# Fate and transport of titanium dioxide nanoparticles in porous media

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# Introduction:

- What are ENPs? size 1–100nm.
- $nTiO_2$ (metal oxide based) global production is the highest (5000 tons/year) (*Park et al.,2017*)
- Highest estimated soil concentration (0.4 ug/kg) (*Park et al.,2017*)
- $nTiO_2$ applications:

  sunscreen lotions, burn treatment, dental, antibacterial, photocatalytic, paint pigment
- Sources of $nTiO_2$ discharge into the subsurface:

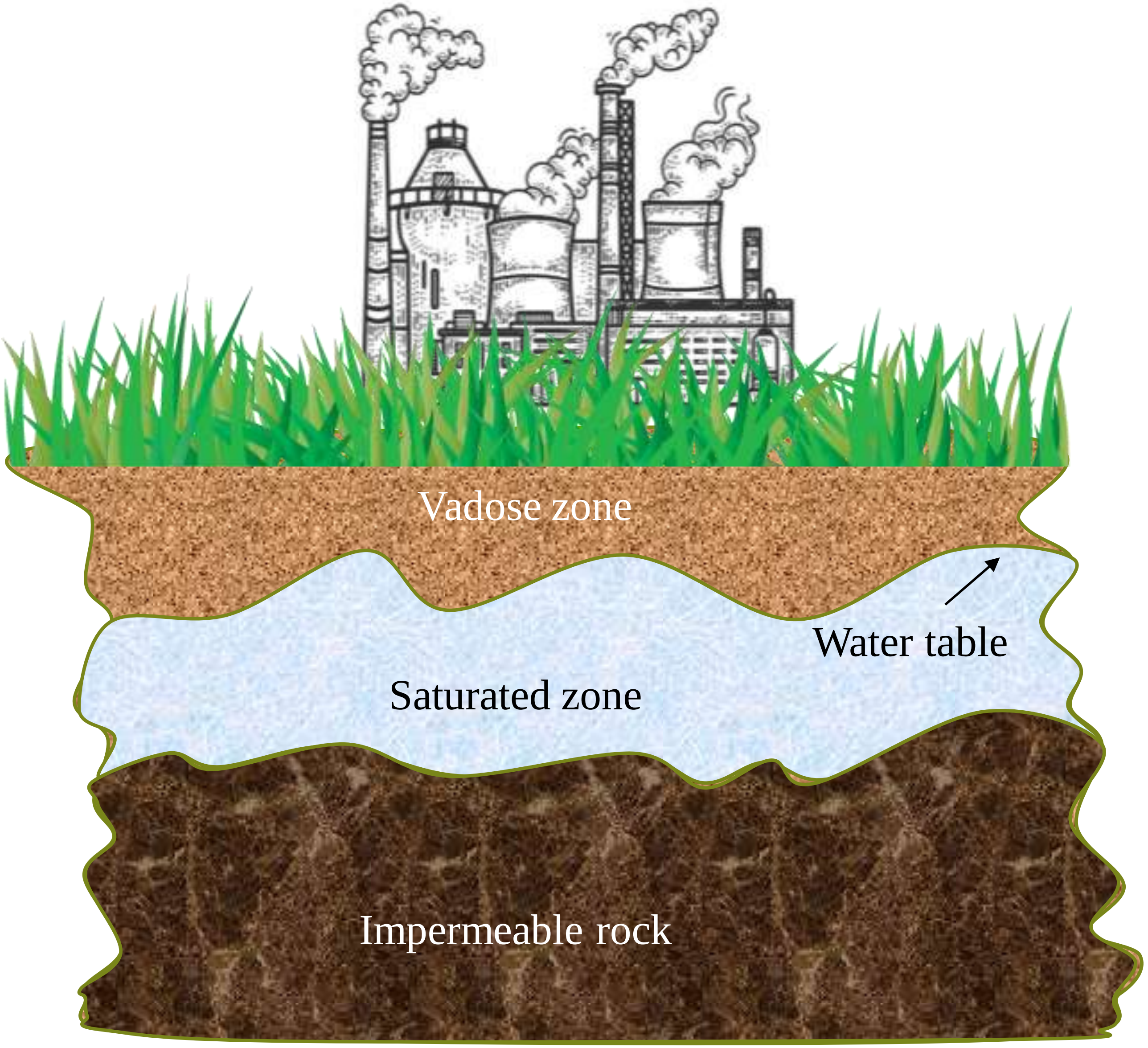
  untreated industrial & agricultural waste,

