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# NEURAL-ODE SURROGATES FOR FUEL DEGRADATION PROCESSES IN NUCLEAR WASTE REPOSITORY SIMULATIONS

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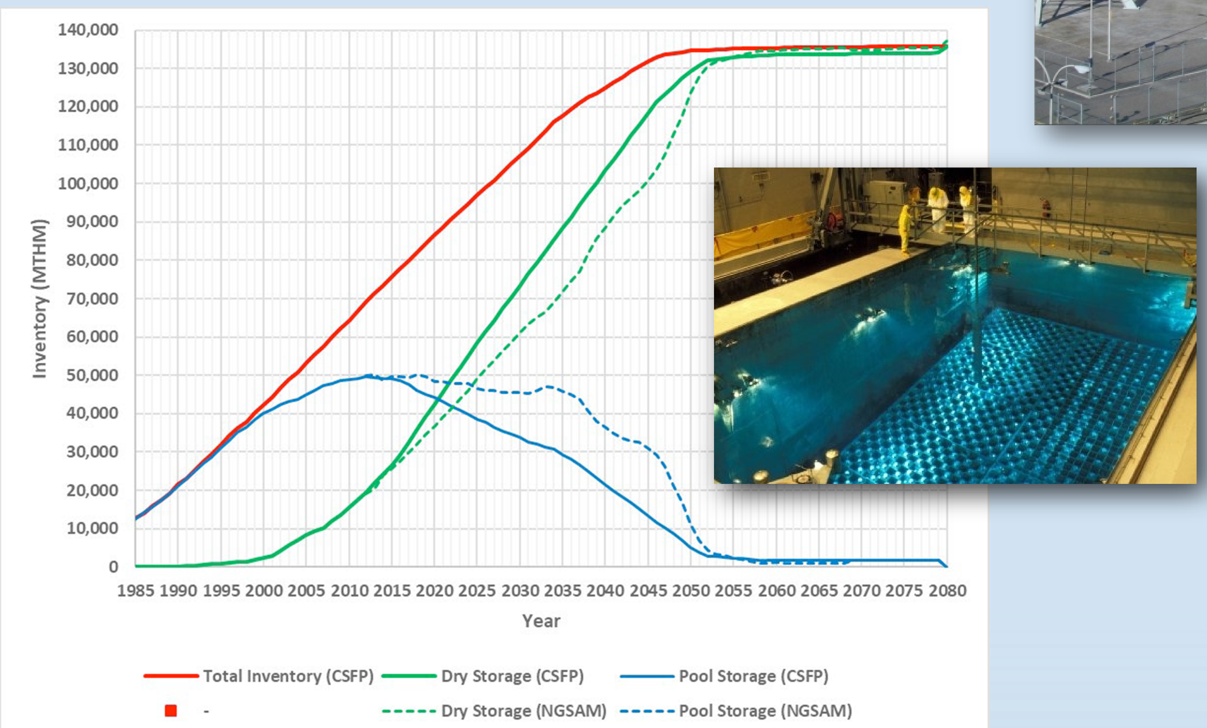
## ABSTRACT

Assessment of subsurface nuclear waste repositories requires the simulation of uranium fuel degradation in thousands of waste packages over hundreds of thousands of years. A comprehensive simulation using a detailed process model would be too computationally expensive, so we employ machine learning surrogate models. Since the internal state of the waste package is a dynamical system, we use neural ordinary differential equations (neural ODEs) to learn the dynamics rather than the system state. Then, to evaluate the system state, we use an ODE solver and the initial conditions of the waste package. We examine the accuracy of the neural-ODE surrogate's predictions of uranium flux.

