Feasibility of Neural Network Metamodels for Emulation and Sensitivity Analysis of Radionuclide Transport Models

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Outline

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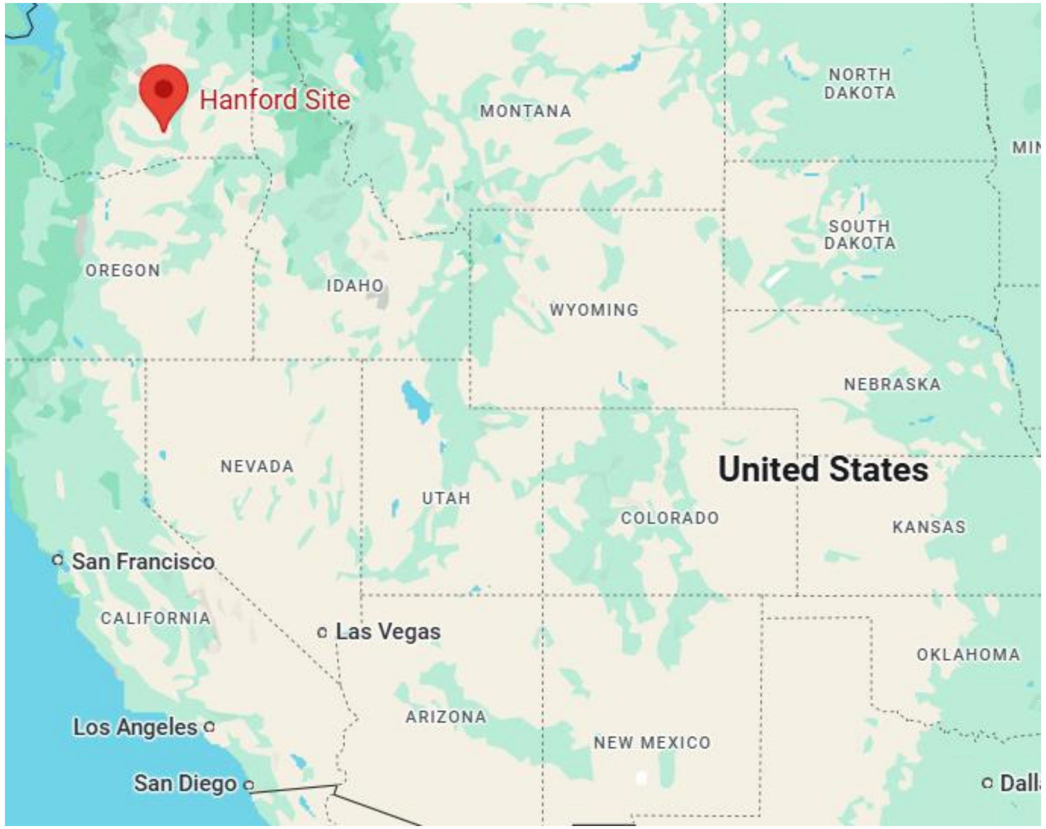
Introduction

Introduction

The leakage of nuclear materials, such as cesium-137 (137Cs) and strontium-90 (90Sr), poses significant environmental and health risks.

Incidents like the Chernobyl disaster and the ongoing challenges at the Hanford site underline the importance of understanding how radionuclides interact with soil and groundwater.



