Universal Differential Equation for Diffusion-Sorption Problem in Porous Media Flow (EGU21-49)

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Sharing is encouraged

Introduction

Goals:
- Model spatio-temporal problems
- Learn constitutive relationships

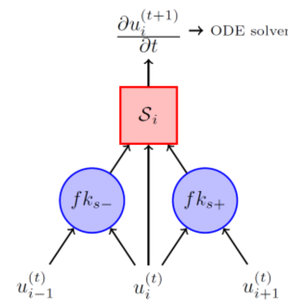
Problem:
Sparsely available experimental data!

Methods

Application:
Subsurface contaminant transport

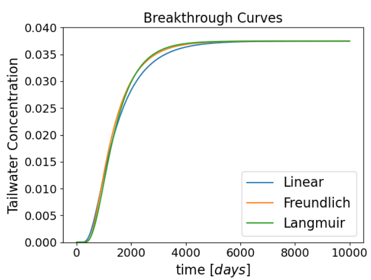
$$\frac{\partial c}{\partial t} = \frac{D_{eff}}{R} \frac{\partial^2 c}{\partial x^2}$$

Hybrid model:
Finite Volume
Neural ODE

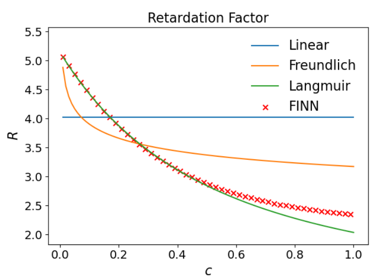


Results

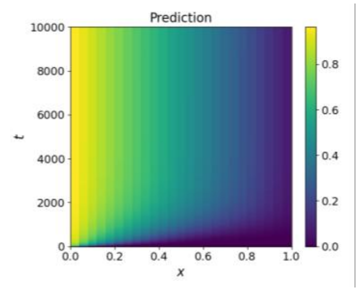
Training data (partial information)



Learn retardation factor



Reconstruct full field solution



[Application to experimental data]

Conclusion

- Excellent structural explainability
- Excellent generalization ability

References & acknowledgement

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Introduction

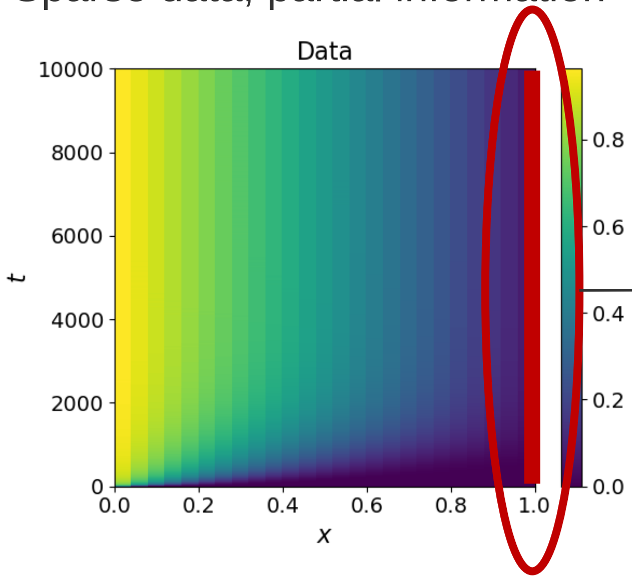
Spatio-temporal problems governed by PDE
(i.e. diffusive type problems)

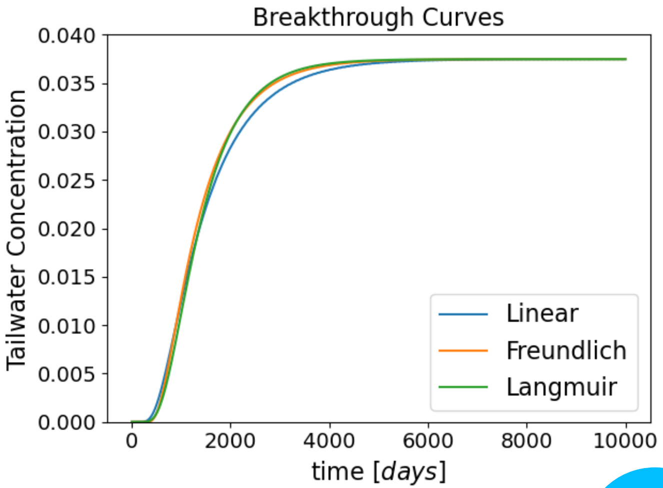
$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\boxed{D(u)}\frac{\partial u}{\partial x}\right) + q$$

