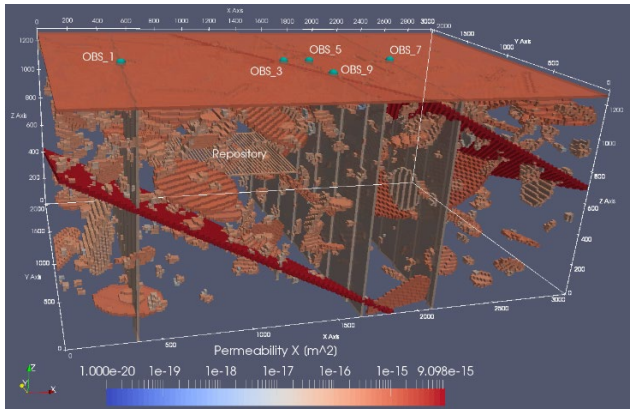

Fuel Matrix Degradation Modeling in Repository Reference Cases

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Sandia National Laboratories

Spring 2024 Fact-finding Meeting on Corrosion of Commercial Spent Nuclear Fuel

April 25, 2024

Virtual Teams Meeting

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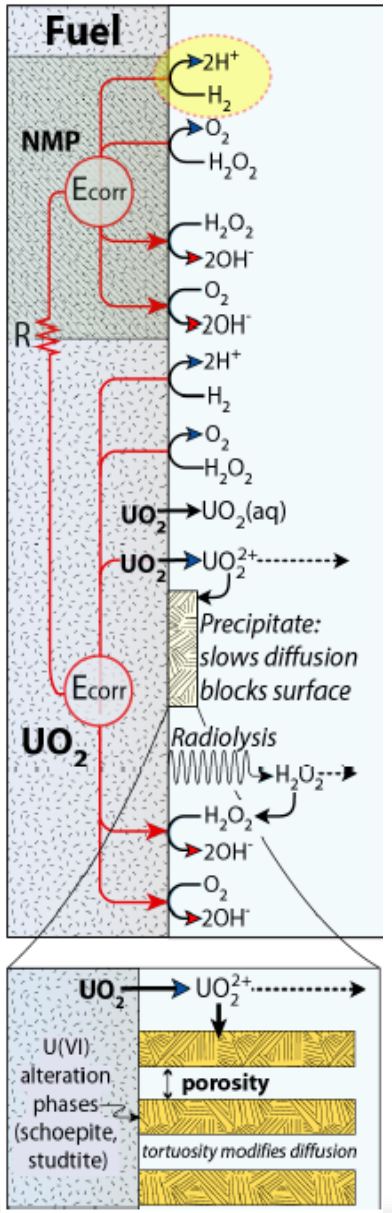
U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Spent Fuel and Waste Science and Technology (SFWST)

