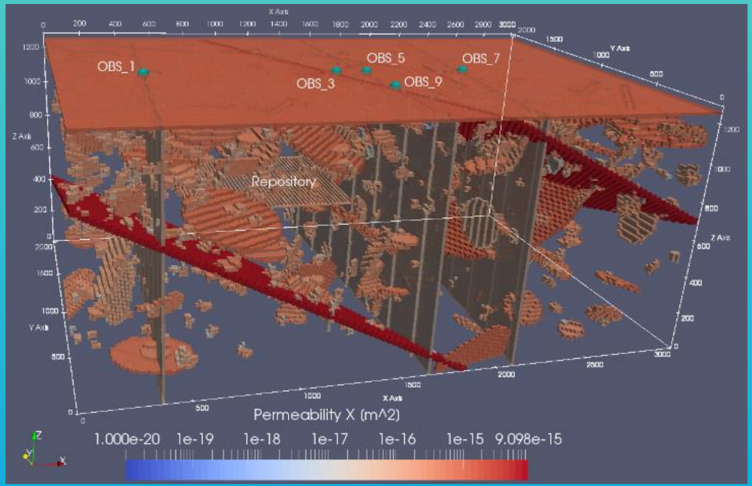


Integration of the Fuel Matrix Degradation Model (embedded)

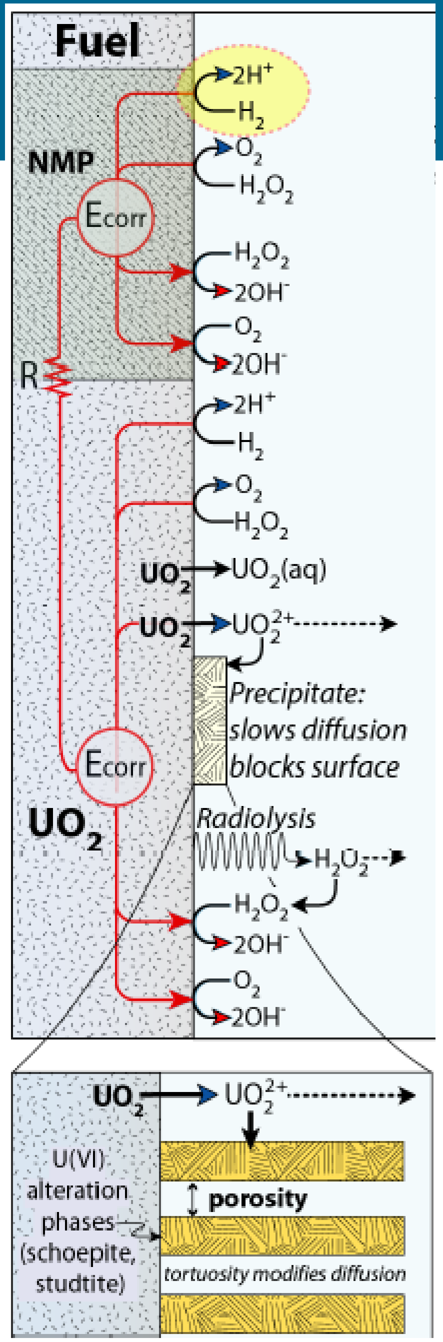
U.S. Nuclear Waste Technical Review Board
Fall Workshop
November 3-4, 2021

Paul Mariner
Sandia National Laboratories

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and 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.
SAND2021-13705 PE