  landfill leachate,

  WWTP discharge,

  nano-remediation

# Flow pathway of ENPs into the subsurface:



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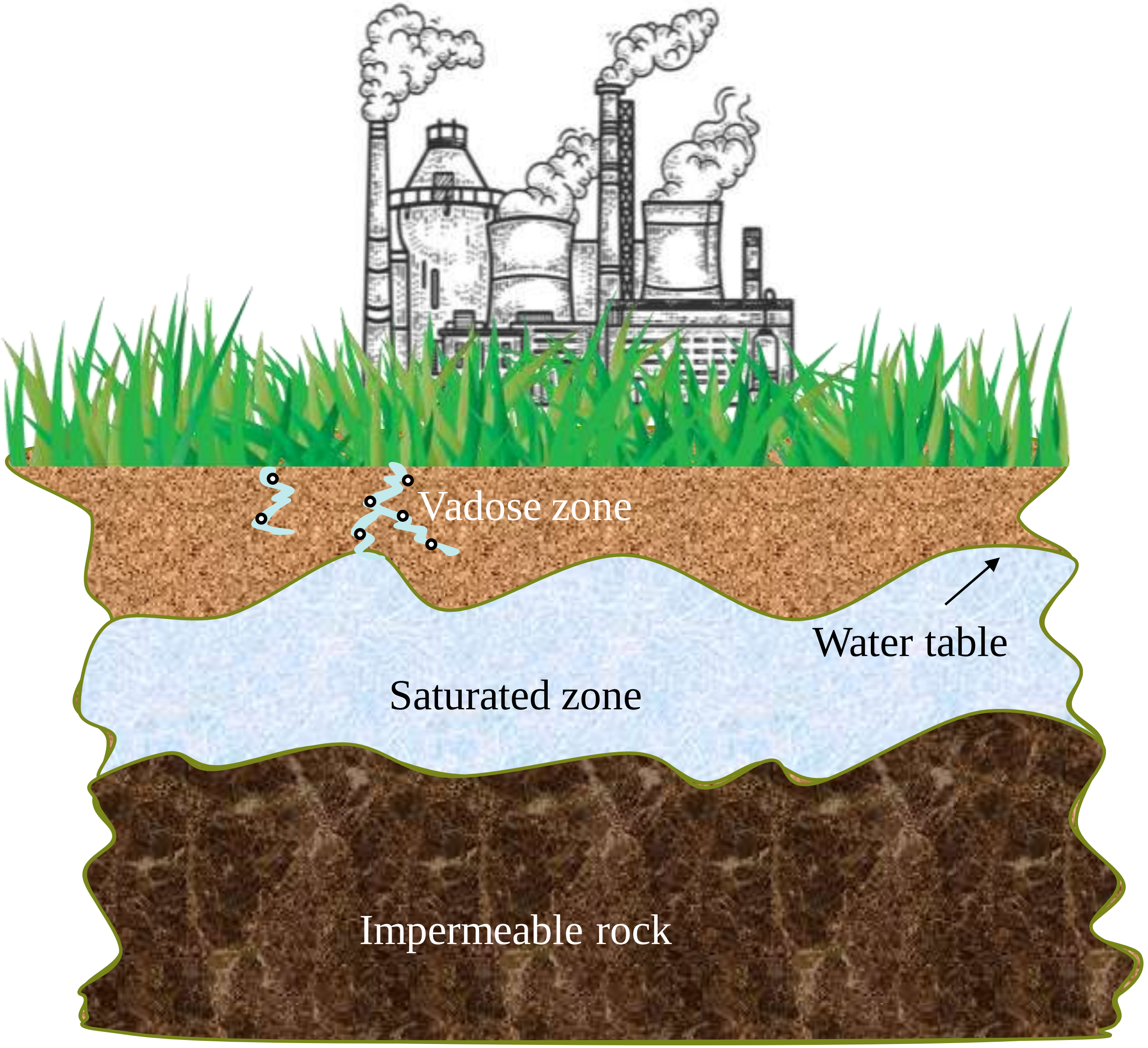