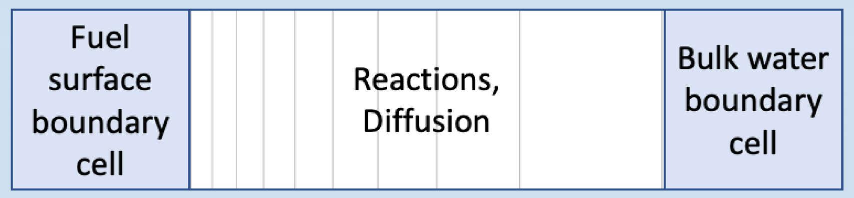

## COMPUTATIONAL MODELING OF SPENT NUCLEAR FUEL

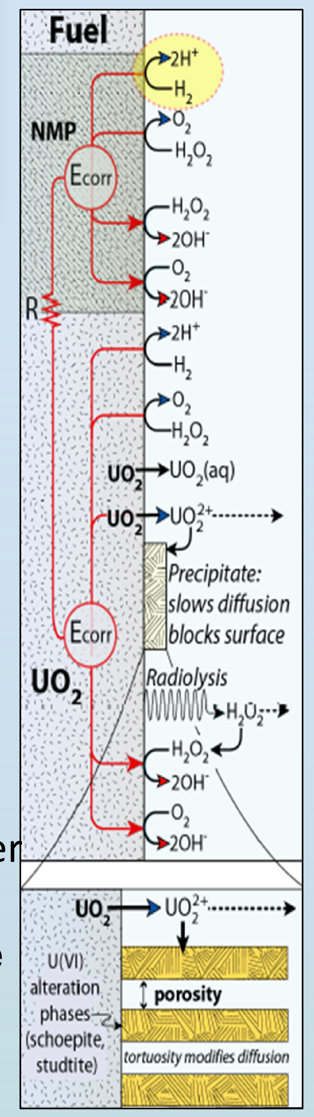
- The US inventory of spent nuclear fuel is rapidly increasing.
- Spent nuclear fuel is moving from pool storage to dry storage in underground repositories.




Freeze et al. (2021, Figure 2-3)

Jerden et al. (2015)