Outline

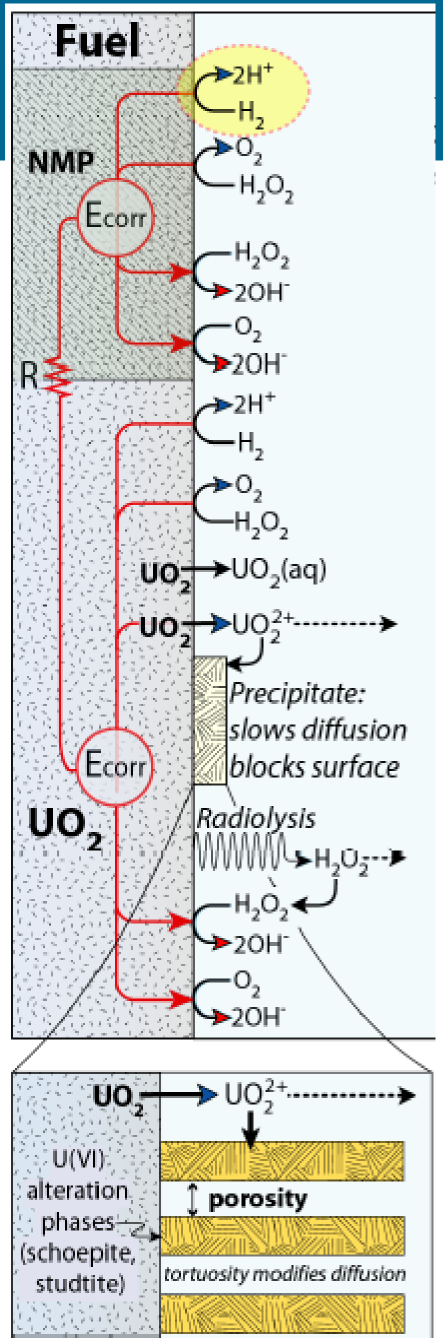
- Fuel Matrix Degradation (FMD) process model
- Motivation for surrogate
- Surrogate approach
- Results and future plans



(Jerden et al. 2017)

Fuel Matrix Degradation (FMD) Process Model

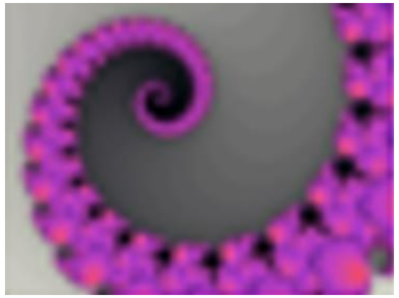
- Complex set of processes
  - Radiolysis
  - Aqueous and surface kinetic reactions
  - Oxidation of H_2 via noble metal particle (NMP) catalyst
  - Growth of an alteration layer
  - 1-D reactive transport through alteration layer
  - Diffusion of reactants and products through the alteration layer
- Expensive to run



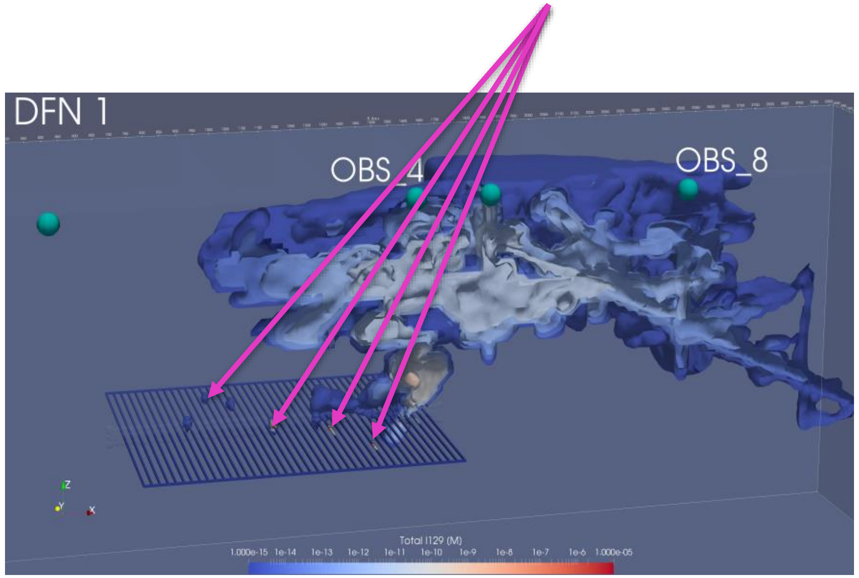
(Jerden et al. 2017)

