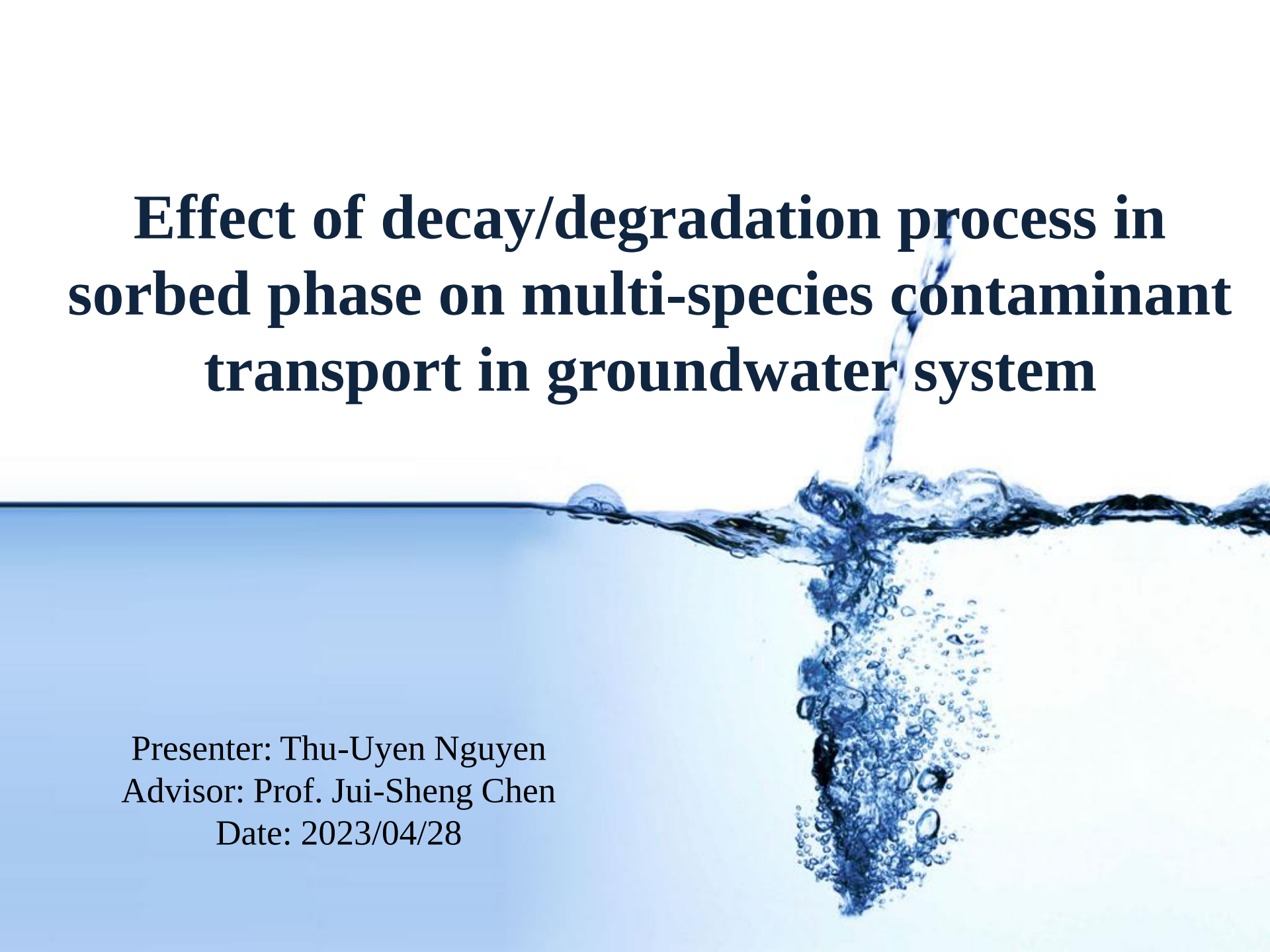
Effect of decay/degradation process in sorbed phase on multi-species contaminant transport in groundwater system



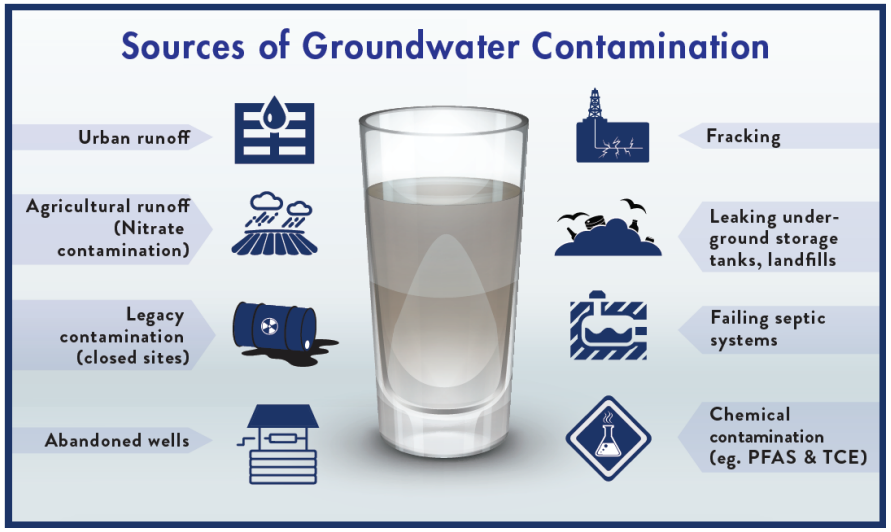
Presenter: Thu-Uyen Nguyen
Advisor: Prof. Jui-Sheng Chen
Date: 2023/04/28

