NEURAL INFORMATION PROCESSING SYSTEMS

AMPHOS 21

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Dynamic weights enabled Physics-Informed Neural Network for simulating the mobility of Engineered Nano-particles in a contaminated aquifer

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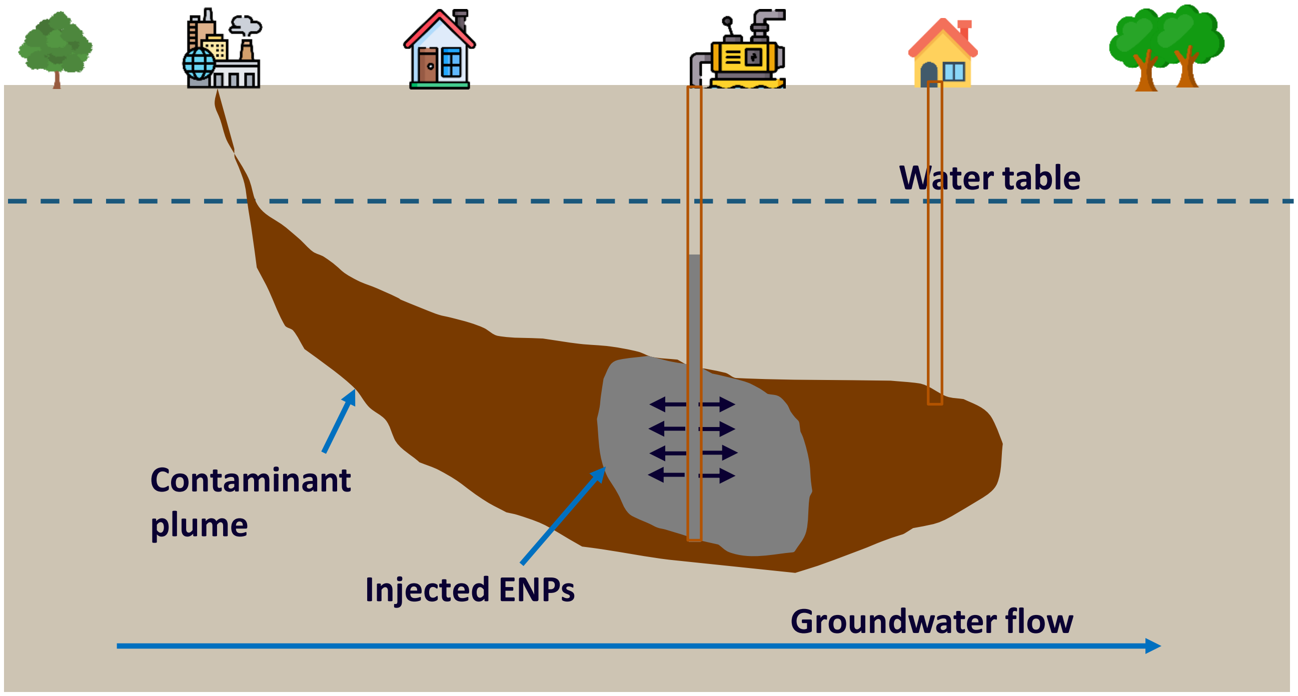
Tackling Climate Change with Machine Learning