Outline

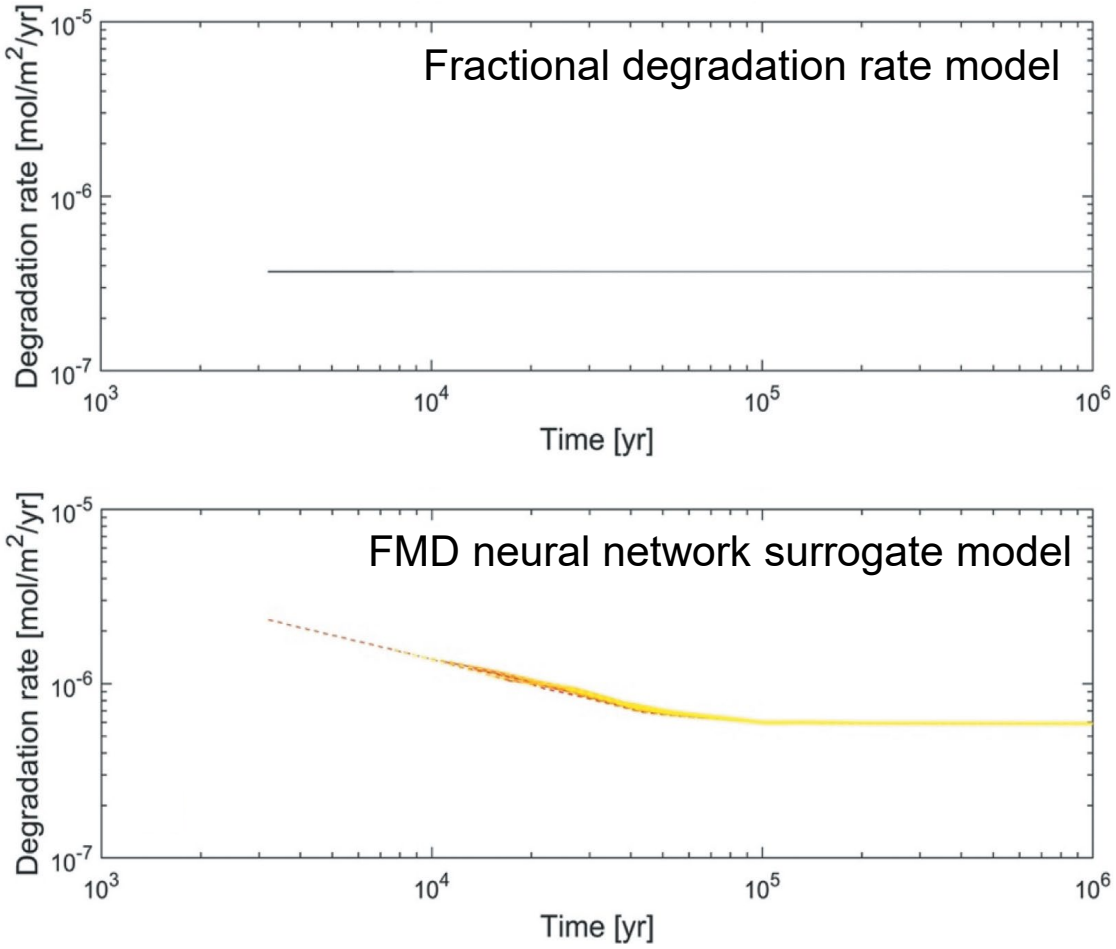
- **Fuel Matrix Degradation (FMD) in repository reference cases**
- **FMD process model surrogate approaches**



(Jerden et al. 2017)

Fuel Matrix Degradation in Repository Reference Cases

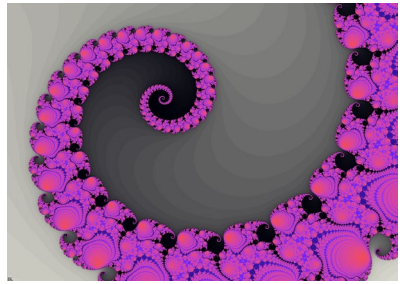
- Fractional degradation rate (FDR)
- Fuel matrix degradation (FMD) surrogate models
- Instant fuel matrix degradation
- Instant radionuclide release fractions



Fuel degradation rates calculated for 2000 failed 4-PWR waste packages in a shale repository simulation (Debusschere et al. 2023)

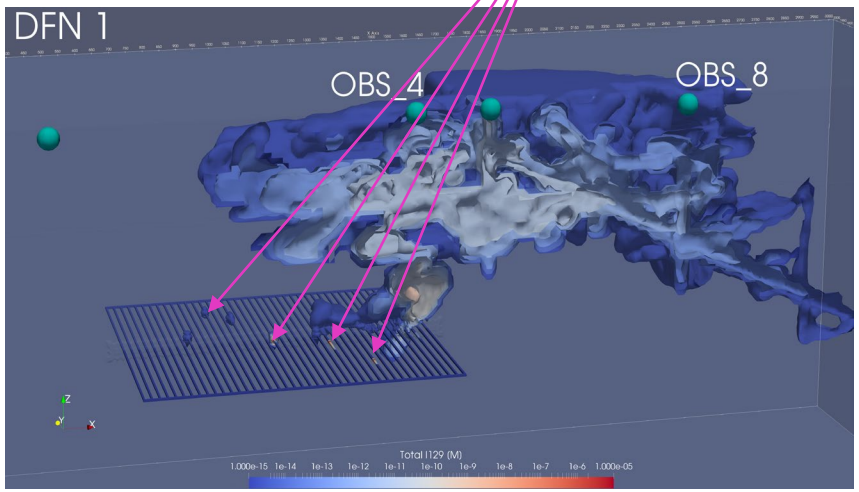
FMD Surrogate Models

- **Repository performance can be highly sensitive to fuel degradation rates**
- **Fuel degradation rates**
  - Sensitive to
    - Temperature
    - Dose rate (radiolysis)
    - H_2, O_2, Fe^{2+}, CO_3^{2-} concentrations
  - Change over repository lifetime
- **FMD process model**
  - Too expensive for repository simulations
- **FMD surrogate models**
  - Rapidly emulate the FMD process model
  - Test the operation of the FMD process model