constitutive relationship

Sparse data, partial information

(data only at $x = L$)





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Methods

Application

Contaminant diffusion-sorption in porous media

$$\frac{\partial c}{\partial t} = \frac{D_e}{R}\frac{\partial^2 c}{\partial x^2}$$

$$\frac{\partial c_t}{\partial t} = D_e \phi \frac{\partial^2 c}{\partial x^2}$$

- R defined with three different sorption isotherms: linear, Freundlich, Langmuir
- Dirichlet and Cauchy BC
- Available data: breakthrough curve and destructive sampling

c	: dissolved TCE concentration
c_t	: total TCE concentration
D_e	: effective diffusion coefficient
R	: retardation factor
ϕ	: porosity

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Methods

Hybrid model

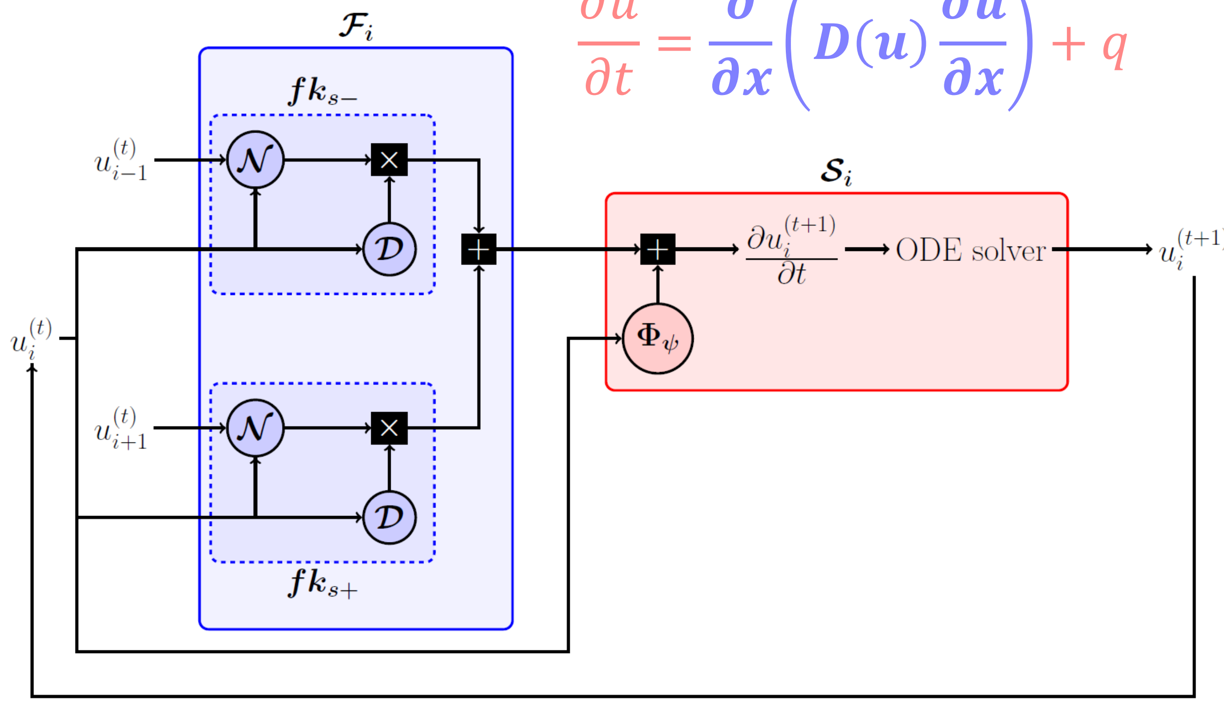
Physics-informed structure:

- Finite Volume Method discretization (spatio)
- Neural Ordinary Differential Equation (temporal)

$\mathcal{F}$: Flux Kernel (calculate fluxes and BCs, learn constitutive relationships)

$\mathcal{S}$: State Kernel (learn reaction term, integrate with ODE solver)

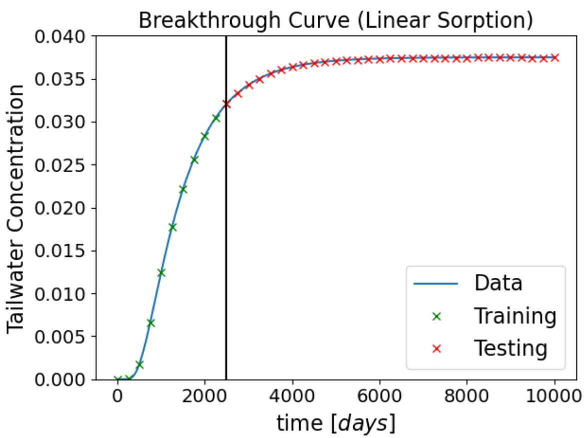
$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D(u)\frac{\partial u}{\partial x}\right) + q$$



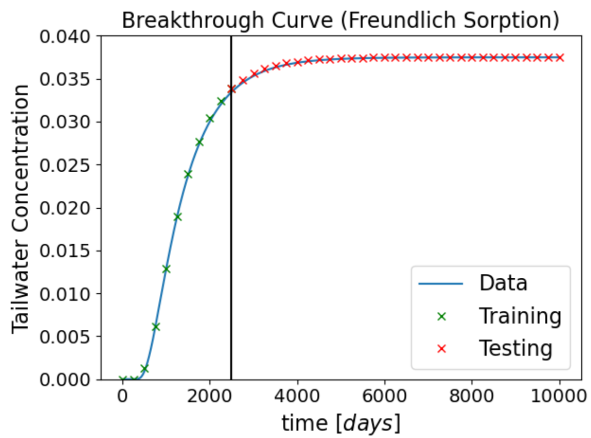