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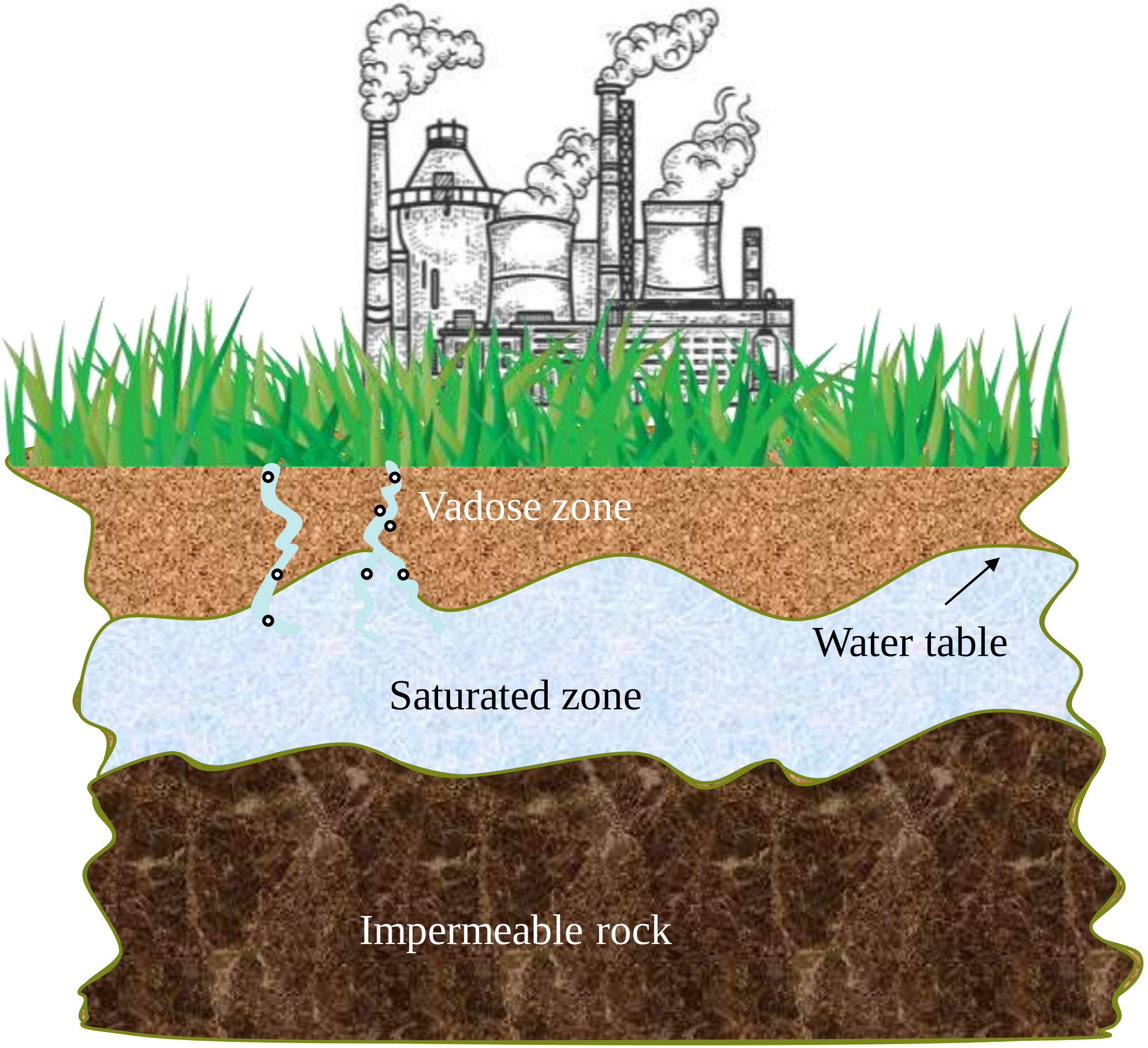