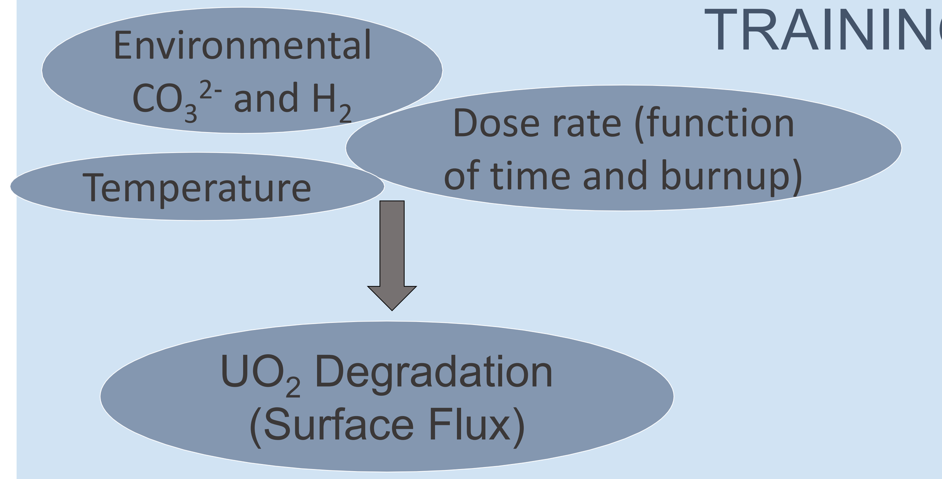


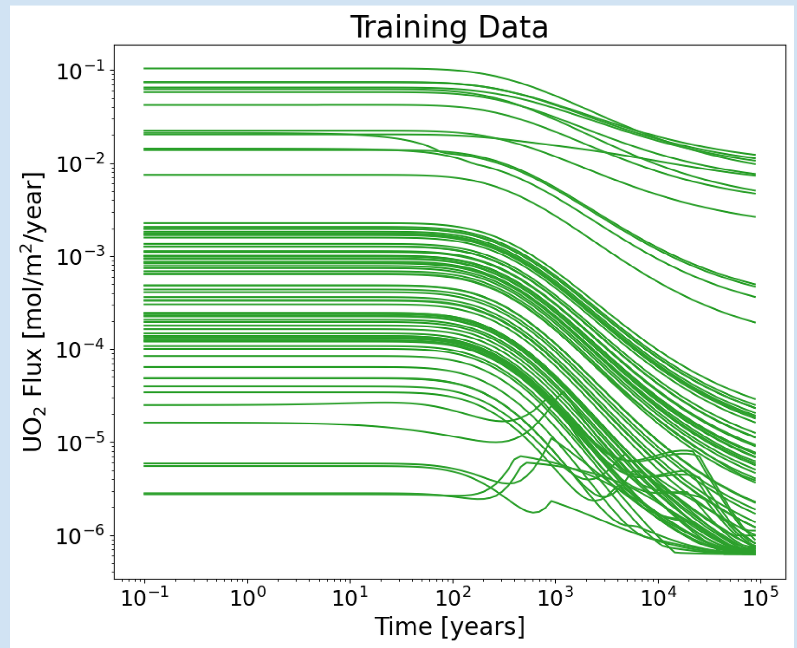

Jerden et al. (2015)

- The Fuel Matrix Degradation Model (FMDM) is a one-dimensional reactive transport model of a waste package (specifically, of water between the fuel surface and the bulk water in contact with the fuel).
- The FMD model is needed for each breached package in the repository at each time point for 100,000 years.
- It is computationally intensive to calculate the quantity of interest, $UO_2$ degradation rates.
- Surrogate models map inputs to outputs with less computational cost