Background

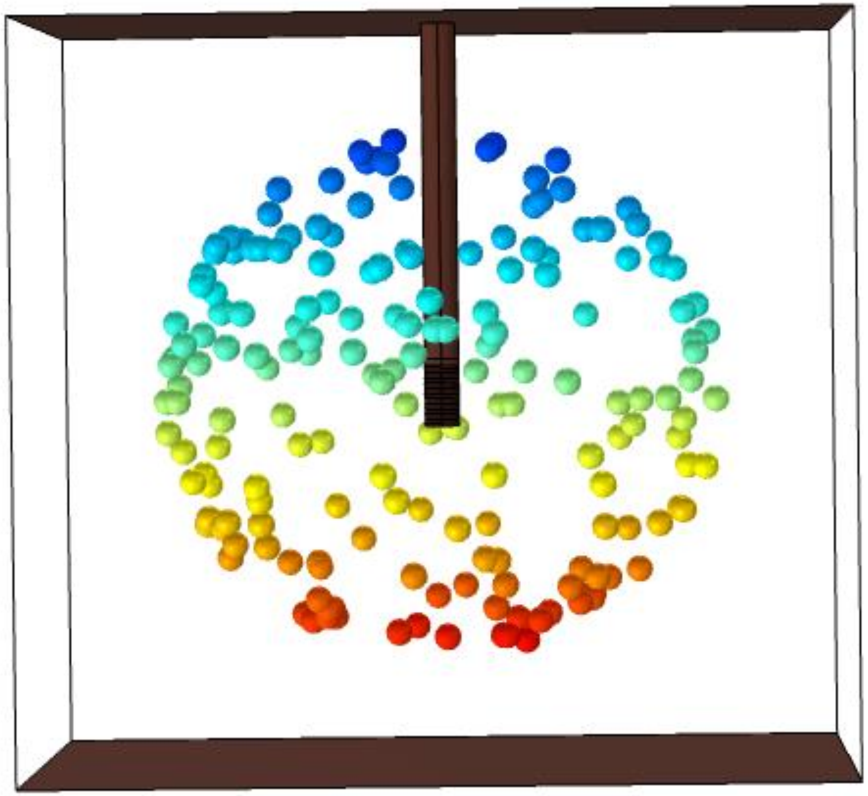
- More than 340000 aquifers are contaminated due to anthropogenic activities just in Europe (Jarsjö et al., 2022)
- The aquifer contamination aggravate climate change due to degradation of soil quality, costal ecosystem and deforestation.
- A promising techniques for remediating the groundwater is by injecting Engineered nano particles (ENPs) that eliminates the contamination



Groundwater remediation strategy

$$\frac{\partial(\theta c)}{\partial t} + \frac{\partial(s)}{\partial t} = -\nabla(vc) + \nabla((D_e + \propto v)\nabla c)$$

$$\frac{\partial(s)}{\partial t} = \theta k_a c - k_d s$$



θ: porosity, v: flow rate, $\propto$: dispersivity, c: aqueous ENPs, s: retained ENPs, k_a: attachment coefficient, k_d: detachment coefficient

Source of column sand figure: Tan et.al, 2020

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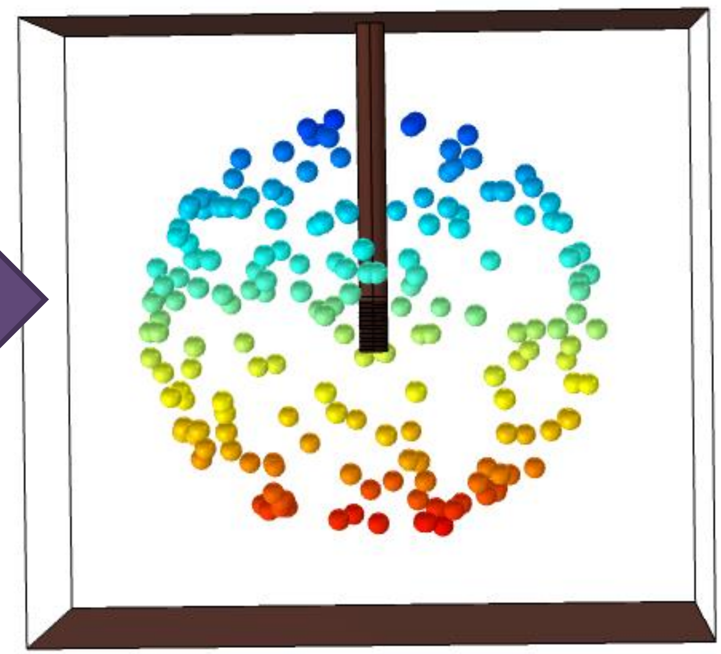
ENPs injection

ENPs observed

Parameter estimation



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Simulation workflow

Aim: To develop a simulator for parameter estimation

↓

PINN formulation

↓

Verification with Comsol

↓

Inverse modeling

$$\frac{\partial(\theta c)}{\partial t} + \frac{\partial(s)}{\partial t} = -\nabla(vc) + \nabla((D_e + \propto v)\nabla c)$$

$$\frac{\partial(s)}{\partial t} = \theta k_a c - k_d s$$

$$c(0,t) = \left(\frac{1}{1+e^{-0.02(t-500)}}\right) \times \left(\frac{1}{1+e^{0.02(t+500)}}\right)$$