Study area of Hanford site

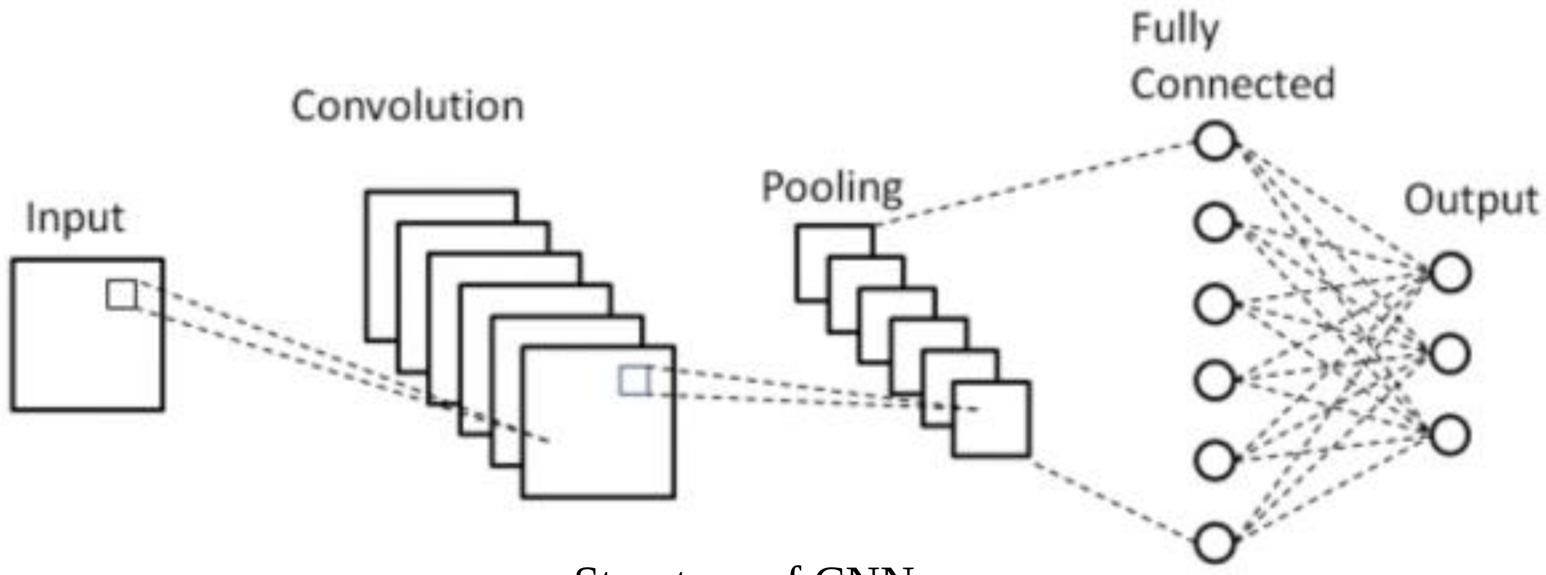
Problem Statement

Traditional numerical models, such as partial differential equations (PDEs), are widely used to simulate radionuclide transport due to their accuracy. However, computation will take a lot of time.

Despite their accuracy, PDEs are not ideal for sensitivity analysis due to the high computational cost, making efficient alternatives like neural network metamodels increasingly attractive.

What is CNN?

Convolutional Neural Network (CNN) is a type of deep learning model used in image processing and pattern recognition.



Structure of CNN

What is Sensitivity Analysis?

Sensitivity analysis is essential to understand how variations in input parameters impact model outputs. It helps identify key parameters, prioritize data collection, and quantify uncertainty, ensuring that the model remains robust and reliable.

The two main uses of sensitivity analysis :

1. **Parameter optimization**: To identify which parameters have the most impact on the model results, allowing for further optimization or study of these key parameters.
2. **Uncertainty quantification**: To help identify and reduce uncertainties in the model, ensuring that the results are more accurate and predictive.

Objective

- Explores the feasibility of using neural network metamodels for simulating and performing sensitivity analysis on radionuclide transport models.

- CNN were used to simulate the transport of radionuclide cesium-137, and the results were compared with numerical solutions based on PDE models.

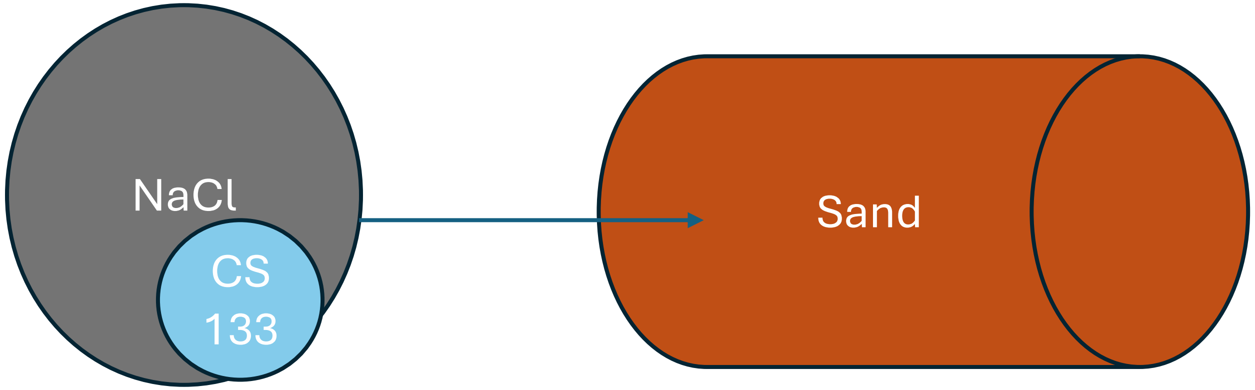
Methods

Cs_{137} Transport Model

The transport of 133Cs was described by the one-dimensional advection-dispersion equation (ADE) model:

$$\theta \frac{\partial C}{\partial t} + \rho \frac{\partial S}{\partial t} = \theta D \frac{\partial^2 C}{\partial z^2} - \theta V \frac{\partial C}{\partial z}$$

Parameter	Symbol
Time	t
Distance	z
Volumetric (saturated) water content	θ
(Sand) bulk density	ρ
Dispersion coefficient	D
Pore water velocity	V



Research data base on **Saiers, J. E. & Hornberger, G. M. (1996)**, transport of Cs-137 through quartz sand and related models proposed.