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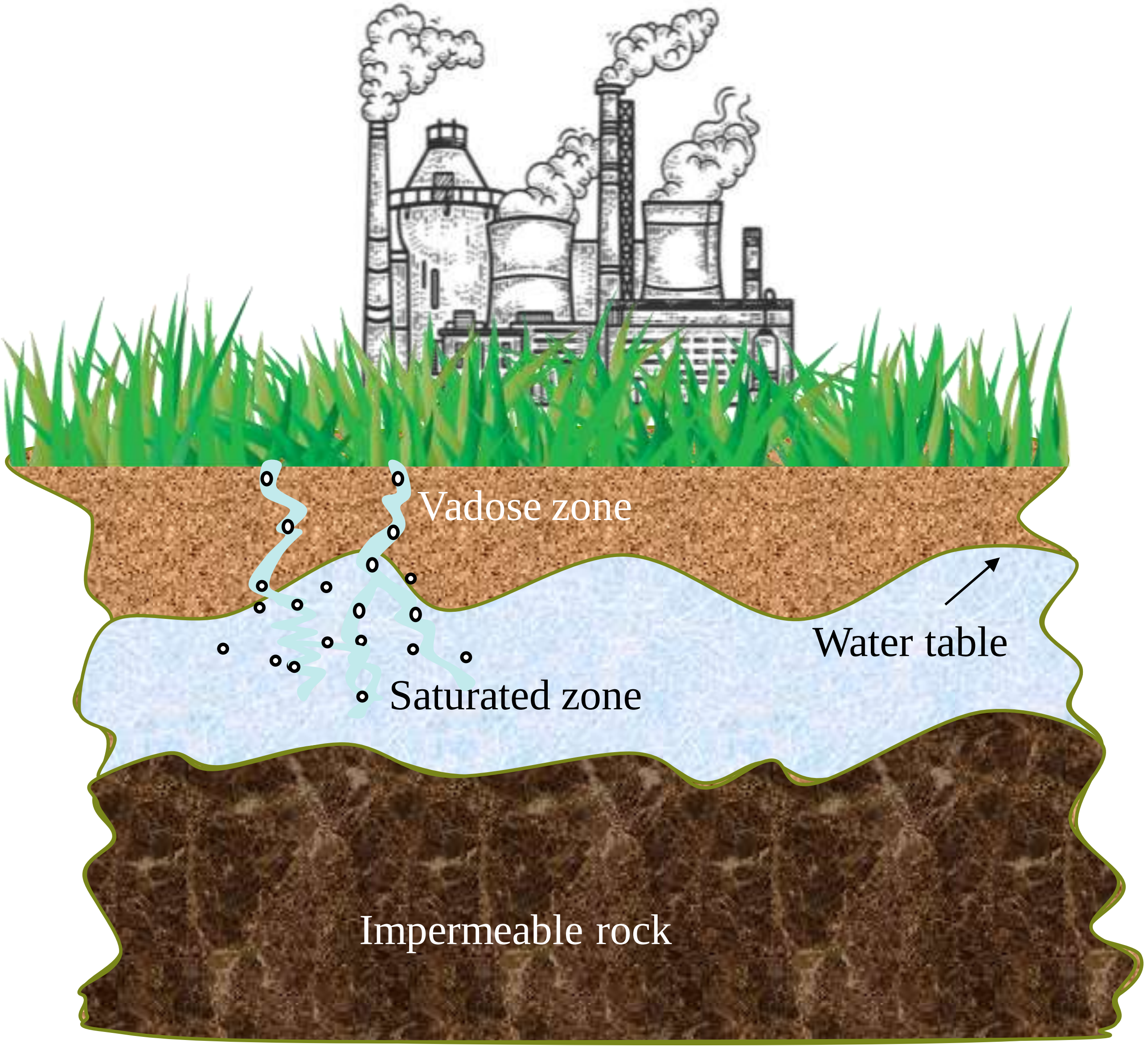

