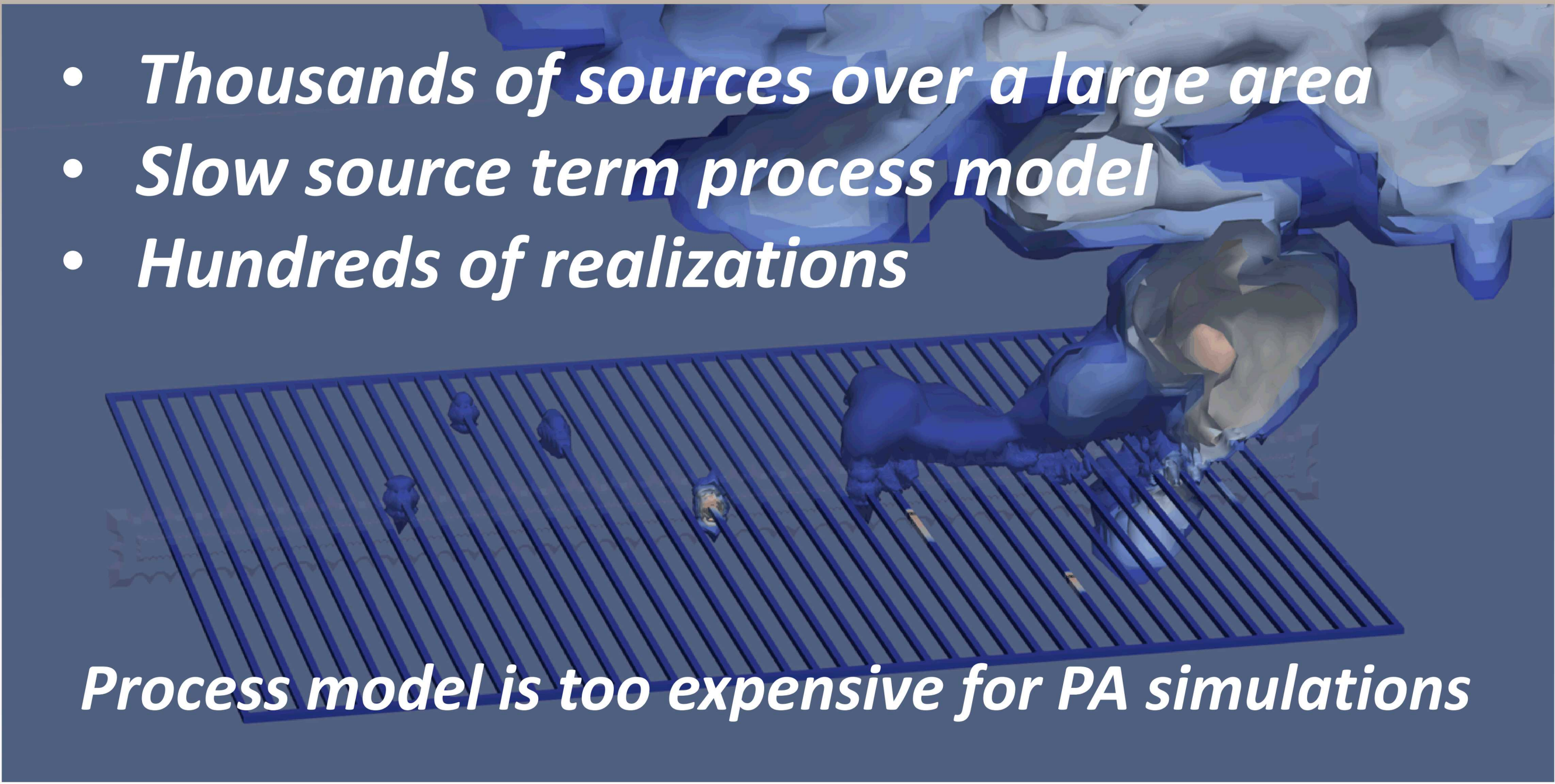


Figure 1. PFLOTRAN simulation of ¹²⁹I plumes in a crystalline rock nuclear waste repository containing 3360 waste packages.