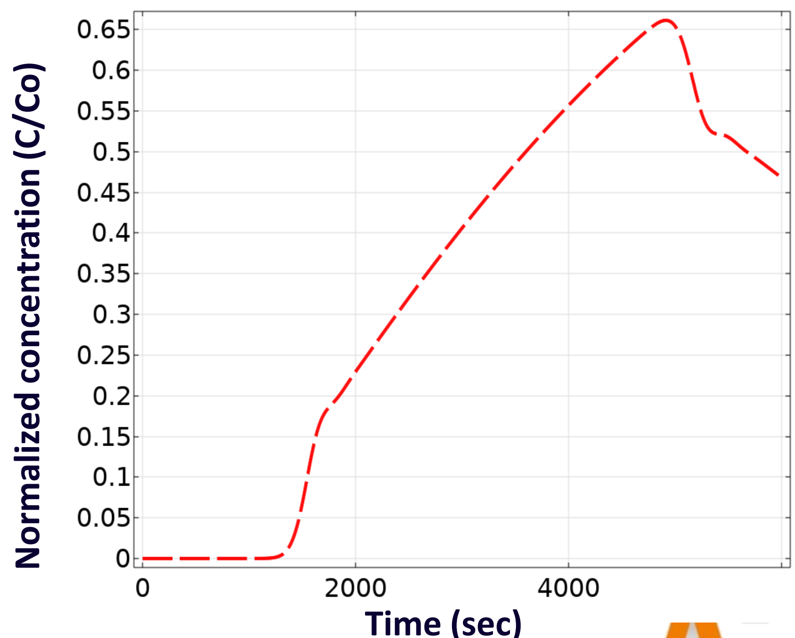
$$\nabla((D_e + \propto_L v)\nabla c(1,t)) = 0$$

$$c(x,0) = s(x,0) = 0$$

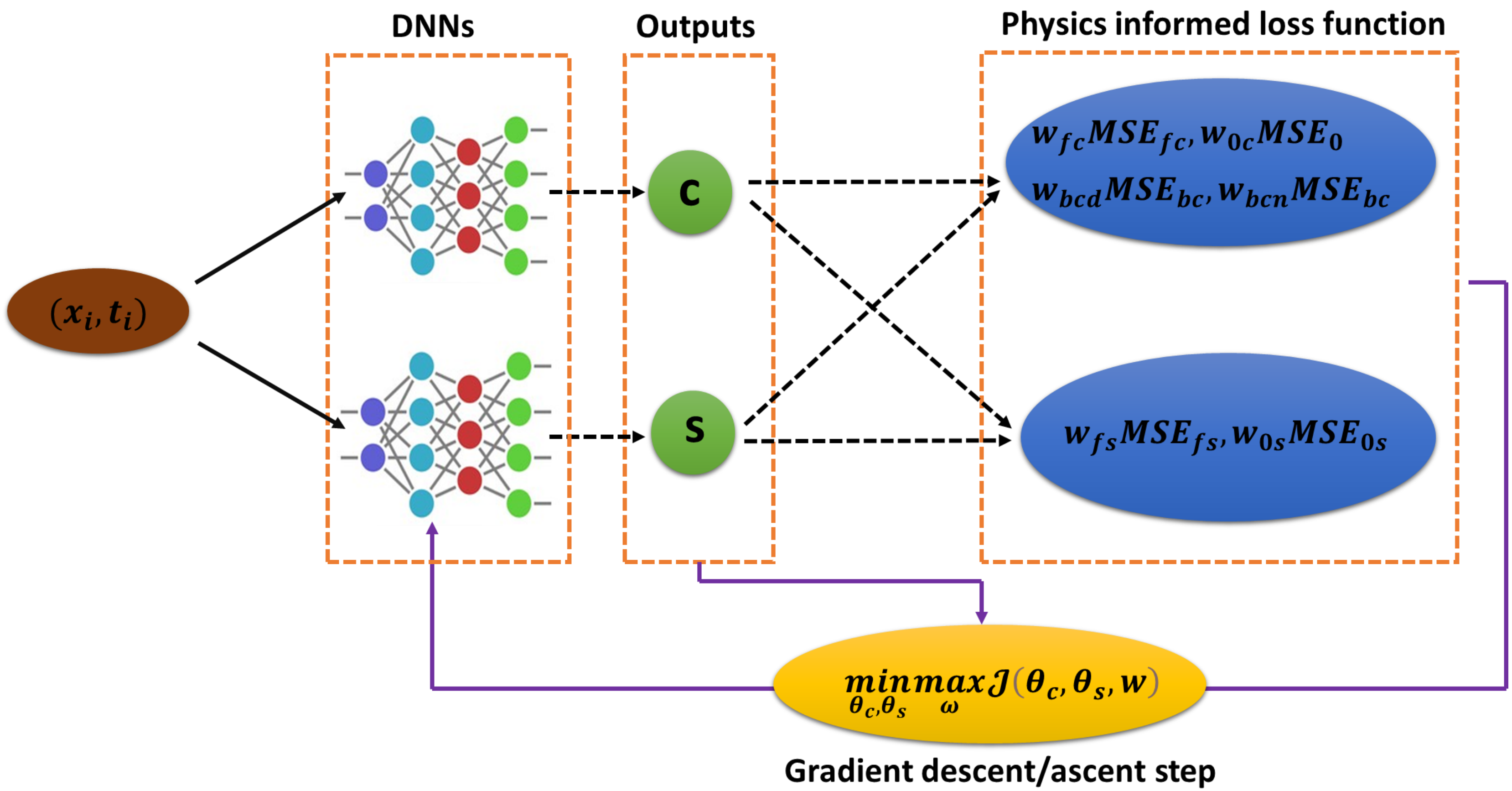
Second Inverse model:

θ = ✓ $\propto$ = ✓ $k_a = ?$, $k_d = ?$

1D simulated domain to estimate:
θ, $\propto$, k_a, k_d

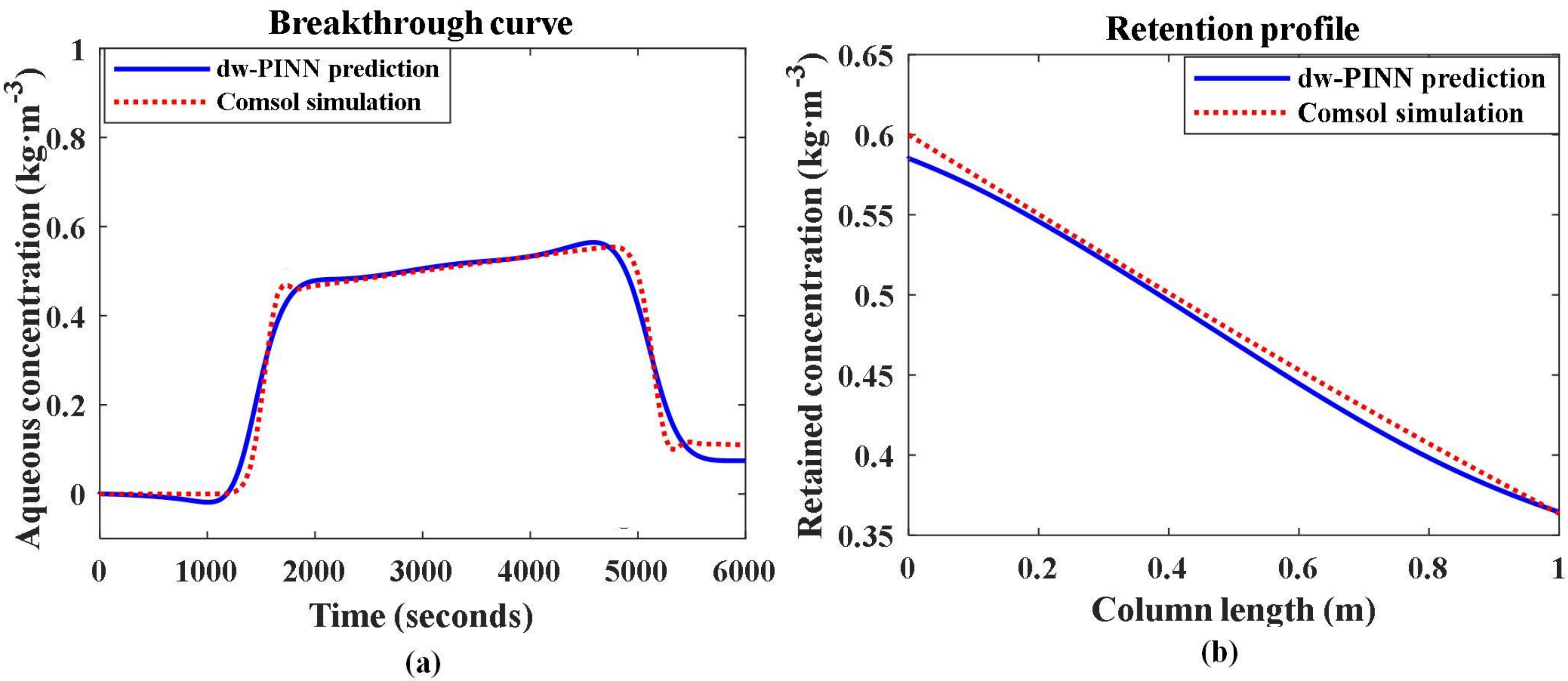


Applied PINN framework



Flowchart of dw-PINN framework representing two Deep Neural Networks with time and spatial points as input and concentration of aqueous and retained ENPs as output