Process model

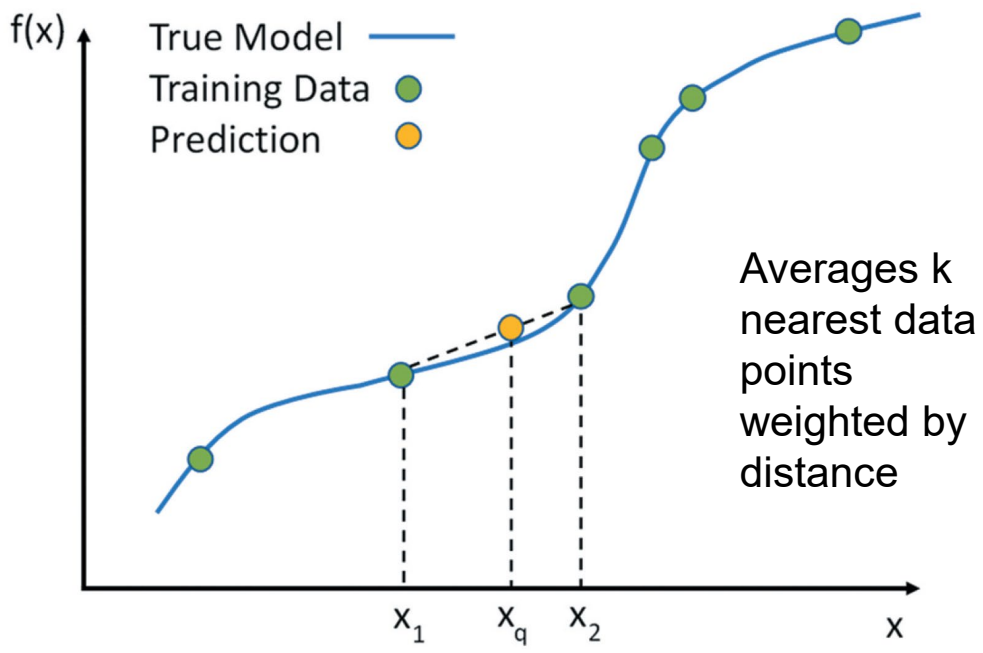
Surrogate model



Performance assessment (PA) model

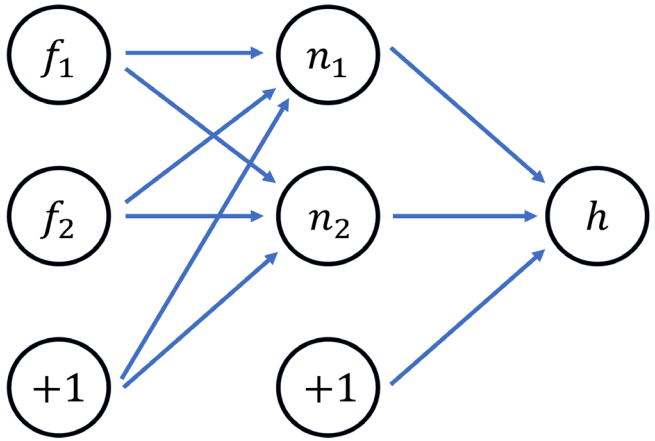
Surrogate Model Approaches

k Nearest Neighbors Regression (kNNr)