Motivation for FMD Surrogate Model

Process model



Surrogate model

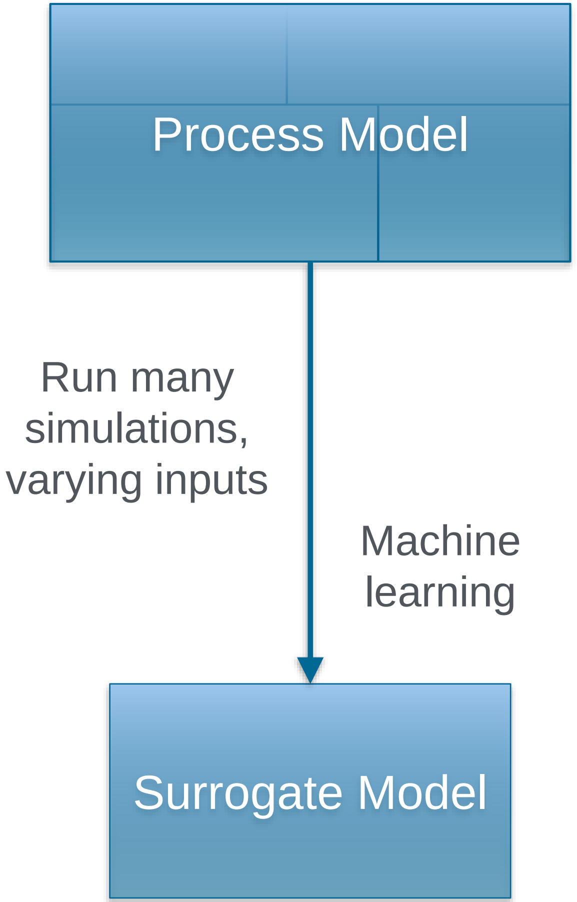


Performance assessment (PA) model

- Fuel degradation rates
  - Change by orders of magnitude
  - Highly sensitive to local conditions (temperature, burnup, dose rate, concentrations of H_2, O_2, Fe^{2+} and CO_3^{2-})
- Performance metrics highly sensitive to fuel degradation rates
- Process model too expensive to run on individual waste packages

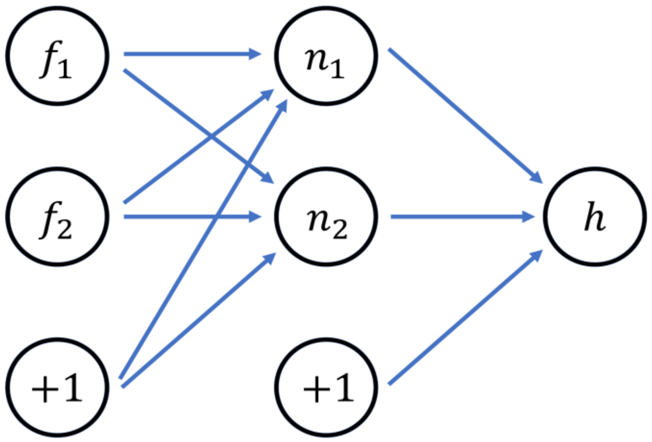
Surrogate Models

- Process models
  - Simulation of system components and the physical processes governing their interactions
- Surrogate models
  - Prediction of system output values from system input values
  - Examples
    - Lookup table
    - K-Nearest Neighbors regression
    - Polynomial regression
    - Artificial Neural Network