→ Surrogate Models

Testing three source term surrogate models:

- Polynomial regression
- Artificial neural network regression
- k-nearest neighbors regression (kNNr)

Process Models & Codes

Fuel Matrix Degradation (FMD) Model

- Radiolysis, oxidation of H₂ via noble metal particle (NMP) catalyst, growth of the alteration layer, 1-D reactive transport and diffusion through the alteration layer



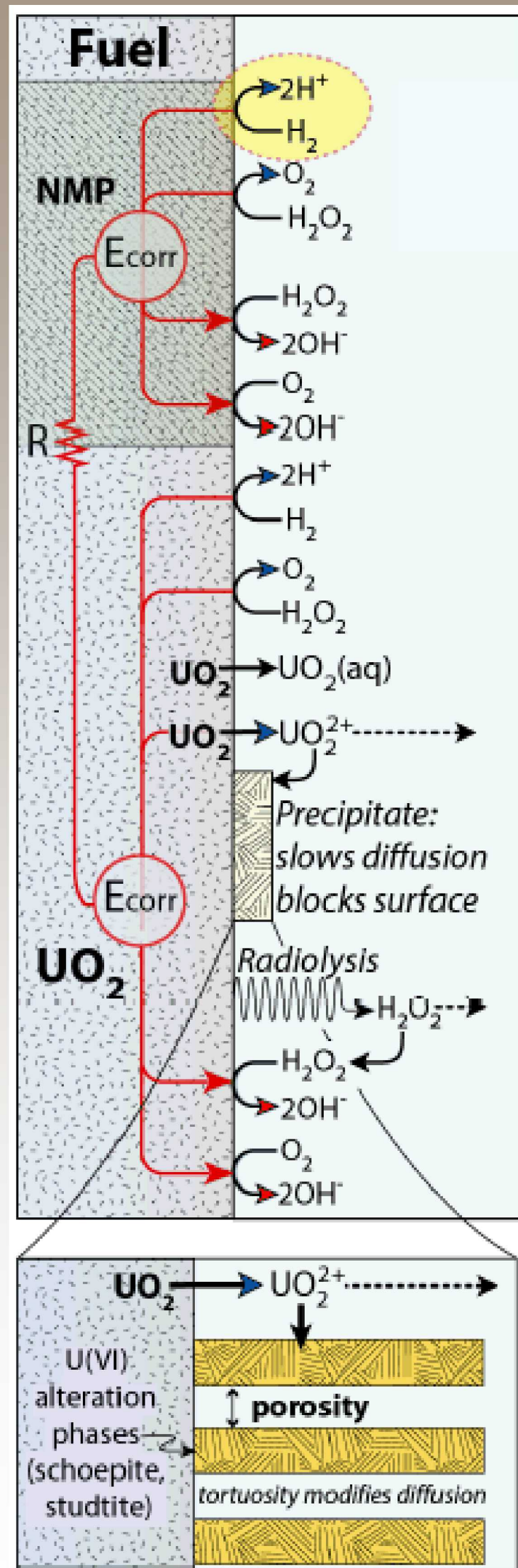
- Thermal-hydrological flow and transport through geologic media



- Uncertainty sampling – multiple realizations
- Parametric surrogate model development
 - Polynomial and neural network



- kNNr surrogate model development



(Figure adapted from Jerden et al. 2017)

Training/Testing Data

Table 1. Performed thousands of process model simulations to define the 6-D response surface.

Parameter	Distribution	Minimum	Maximum
Temperature (C)	Uniform	298	373
Burnup (Gwd/MTU)	Uniform	20	90
Environmental CO ₃ ²⁻ (mol/m ³)	Log-uniform	10 ⁻⁶	10 ⁰
Environmental O ₂ (mol/m ³)	Log-uniform	10 ⁻⁶	10 ⁻¹
Environmental Fe ²⁺ (mol/m ³)	Log-uniform	10 ⁻⁶	10 ⁻⁵
Environmental H ₂ (mol/m ³)	Log-uniform	10 ⁻⁶	10 ⁻¹