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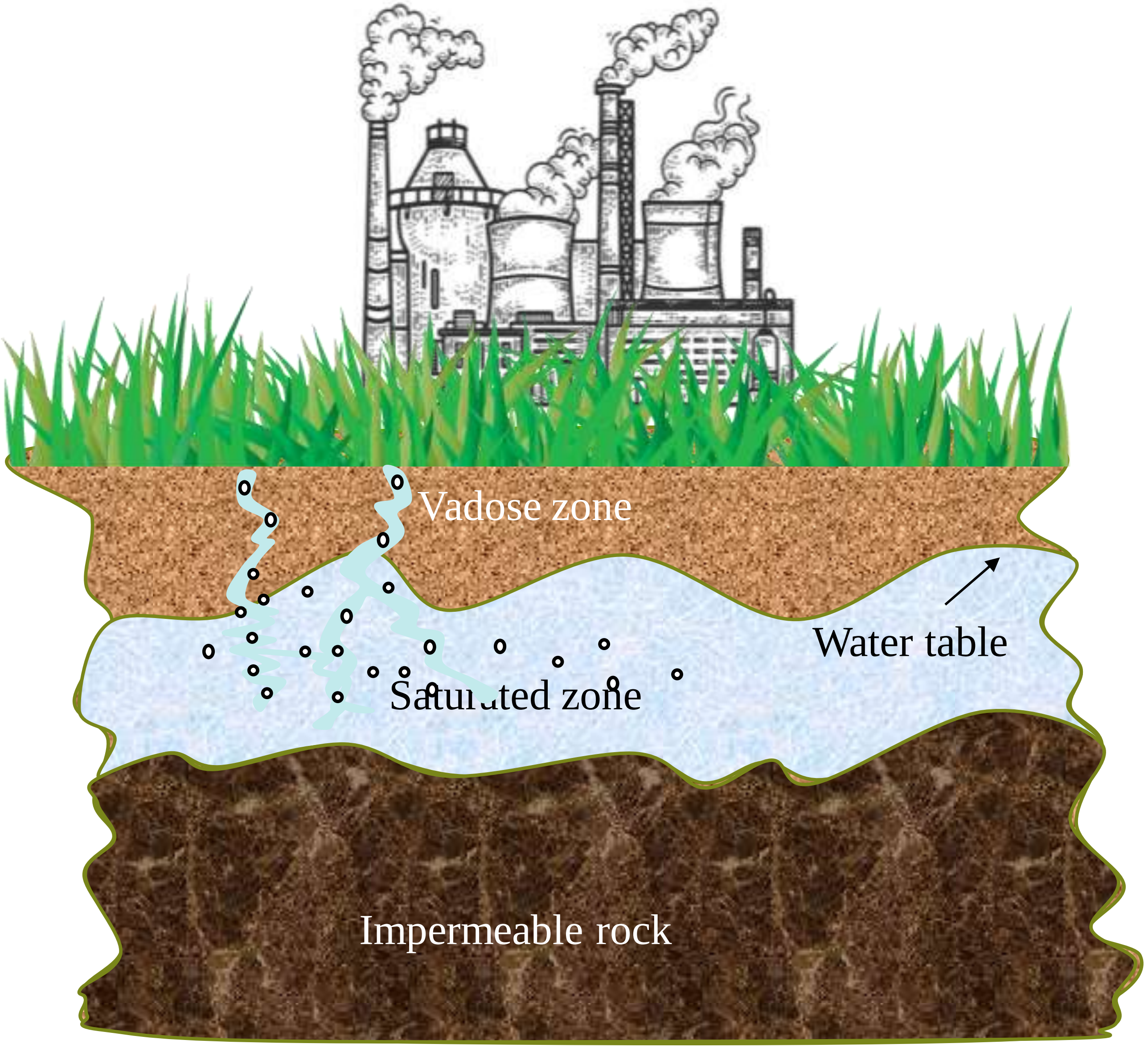


# Objective:

- To understand $nTiO_2$ fate and transport in porous media through column experiments and modeling

# Methodology:

## *nTi$O_2$: Column transport experiments:*

***Experimental conditions:***

- Clean acid washed sand
- *Tracer experiment*

  0.1 M NaCl solution: 3 PV, DIW: 3 PV

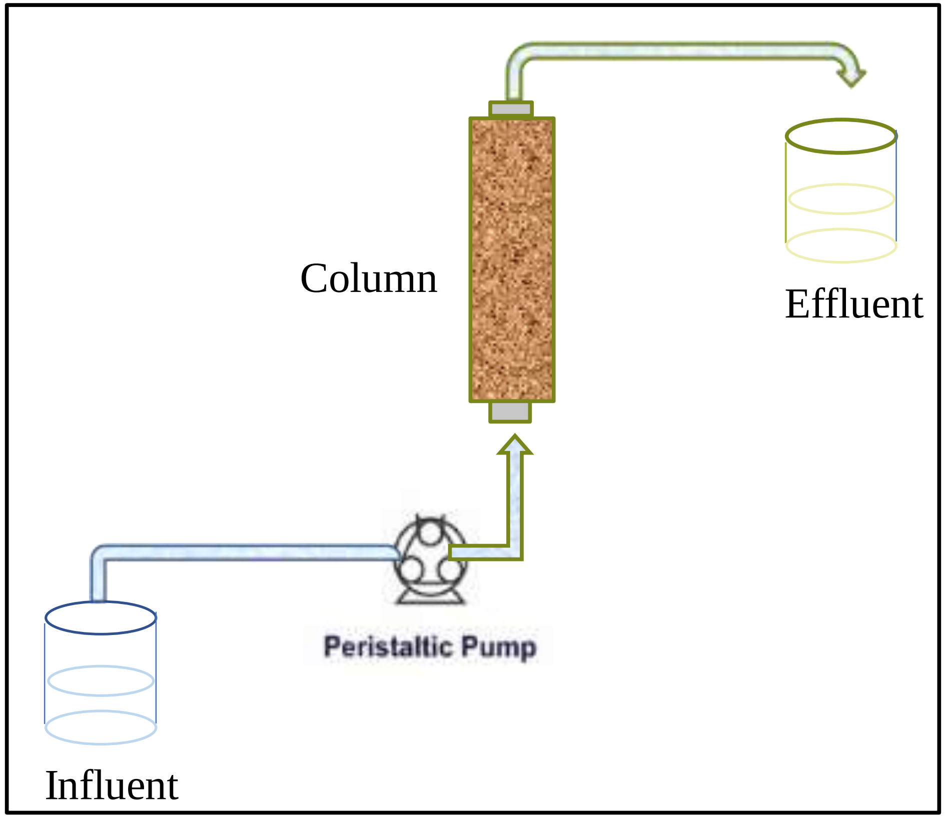
  flow velocity: 1 ml/min
- *nTi$O_2$ experiment*