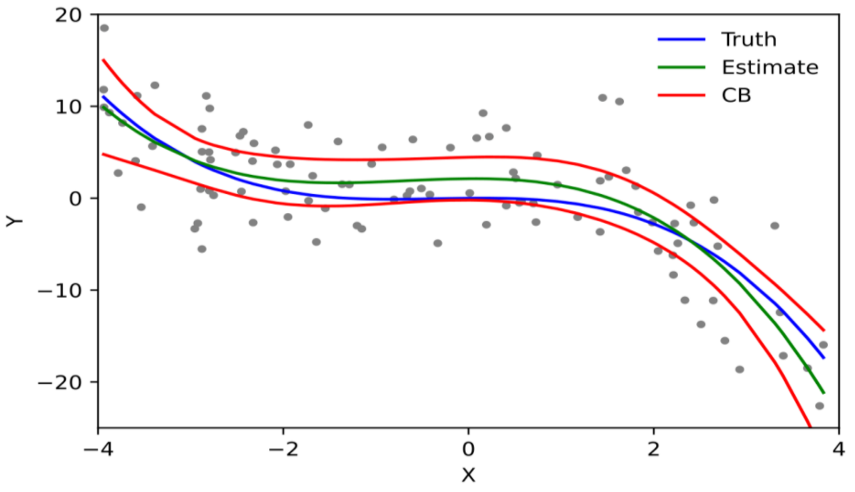


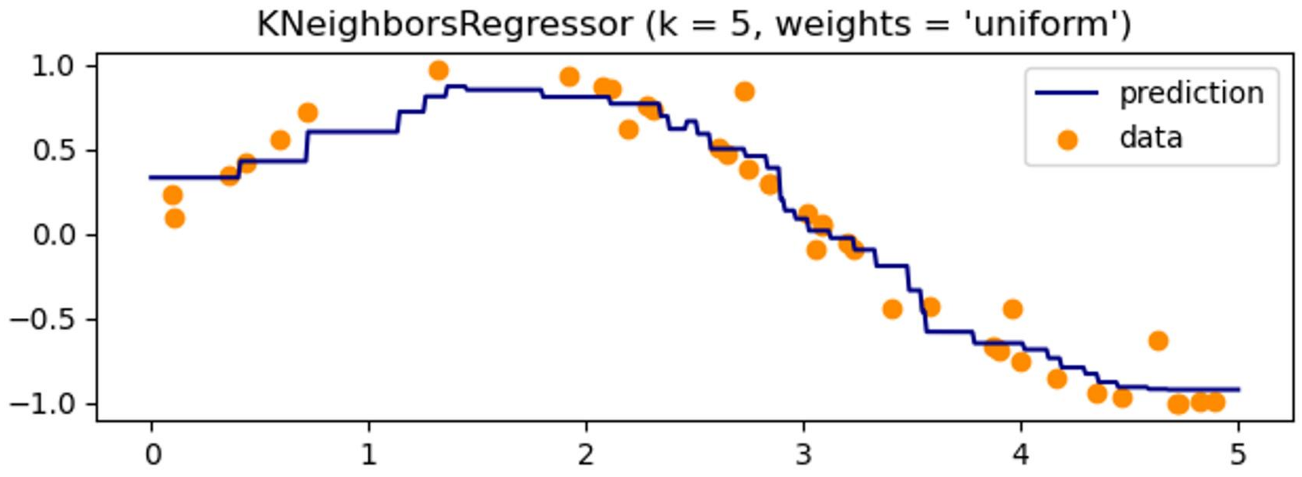
Surrogate Model Approaches

- Three FMD surrogate models tested
  - Artificial Neural Network (ANN)
  - K-Nearest Neighbors (kNNr)
  - Polynomial regression



Single layer feed-forward neural network with 2 input features and 2 neurons in the hidden layer





Development and Integration of Surrogate Models

- Surrogate training/testing data
  - Generated from Matlab process model
  - Latin Hypercube Sampling (LHS)
    - 30,000 runs (samples), 100 points per run
  - 3,000,000 training data points
  - 300,000 test data points
- PFLOTRAN integration
  - Artificial Neural Network (ANN)
    - Trained coefficients read in from file
    - Direct calculation
  - K Nearest Neighbors (kNNr)
    - Scan search tree for k nearest neighbors (e.g., k = 250)
    - Calculate response using inverse distance rule

Input Features	Training/Testing Range
Initial Temp. (K)	298 – 393
Fuel Burnup (GWd/MTHM)	20 – 70
CO_3^{2-} (mol/m^3)*	$10^{-4} – 10^{-1}$
O_2 (mol/m^3)*	$10^{-7} – 10^{-3}$
Fe^{2+} (mol/m^3)*	$10^{-3} – 10^{-2}$
H_2 (mol/m^3)*	$10^{-7} – 10^{-1}$