Equation of sorbed-phase

$$S = S_1 + S_2$$
$$S_1 = fKC^n$$
$$\frac{\partial S_2}{\partial t} = a[(1-f)(KC^n - S_2)]$$

S1 and S2 are the sorbed-phase concentrations for equilibrium and nonequilibrium sorption sites.

Sensitivity analysis was conducted on the following four parameters.

Parameter	Symbol
Sorption rate coefficient	α
Fraction of equilibrium sorption sites	f
Sorption coefficient	K
Freundlich exponent	n

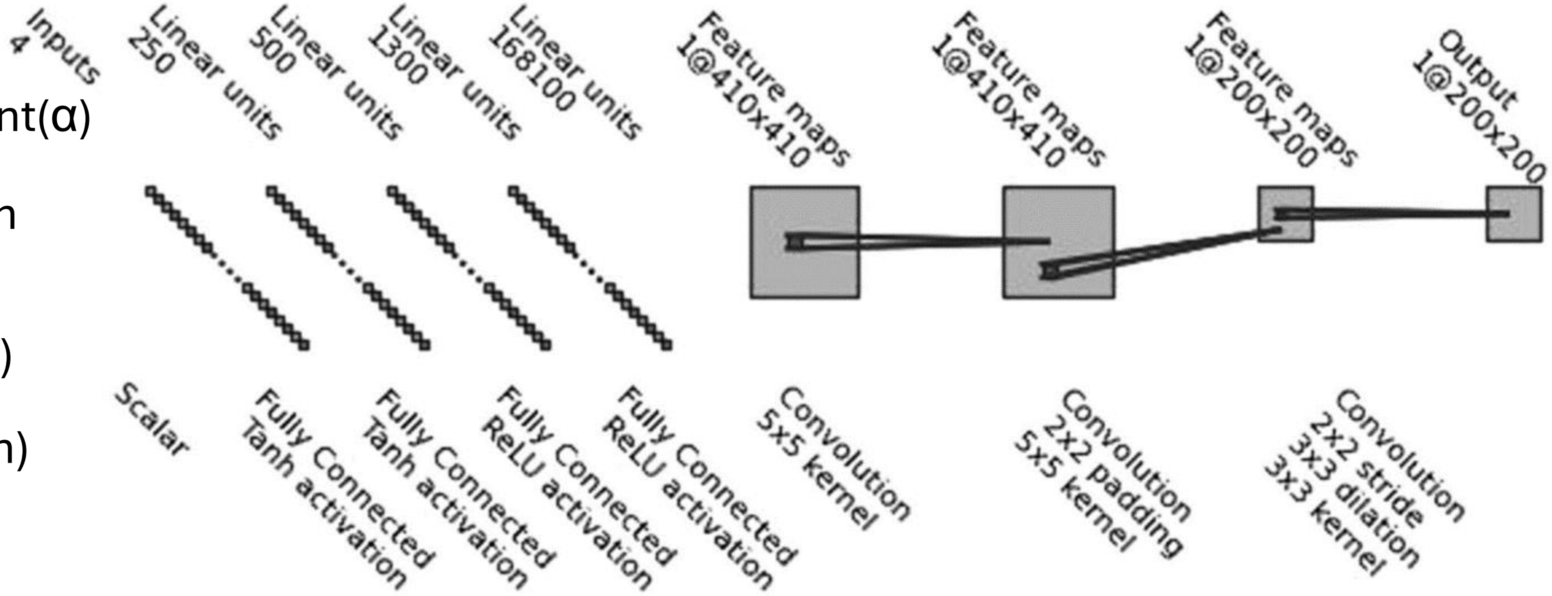
Proposed neural network architecture

Sorption rate coefficient(α)

Fraction of equilibrium sorption sites(f)

Sorption coefficient(K)

Freundlich exponent(n)