  pH =7

  DIW: 10 PV, BS (0.01 M NaCl): 10 PV

  nTi$O_2$ influent concentration: 15 mg/L

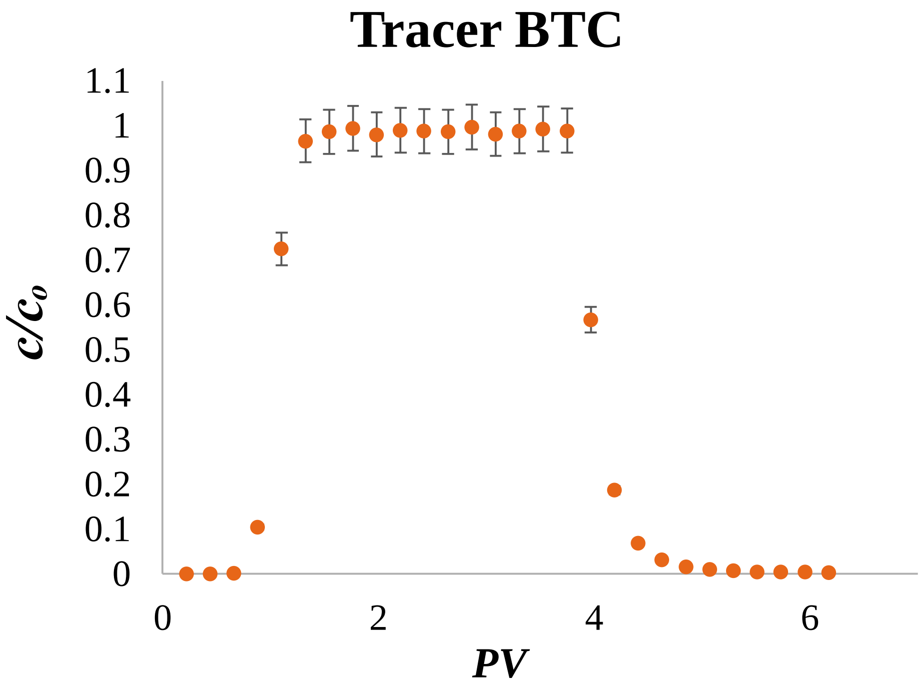
  nTi$O_2$: 3 PV, BS: 3 PV
- Measurements by Turbidimeter