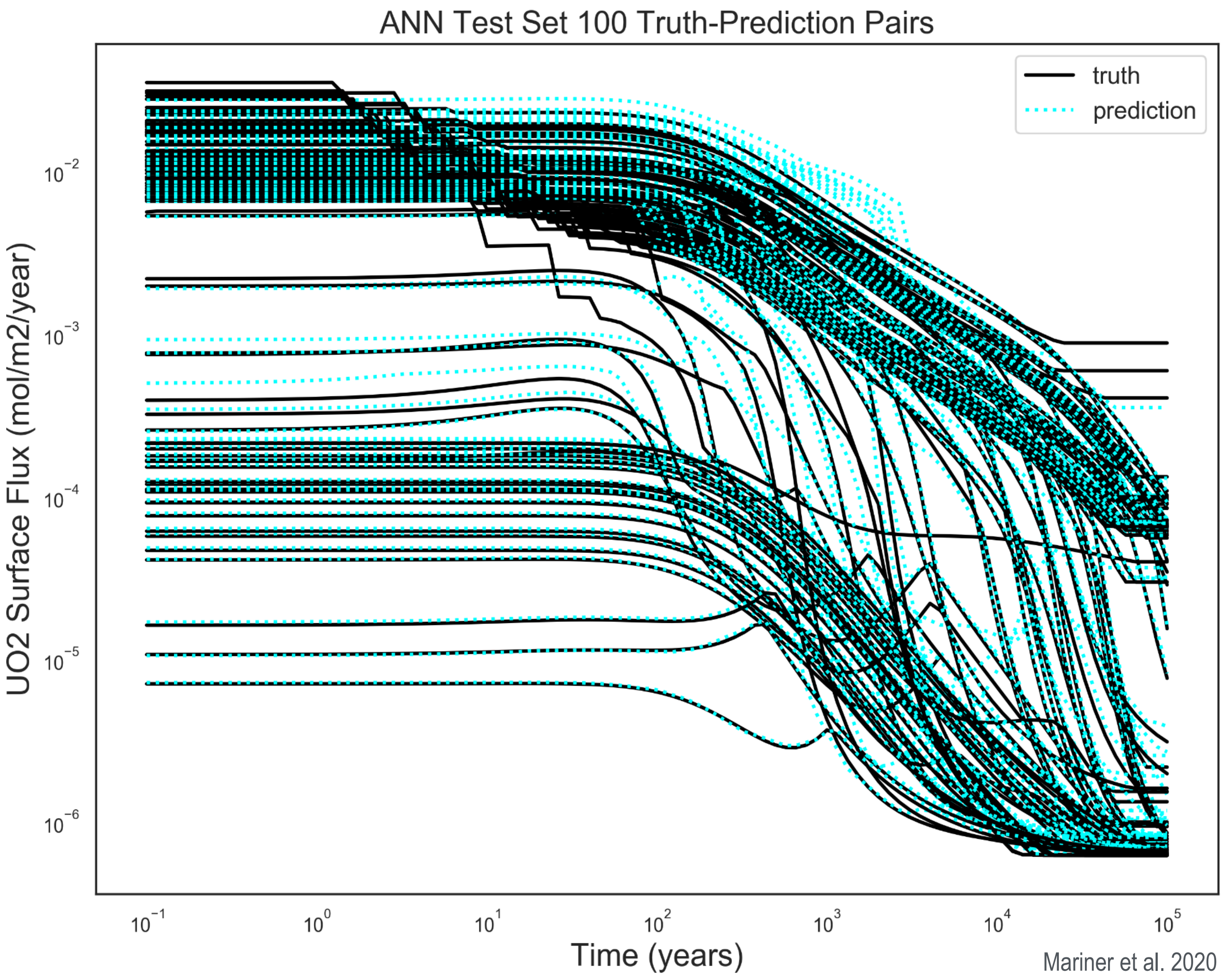
* Log-uniform sampling distribution

Mariner et al. 2020

Surrogate Performance – Accuracy

- Trained surrogates tested against independently generated test data
- ANN and kNNr error much lower than polynomial surrogate error