Results

Retardation Factor

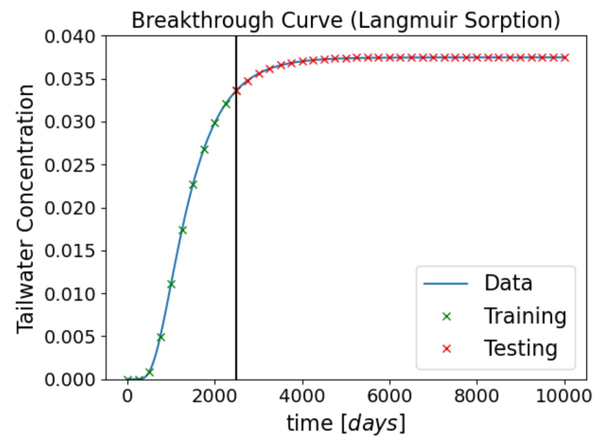
Linear



Freundlich



Langmuir



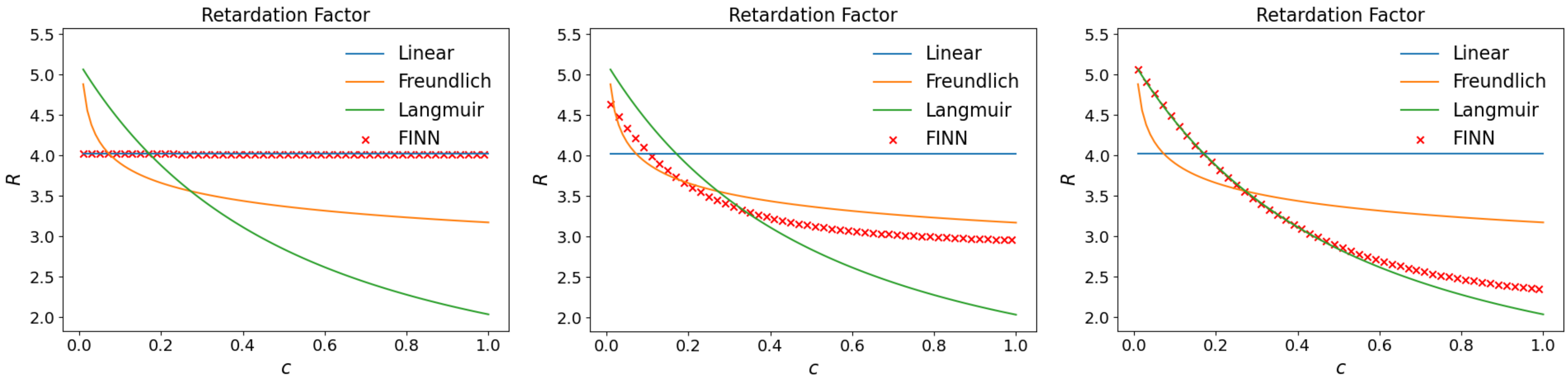
Similar breakthrough curves, but…

Results

Retardation Factor

we can still learn the difference in the retardation factor, …

Linear | Freundlich | Langmuir



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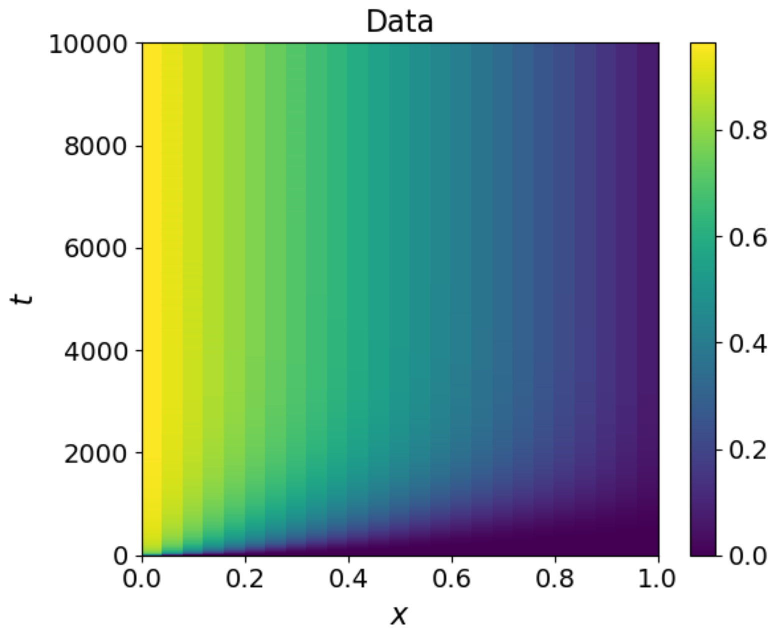
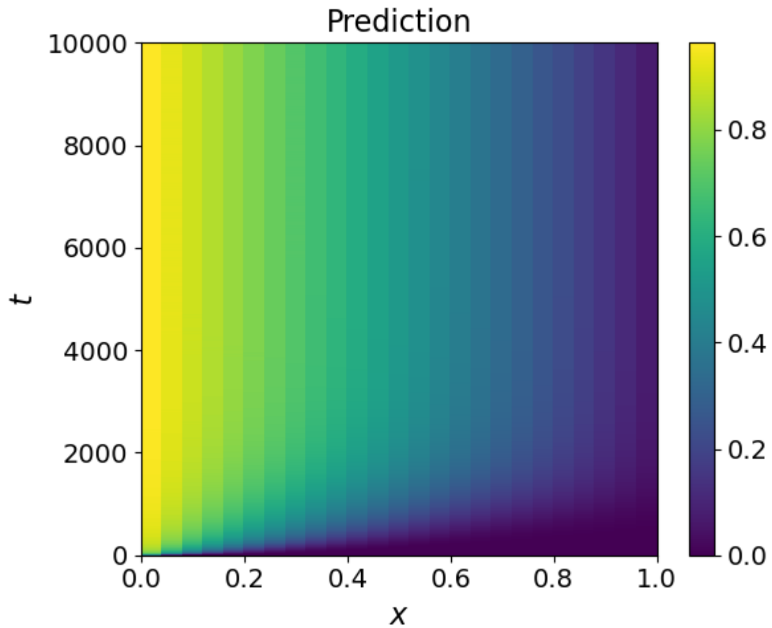
Results