## TRAINING DATA



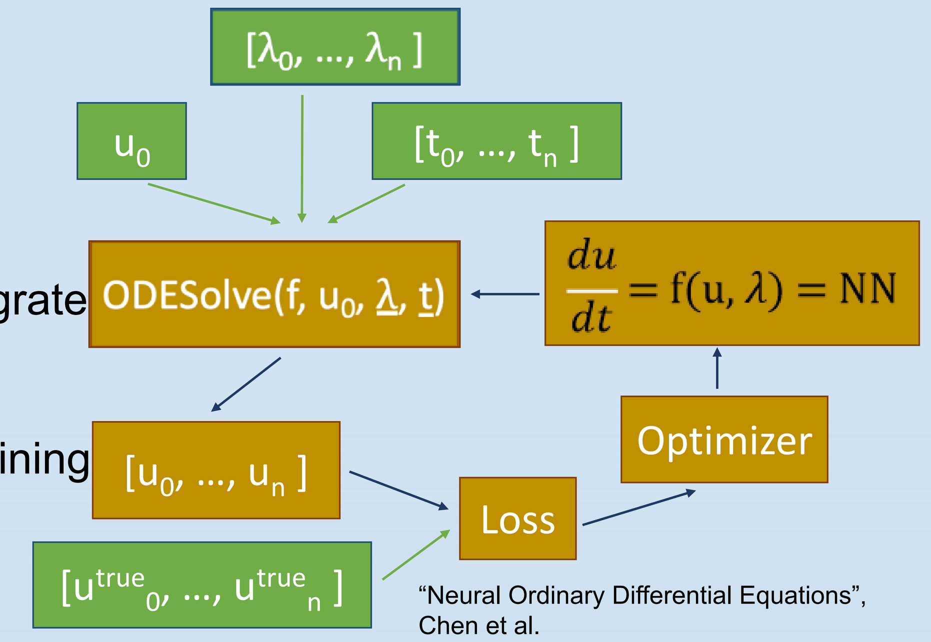

| Parameter | Distribution | Min. | Max. |
|---|---|---|---|
| Init. Temp. (K) | Uniform | 300 | 600 |
| Burnup (Gwd/MTU) | Uniform | 40 | 80 |
| Delay Time (years) | Log-uniform | $10^2$ | $10^4$ |
| Env. $CO_3^{2-}$ (mol/m³) | Log-uniform | $10^{-3}$ | $2x10^{-2}$ |
| Env. $O_2$ (mol/m³) | Log-uniform | $10^{-7}$ | $10^{-5}$ |
| Env. $Fe^{2+}$ (mol/m³) | Log-uniform | $10^{-3}$ | $10^{-2}$ |
| Env. $H_2$ (mol/m³) | Log-uniform | $10^{-5}$ | $2x10^{-2}$ |




- Process model input parameters are sampled from expected ranges in reservoir simulations to generate training data time-trajectories.

## TRAINING PROCESS

- Neural ODEs approximate the derivative of the system state as a neural network.
- We predict the system state by putting the neural network through the ODE solver.
- Random points from a trajectory are selected to serve as batch initial conditions.
- Hyperparameters to tune:
  - Learning rate
  - Number of layers
  - Number of neurons per layer
  - Number of batches (batch_size)
  - Number of time steps to predict/integrate during training (batch_time)
  - Amount of training data
  - Number of time points to use from training data
  - Choice of numerical ODE solver




"Neural Ordinary Differential Equations", Chen et al.