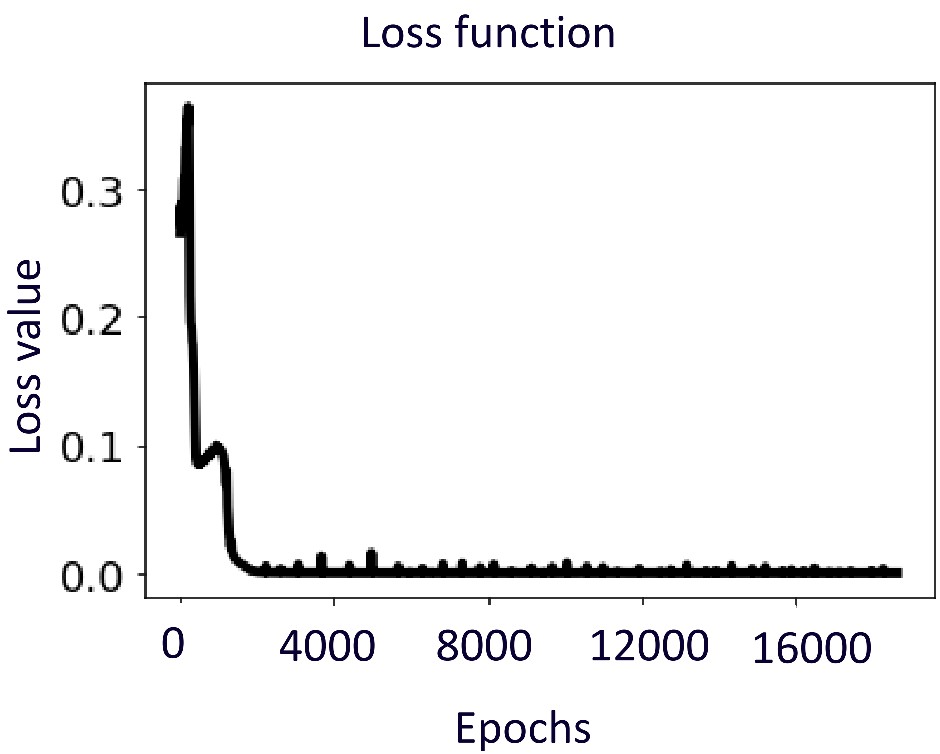
Stage 1: Forward modeling verification

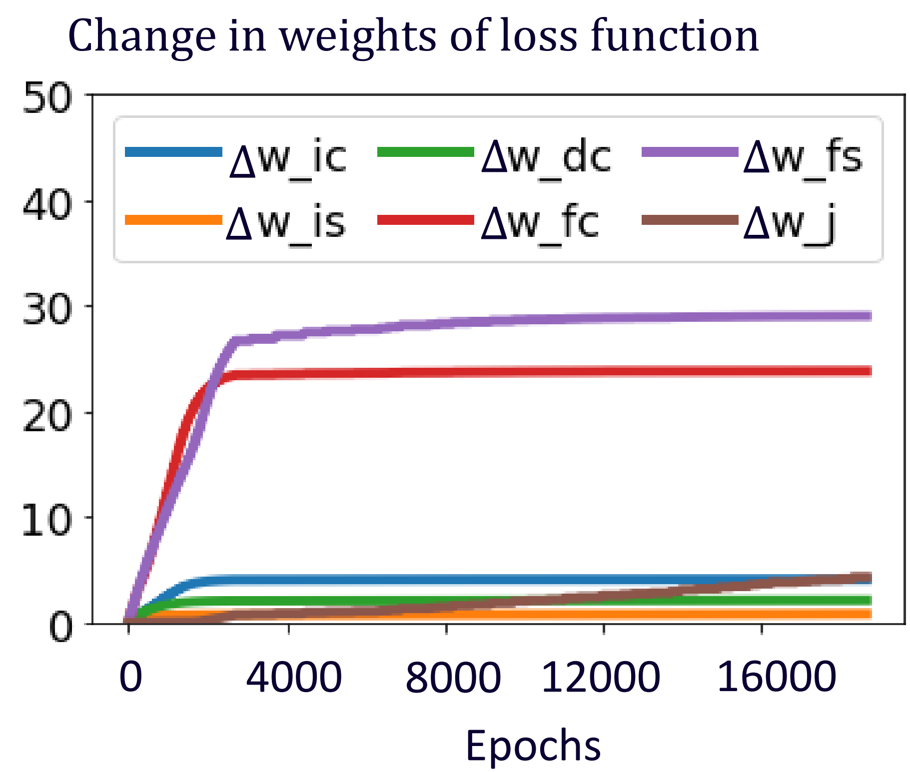


Result comparison of dw-PINN and Comsol model; (a) breakthrough curve (b) retention profile