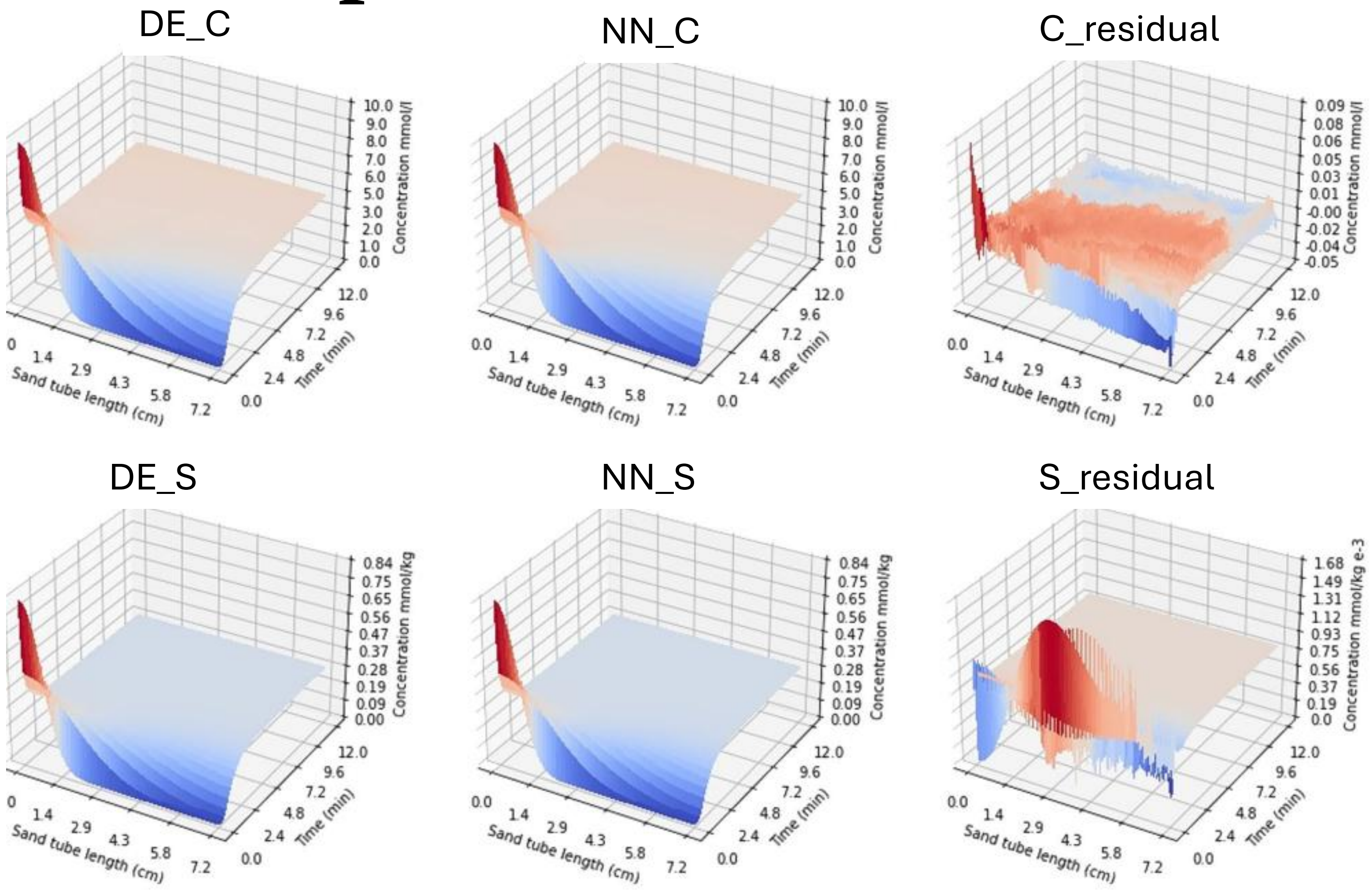


liquid concentration (C)

sorbed concentration (S)