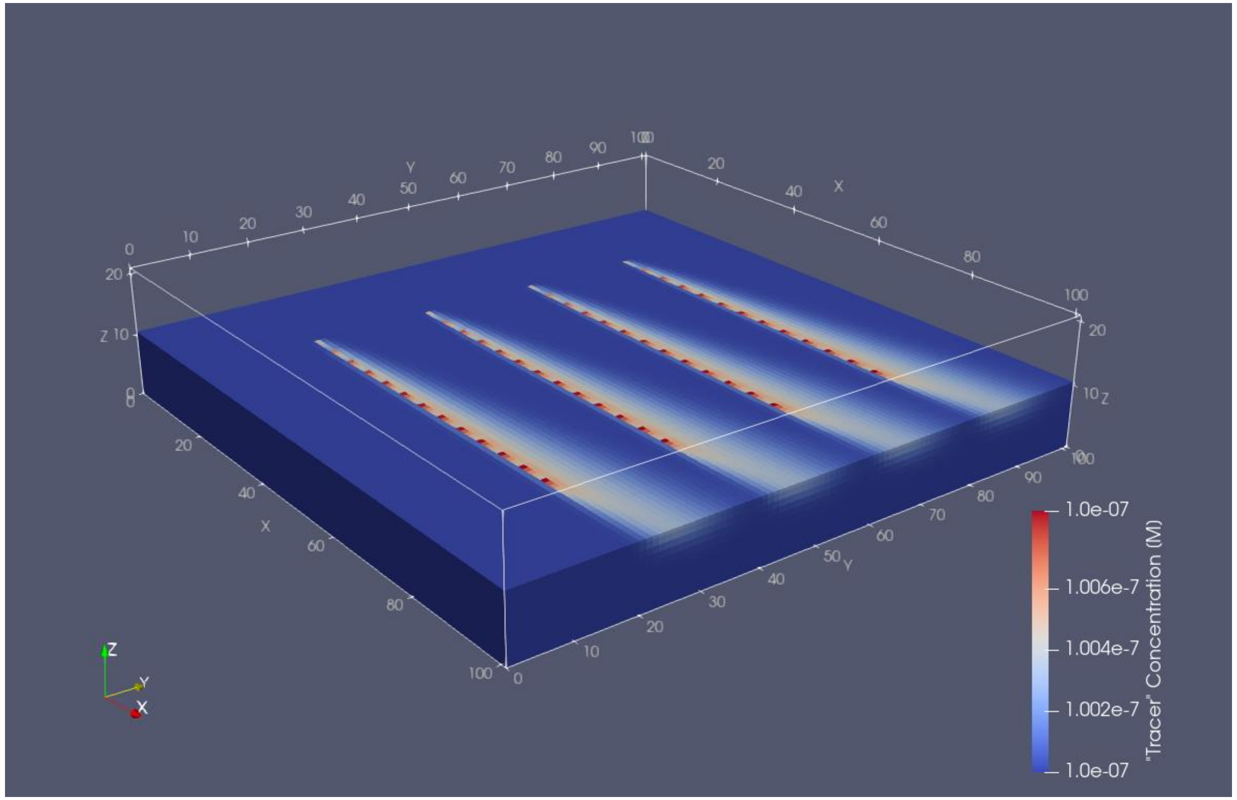
Error Metric	ANN (2020)	kNNr (2020)
Mean Square Error $(mol/m^2/yr)^2$	3.56e-6	5.95e-6
Mean Absolute Error $(mol/m^2/yr)$	9.30e-4	1.25e-3
Mean Absolute Percentage Error	31.2%	78.4%



Mariner et al. 2020

Surrogate Performance – Speed

Test problem: 52 failed waste packages in a flow field (Mariner et al. 2015)