Reconstruction of full field solution

and reconstruct the solution at all location x!





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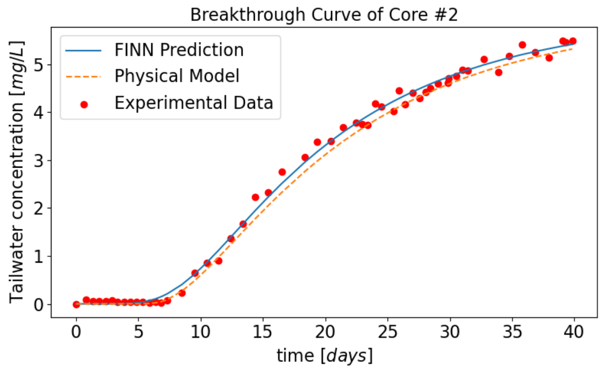
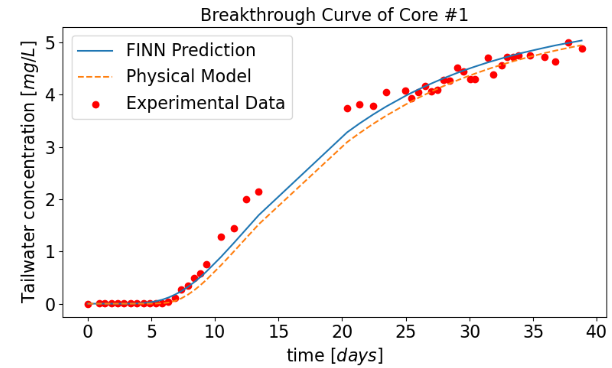
Results

Experimental data (core samples extracted from same geographical area)

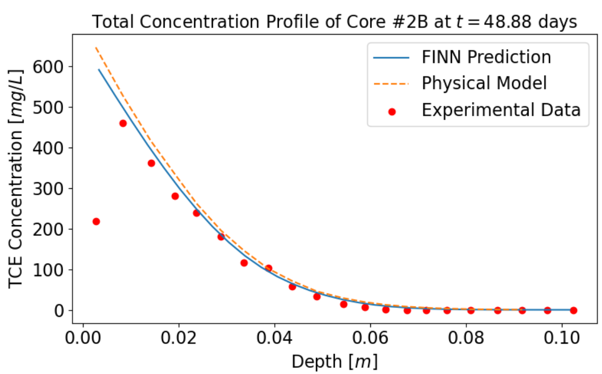
Train with core #2



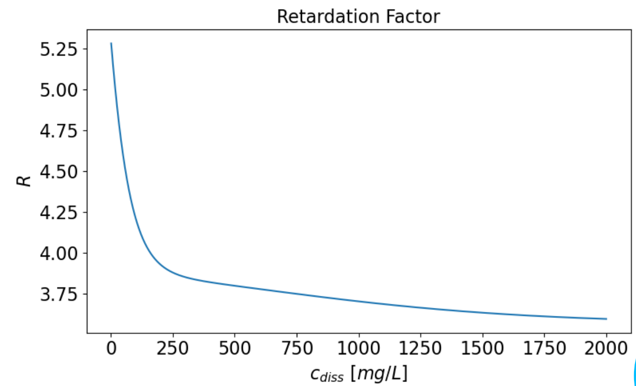
Test with core #1



Test with different BC (#2B)



Learned retardation factor



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References & Acknowledgement

References:

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