Accurate & Fast

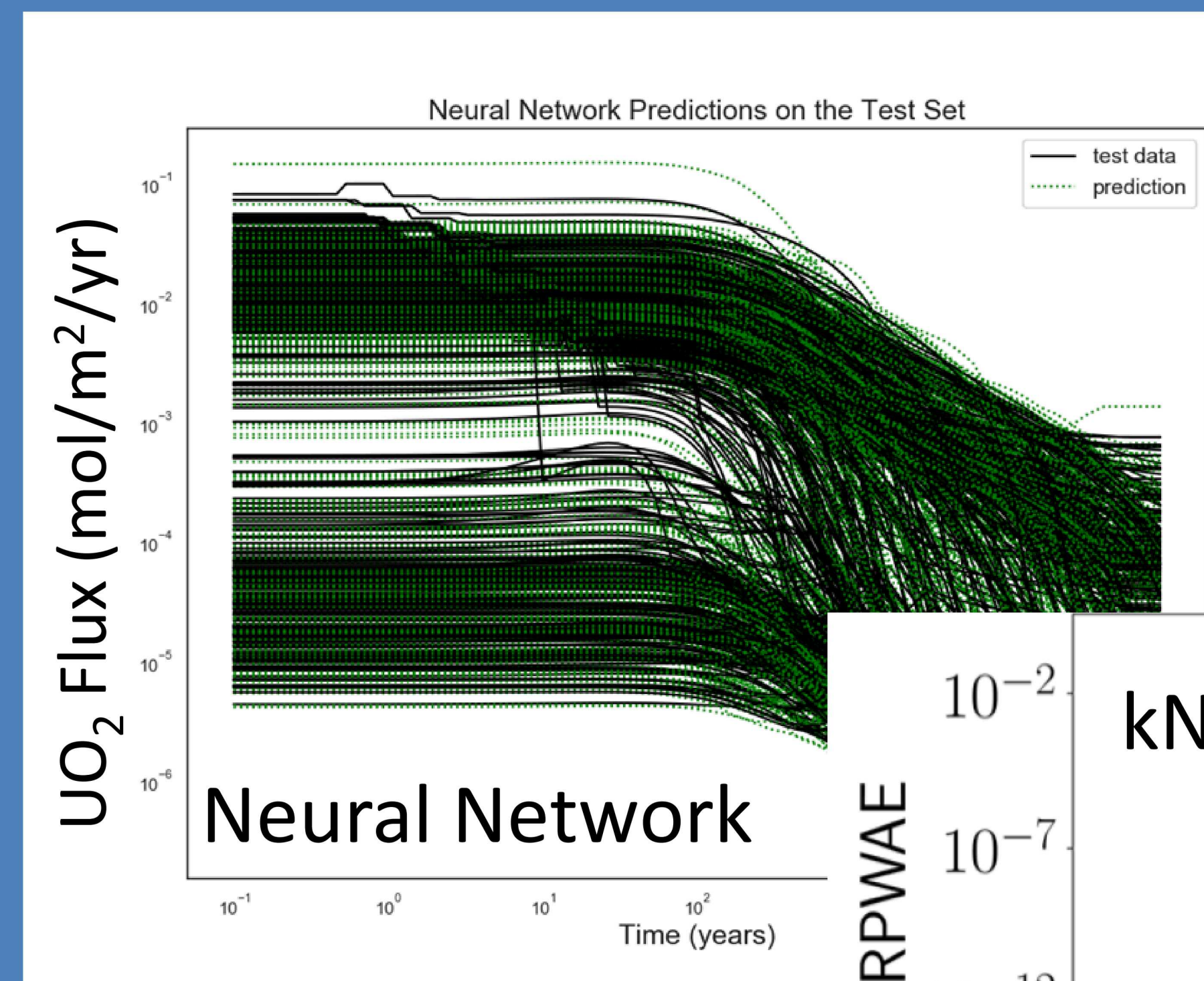


Figure 2. Neural network and kNNr surrogate results compared to test data from the FMD process model.