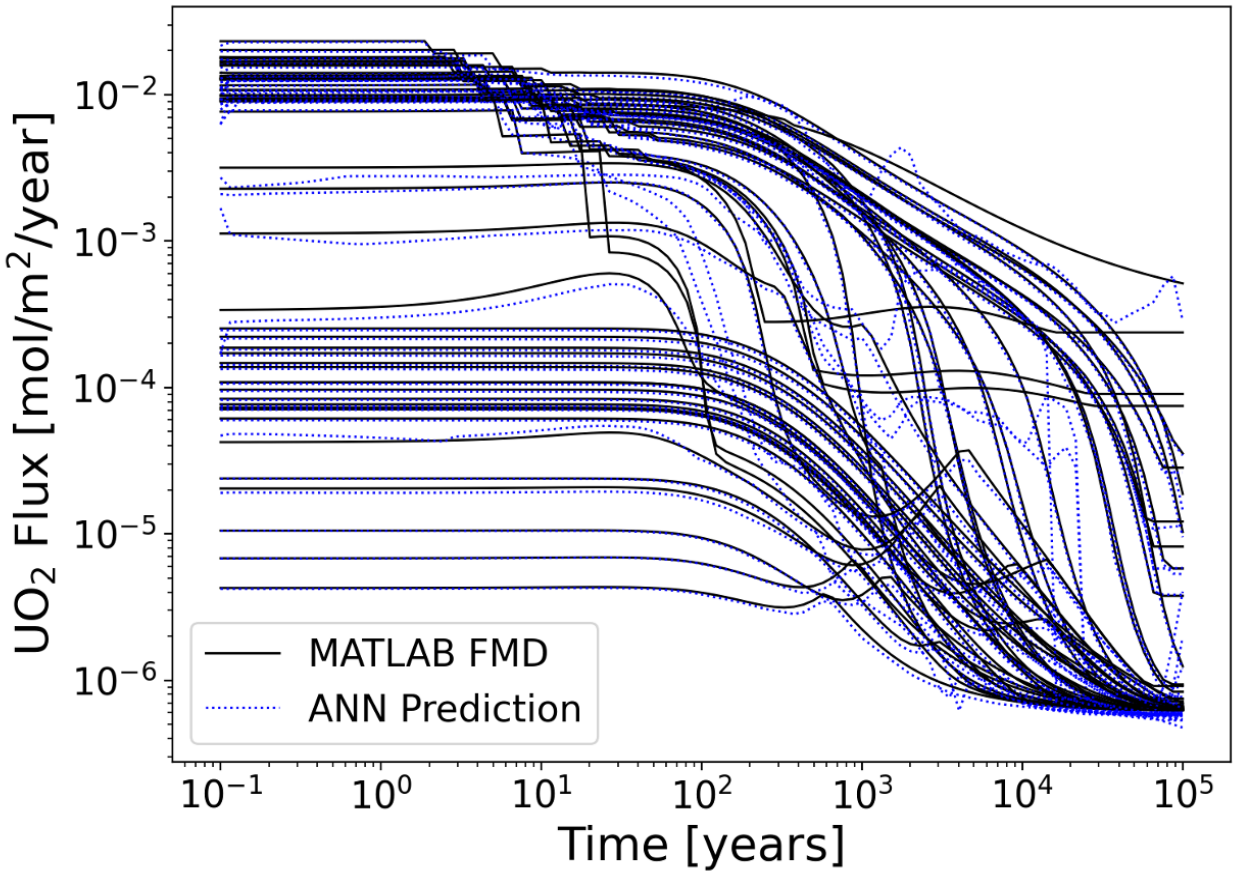
Averages k nearest data points weighted by distance

Artificial Neural Network (ANN)



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

Surrogate Accuracy



Input Ranges

Input Features	Training/Testing Range
Initial Temp. (K)	300 – 400
Fuel Burnup (GWd/MTHM)	40 – 65
Env CO_3^{2-} Conc (mol/m^3)*	10^{-3} – 2×10^{-2}
Env O_2 Conc (mol/m^3)*	10^{-7} – 10^{-5}
Env Fe^{2+} Conc (mol/m^3)*	10^{-3} – 10^{-2}
Env H_2 Conc (mol/m^3)*	10^{-5} – 2×10^{-2}

* Log-uniform sampling distribution

Accuracy

Error Metric	kNNr	ANN
Normalized Mean Square Error	0.11	0.12
Mean Absolute Percentage Error	29%	14%

Mariner et al. 2023

References

- Debusschere, Bert J., D. Thomas Seidl, Timothy M. Berg, Kyung Won Chang, Rosemary C. Leone, Laura P. Swiler & Paul E. Mariner (2023). Machine Learning Surrogates of a Fuel Matrix Degradation Process Model for Performance Assessment of a Nuclear Waste Repository, *Nuclear Technology*, 209:9, 1295-1318, DOI: 10.1080/00295450.2023.2197666
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Questions