Results & Discussion

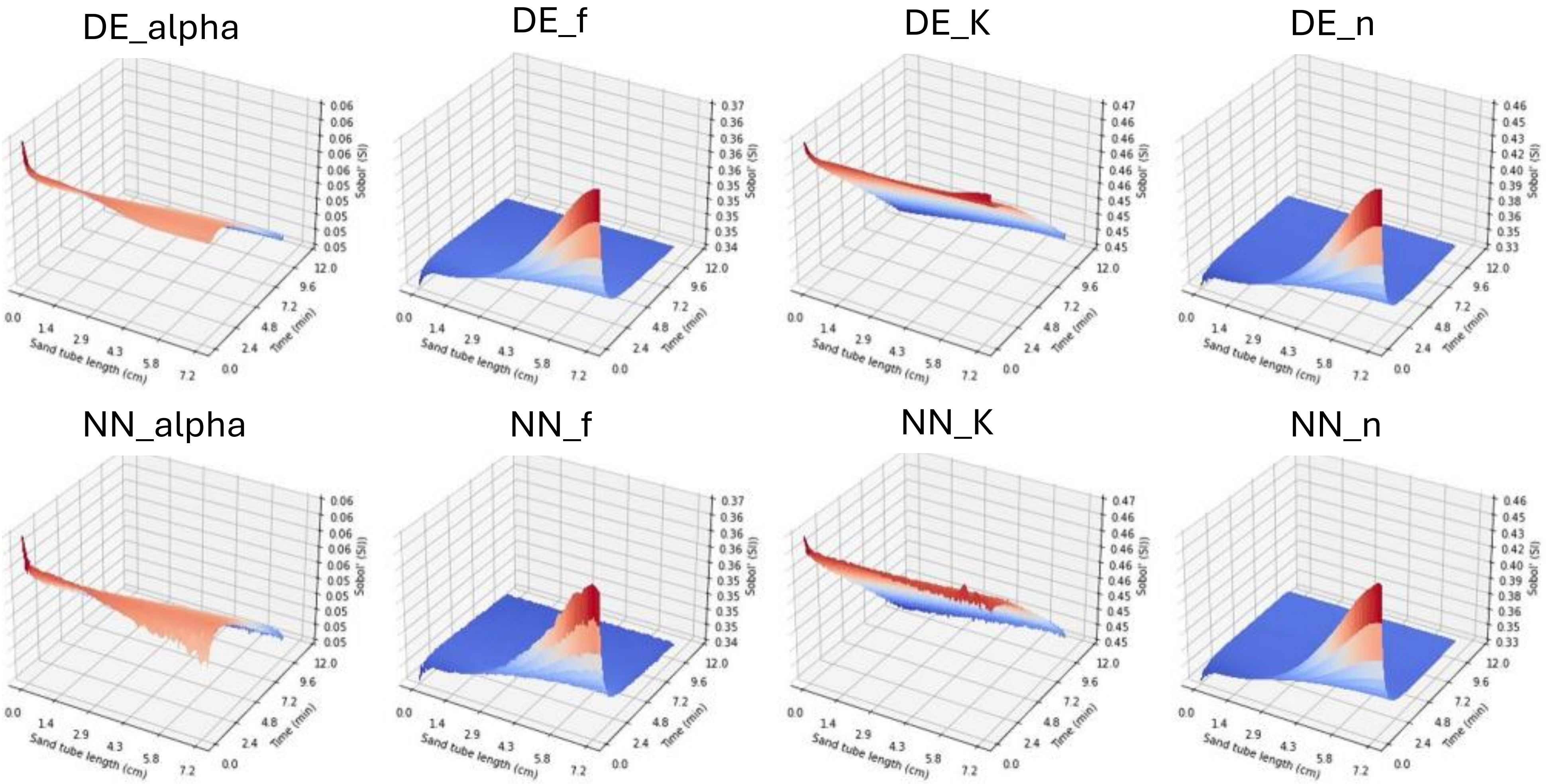
Comparison between DE and NN



A comparison between the PDE and CNN concentration surfaces for liquid (C) and sorbed (S) concentration shows the **error is largest at t < 1 s** ,being at most of the order of 0.1 mmol/l for C and 0.001 mmol/kg for S.

Red means high concentration, blue means low

Sensitivity analysis



The sensitivity analysis results indicate that the sorption coefficient (K) is the most influential parameter for liquid concentration (C). Both PDE and CNN models yield similar sensitivity trends, confirming the CNN model's reliability for parameter analysis.

Sobol's first order sensitivity analysis results for wide tolerances for DE and 40,960-trained NN concentration surfaces for liquid concentration C.

Discussion

Using the PDE model, running 10,240 simulations takes about 235 minutes, while the CNN model requires only 3.5 minutes for the same calculations.

Despite the fast computation speed of the neural network model, finding a suitable model architecture took several months, even in this relatively simple experiment.

Conclusion

Conclusion

1.The CNN model is able to deliver predictions similar to those of the PDE model while significantly reducing computation time.

2.In the future, CNN model can be further optimized to handle different datasets and physical scenarios, enhancing its adaptability and performance across various applications.

Thank you for your attention.

Study Area

Hanford site in Washington State, USA, which is the largest nuclear waste processing facility in the country. During the Cold War, the United States built nuclear weapons in this area, and after the Cold War ended, Hanford became a major storage site for nuclear waste.