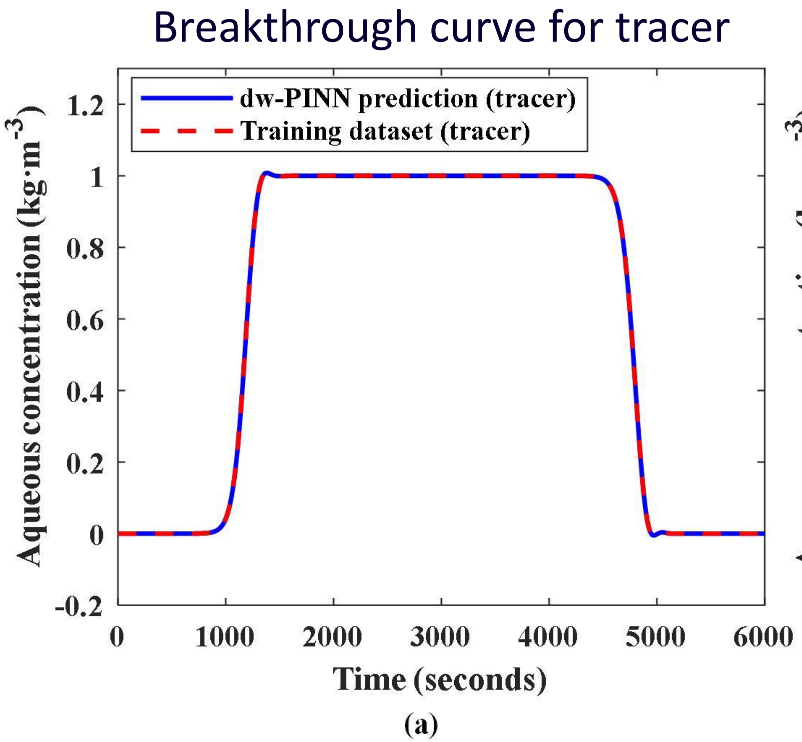
v = 0.0003 m·s^{-1}, D_e = 1e-9 m^2·s^{-1}, $\propto$ = 0.01, k_a = 0.00008 s^{-1}, k_d = 0.0001 s^{-1}, θ = 0.3, Column length = 1 m