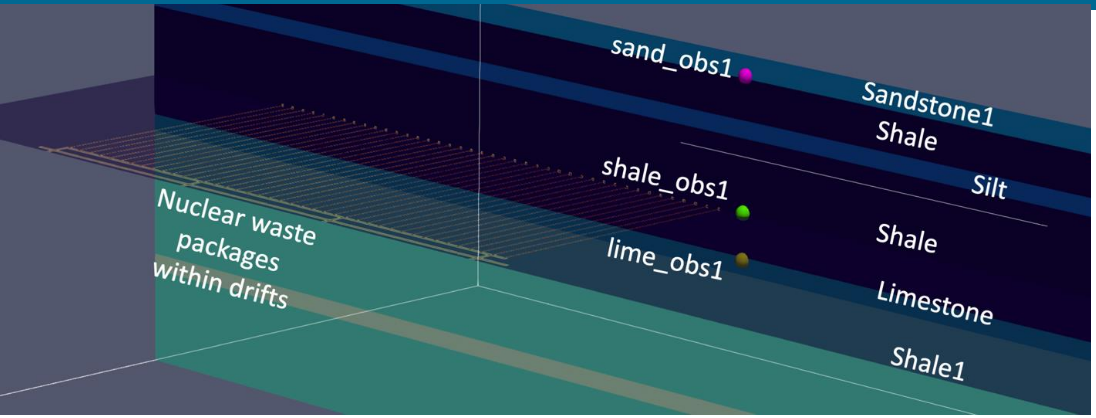
- Speedup of 30,000x (ANN) and 2,800x (kNNr) compared to 2015 coupling of process model

Compute time (sec) and speed-up factor (x)

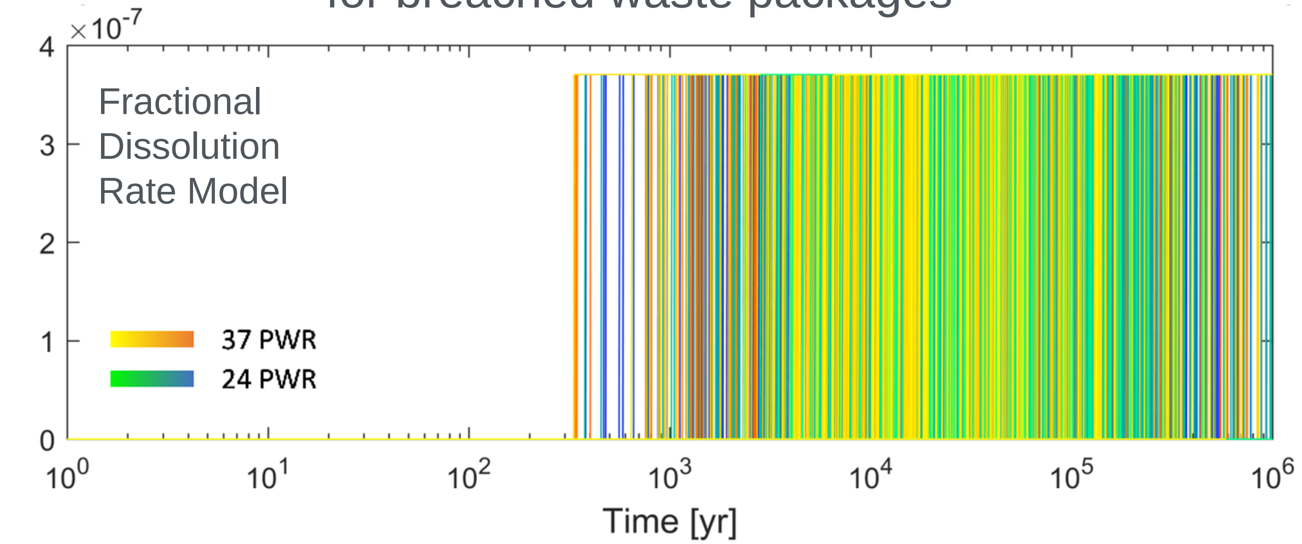
Process	Coupled Process Model (2015)	ANN (2020)	kNNr (2020)
Waste Form	1,522	0.05 (30,440x)	0.54 (2,820x)
Flow	128	61.0 (2.1x)	60.3 (2.1x)
Transport	244	147.8 (1.65x)	117.6 (2.1x)