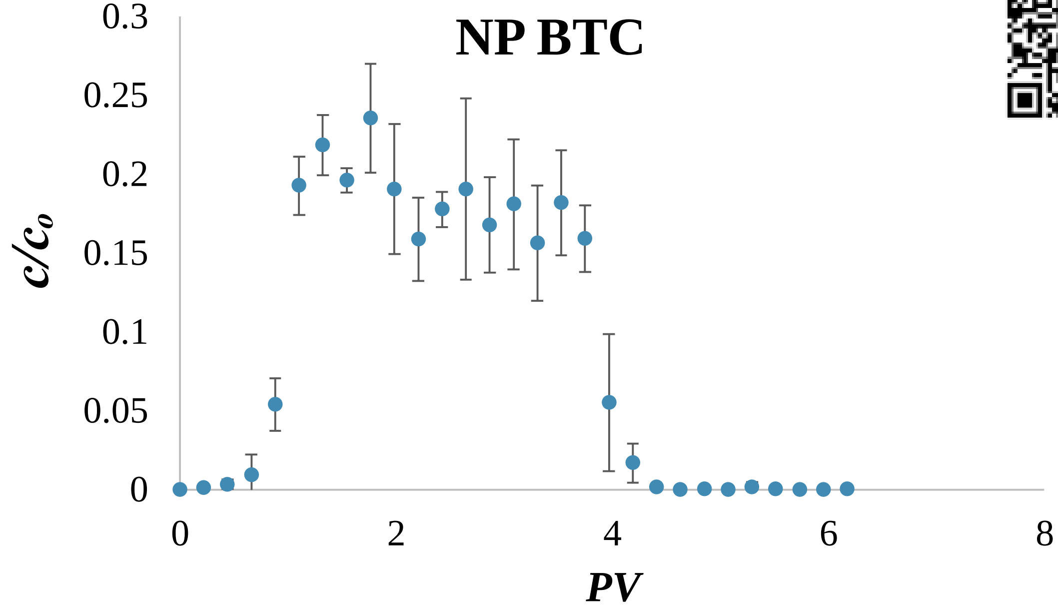


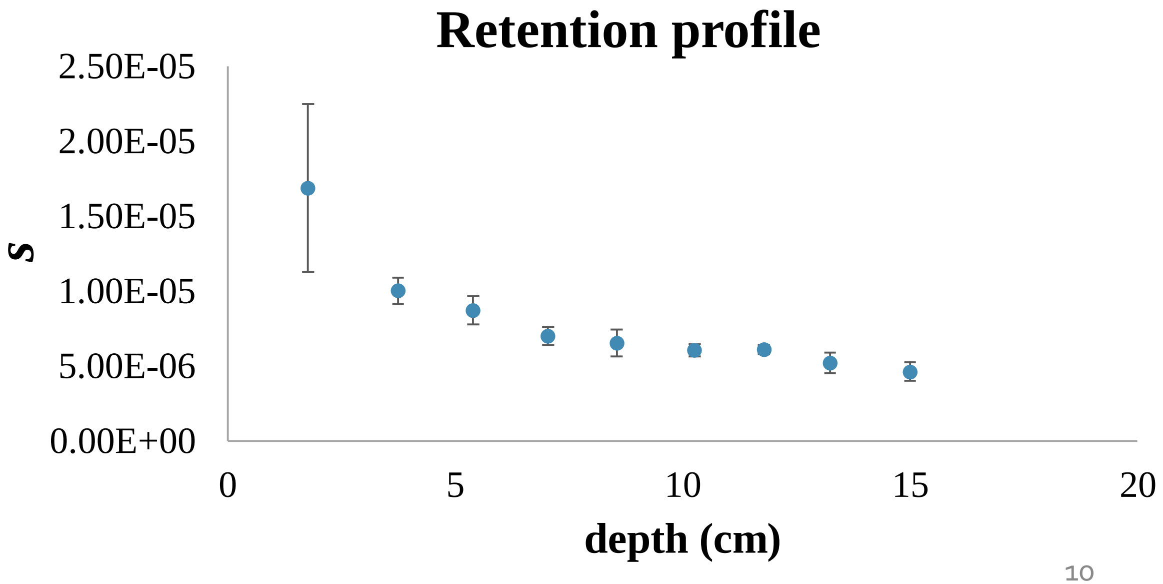

**Column experiment setup**

# Experimental Results:

## *$nTiO_2$ transport experiment:*



# Mathematical Model:

Solution obtained through COMSOL

**Ripening mechanism observed**:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} - k_{att}\psi c + \frac{\rho_b}{\theta}k_{det}s$$

$$\frac{\rho_b}{\theta}\frac{\partial s}{\partial t} = k_{att}\psi c - \frac{\rho_b}{\theta}k_{det}s$$