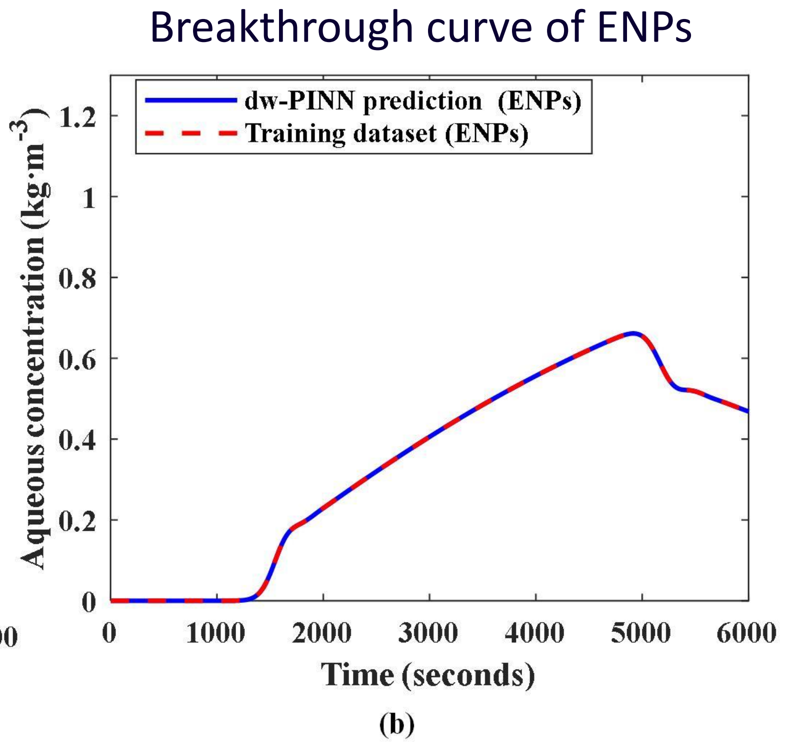
Stage 1: Loss function and Dynamic weights





Stage 2: values estimated and comparison

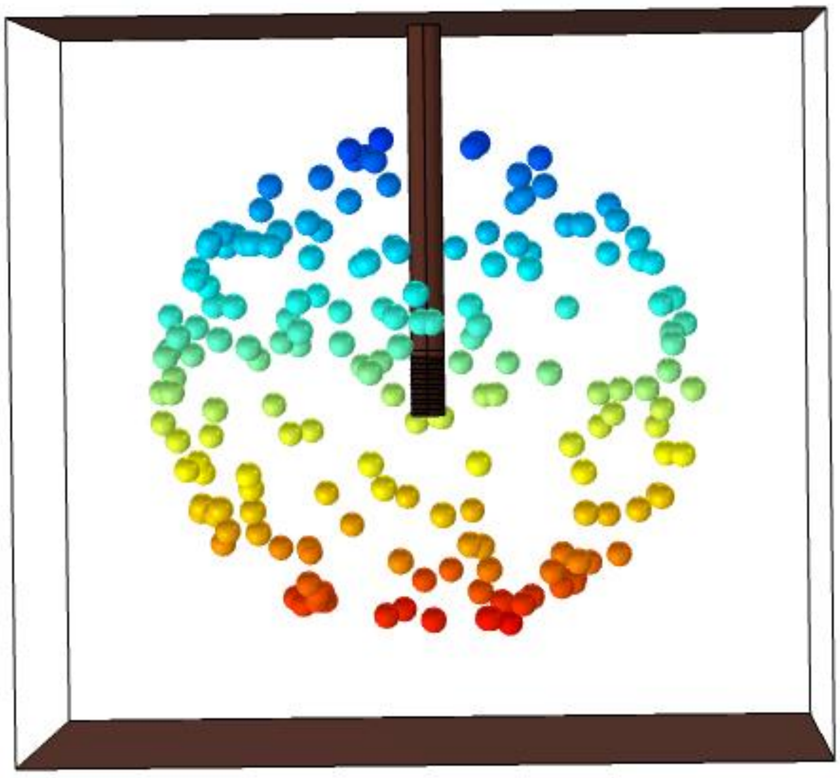




	Porosity	Dispersivity (m)	Attachment Coefficient (s^{-1})	Detachment coefficient (s^{-1})
Ground truth	0.20	0.0050	0.00070	0.00010
Estimated values	0.21	0.0059	0.00071	0.00018

Conclusion and future work

- The model result matches well with the benchmark cases from the numerical simulator, Comsol Multiphysics
- The result demonstrates that the PINN based simulation tool is a viable option for parameter estimations required for upscaling
- Application of simulation tool on real 1D sand-filled column data & forward modeling on 3D system is being explored



Development of ENP´s mobility in a 3D system

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