## REFERENCES

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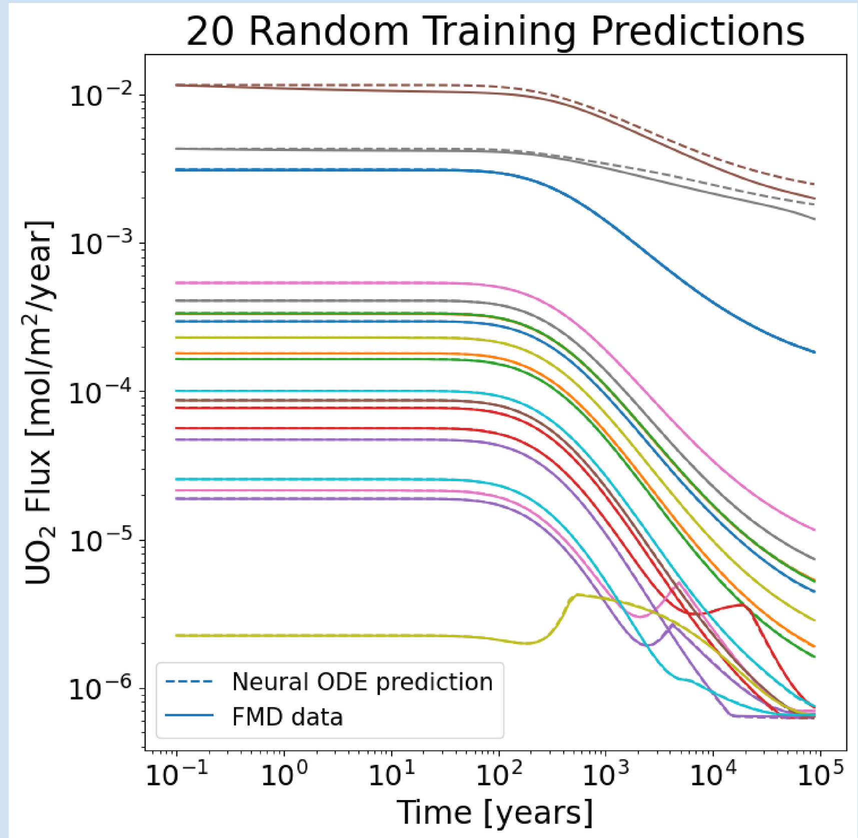
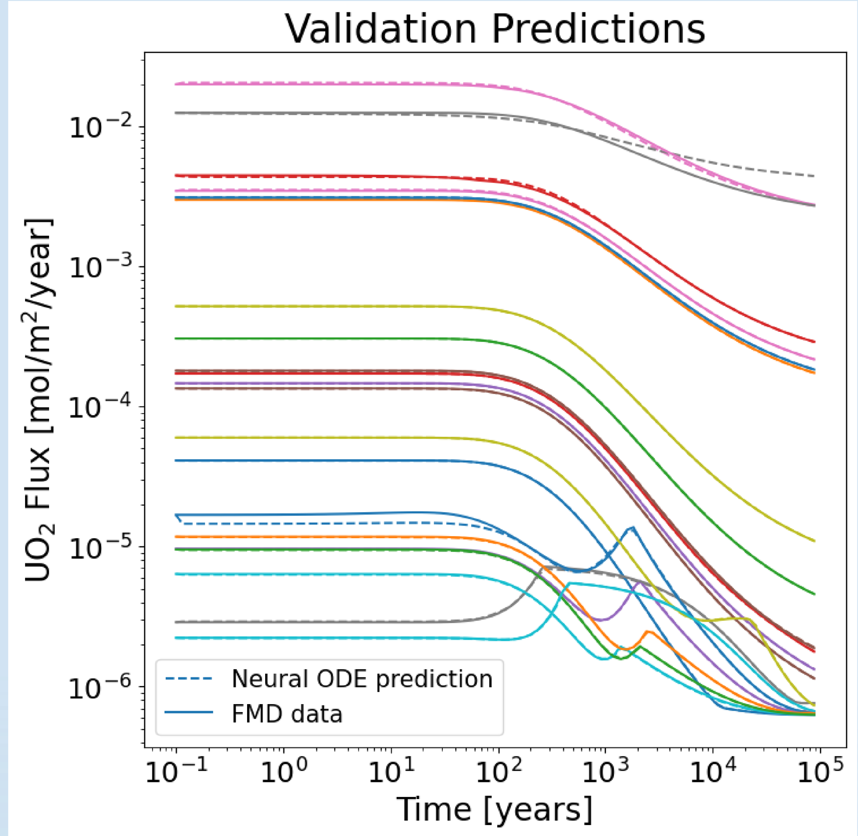
- J. Jerden, K. Frey, and W. Ebert, "A Multiphase Interfacial Model for the Dissolution of Spent Nuclear Fuel," Journal of Nuclear Materials, 462, 135, (2015)
- Chen, Ricky T. Q., Yulia Rubanova, Jesse Bettencourt, and David K. Duvenaud, "Neural Ordinary Differential Equations." Advances in Neural Information Processing Systems 31 (2018).
- J. Harvey et al.: Development of an Efficient Version of the Fuel Matrix Degradation Model, IHLRWM 22 (2022)


## RESULT




- For preliminary hyperparameter tuning, minimizing validation error, we use
  - torchdiffeq.dopri5 solver
  - 100 trajectories (80 training/ 20 validation)
  - 100 time steps
- Tuning shows the optimal hyperparameters are
  - Learning rate = 0.01
  - 2 layers
  - 8 neurons per layer
  - Batch_time = 10
  - Batch_size = 90

| | Mean Absolute Error | Normalized Root Mean Square Error |
|---|---|---|
| Training | 0.0038 | 0.097 |
| Validation | 0.0030 | 0.043 |




## CONCLUSIONS

- Hyperparameter selection, especially of an accurate ODE solver, is crucial for learning the timing of the slope transition.
- Since training may involve local minima in the loss over the training epochs, training for long enough is important to ensure convergence.
- Neural ODEs have shown the ability to learn the dynamics of the FMDM data and predict a time trajectory from its initial condition, and therefore, have potential as a surrogate for this application.

## ONGOING WORK

- Further hyperparameter tuning of the
  - Number of trajectories to use as training data
  - Number of time steps to use from the training data
  - Choice of numerical solver
- 10-fold cross-validation for hyperparameter tuning
- Evaluation of trained surrogate on testing data

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