$$RPWAE = \frac{|y_{pred} - y_{true}|}{y_{true}}$$

Relative pointwise absolute error

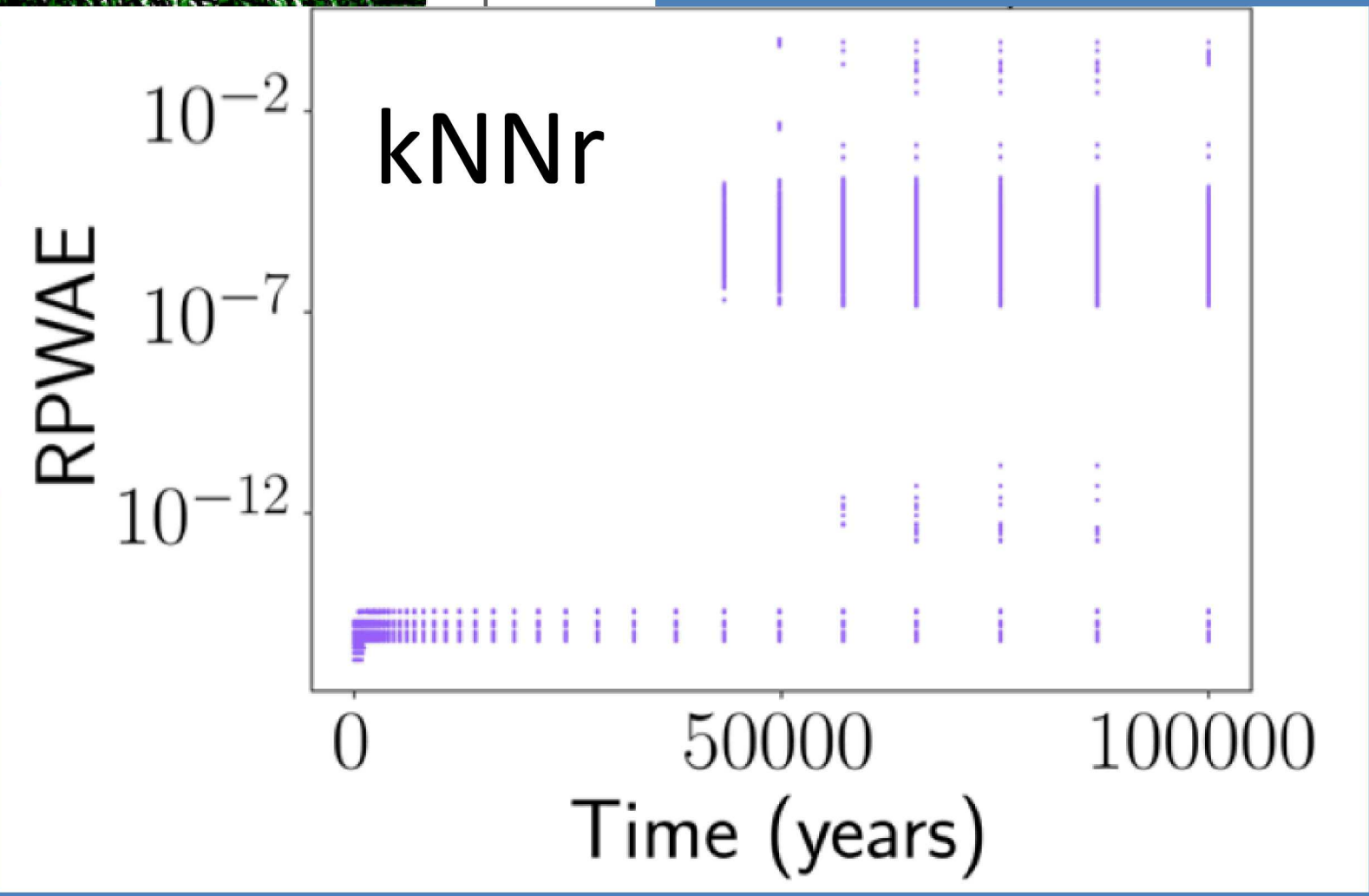


Table 2. Surrogate accuracy comparison (as of 2019).

Surrogate	Terms / Coeffs.	Train Set Size (Runs)	Train R ²	Train Mean RPWAE	Test R ²	Test Mean RPWAE
Polynomial (order 5)	462	1908	0.952	0.858	0.942	0.898
Neural Network	801	1908	0.978	0.40	0.972	0.635
kNNr (k=7)	NA	15169	NA	NA	NA	1 × 10 ⁻⁵

Benefits of a Surrogate Model

- Can calculate a custom UO₂ dissolution rate for each waste package in a probabilistic repository performance assessment (PA) as a function of local conditions at each time step
 - Highly accurate vs. process model (e.g., kNNr above)
- Tremendous speed up (e.g., ~200x faster than process model)
 - Also avoids potential process model convergence issues in PA calculations
- Surrogate model development helps vet the process model
- Capturing source term heterogeneity improves repository PA

References

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