$$\psi = 1 + As^{\beta}$$

Initial condition: $c(x,0) = 0$, $s(x,0) = 0$

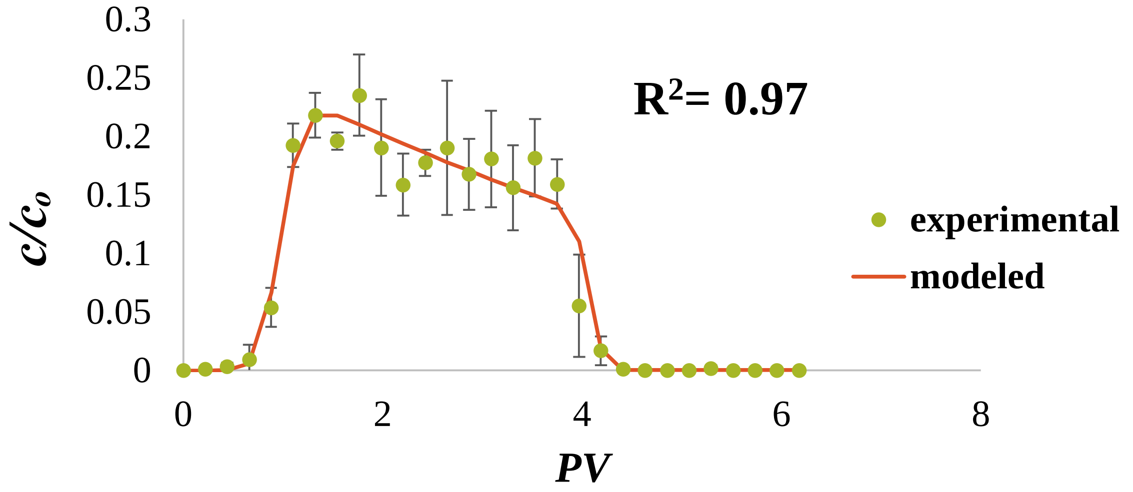
Boundary condition: $c(0,t) = c_o \ (t < t_0)$

$c(0,t) = 0 \ (t \geq t_0)$

$-D\frac{\partial c}{\partial x}(L,t) = 0$

- $\boldsymbol{\theta}$ is the porosity of porous media before the injection of the particles [-],
- $\boldsymbol{k_{att}}$ is the first-order coefficient of particle attachment in the secondary minimum ($T^{-1}$)
- $\boldsymbol{k_{det}}$ is the first-order coefficient of particle detachment from the secondary minimum ($T^{-1}$)
- $\boldsymbol{\psi}$ is dimensionless function accounting for particle ripening
- $\boldsymbol{\beta}$**=1**,is an empirical parameter that controls the shape of the colloid spatial distribution
- $\boldsymbol{A}$ multiplier coefficient

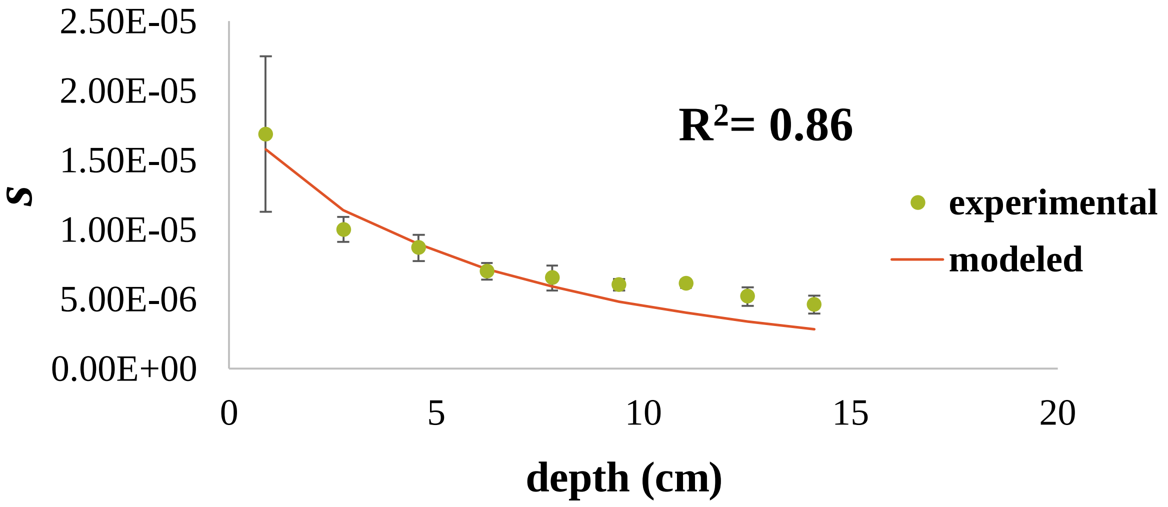
# Comparison of simulated and experimental BTC and retention profile:




Breakthrough curve for $nTiO_2$ through porous media

Optimized parameter values using COMSOL:

$k_{att}$ = 0.052926/min
$k_{det}$ = 1x$10^{-5}$/min
$A$ =50997




Retention profile for $nTiO_2$ through porous media

# Conclusion:

- $nTiO_2$ transport through porous media has been observed to follow ripening mechanism.
- Experimental results were fitted with a 1D model accounting for ripening.

# Future Work:

- Column experiments for studying the transport of $nTiO_2$ in the presence of biofilm is going on, followed by developing a mathematical model.

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# Thank you