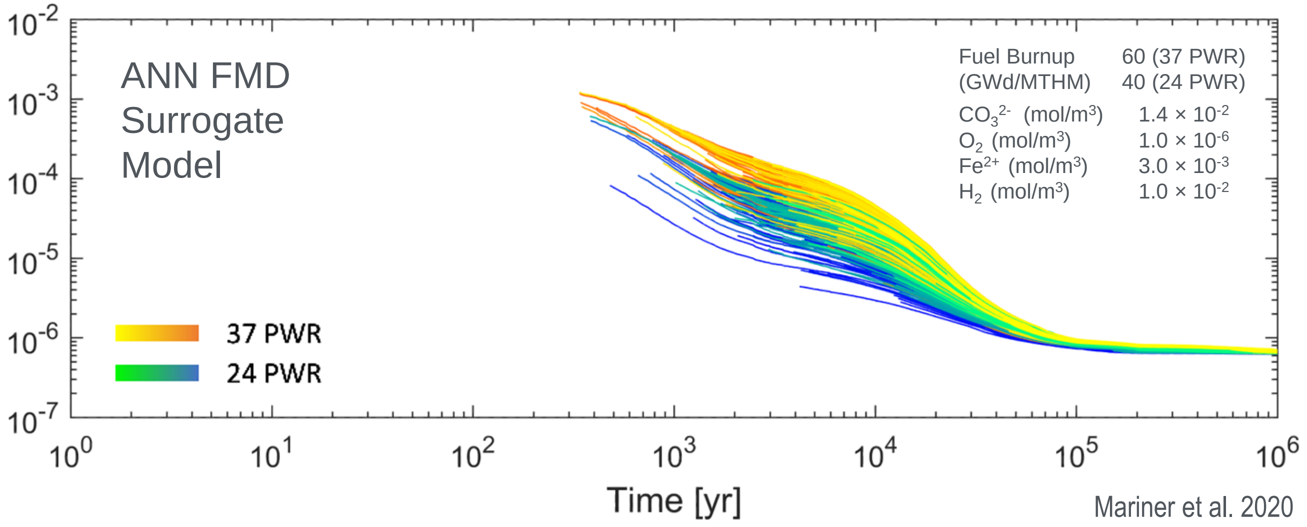
Mariner et al. 2020

Shale Reference Case Demonstration



Degradation rates (mol m^{-2} yr^{-1}) for breached waste packages





Mariner et al. 2020

- Fractional Dissolution Rate (FDR) model ignores local conditions and fuel age
- FMD accounts for fuel age and local conditions

Summary and Future Work

- Summary
  - Surrogate modeling has allowed us to emulate fuel matrix degradation processes at each waste package in full-scale reference case simulations
    - Allows accounting for local environmental conditions (temperature and chemistry) and individual burnups and dose rates
  - Artificial neural network (ANN) and k nearest neighbors regression (kNNr) are quite accurate and extremely fast
- Future work
  - Awaits the next major upgrade of the process model

References

- Jerden, J., V. K. Gattu and W. Ebert (2017). *Progress Report on Development of the Spent Fuel Degradation and Waste Package Degradation Models and Model Integration*. SFWD-SFWST-2017-000091, SFWD-SFWST-2017-000095. Lemont, Illinois, Argonne National Laboratory.
- Mariner, P.E., Berg, T.M., Chang, K.W., Debusschere, B.J., Leone, R.C., and Seidl, D.T. (2020), *Surrogate Model Development of Spent Fuel Degradation for Repository Performance Assessment*. SAND2020-10797 R. Sandia National Laboratories.
- Mariner, P.E., Gardner, W.P., Hammond, G.E., Sevougian, S.D., and Stein, E.R. (2015), *Application of Generic Disposal System Models.* SAND2015-10037R. Sandia National Laboratories.

Questions