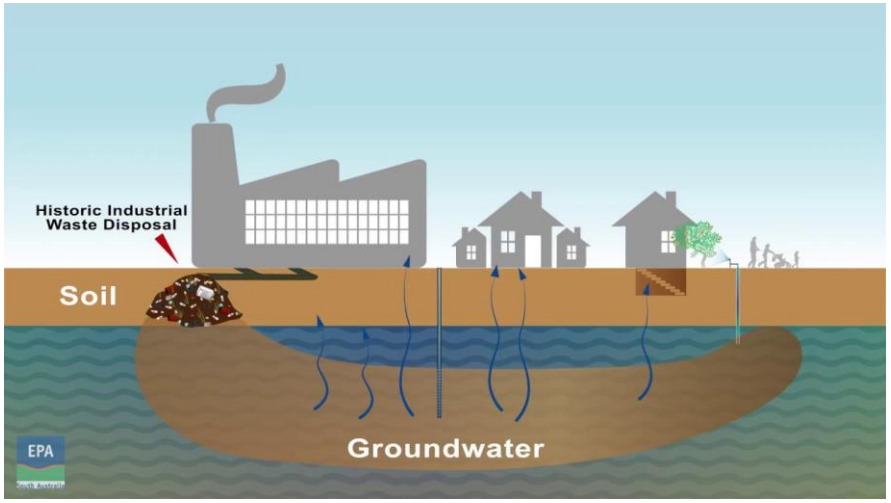
OUTLINE:

1. Introduction
2. Mathematical model
3. Preliminary results
4. Conclusions
5. Future work

1. Introduction

Groundwater contamination





- Drinking contaminated groundwater can have serious health effects.
- Diseases such as hepatitis and dysentery may be caused by contamination from septic tank waste.
- Poisoning may be caused by toxins that have leached into well water supplies.
- Certain types of cancer may also result from exposure to polluted water.

It is important to **understand about fate and transport of contaminant** in groundwater system

Advection-dispersion equations (ADEs)

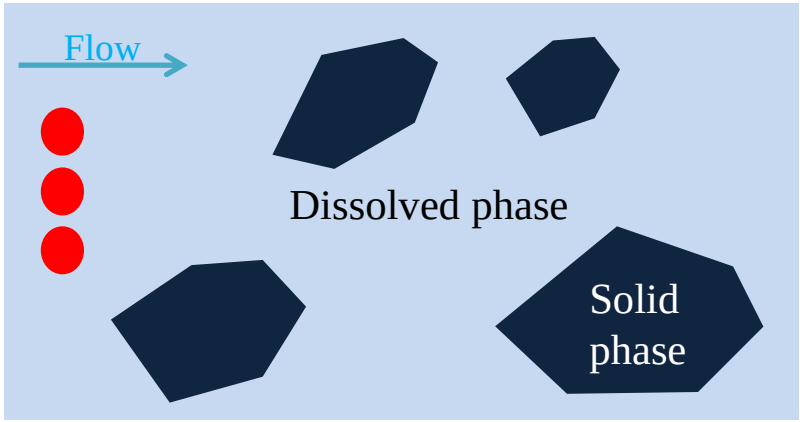
- ADEs describe the transport of dissolved solutes in groundwater.
- Using mathematical methods (numerical methods or **analytical methods**) to solve the advection-dispersion equations (ADEs).

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} \pm F$$

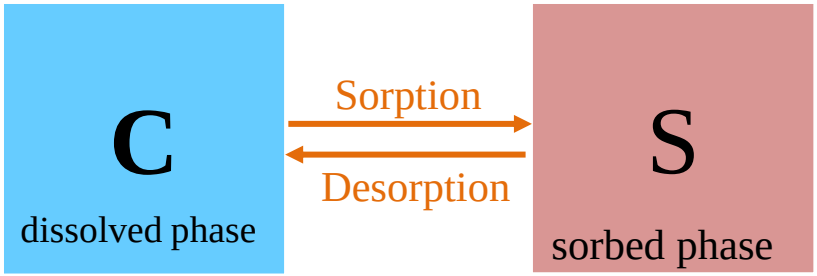
F: all other physical, biological, chemical processes

Advection

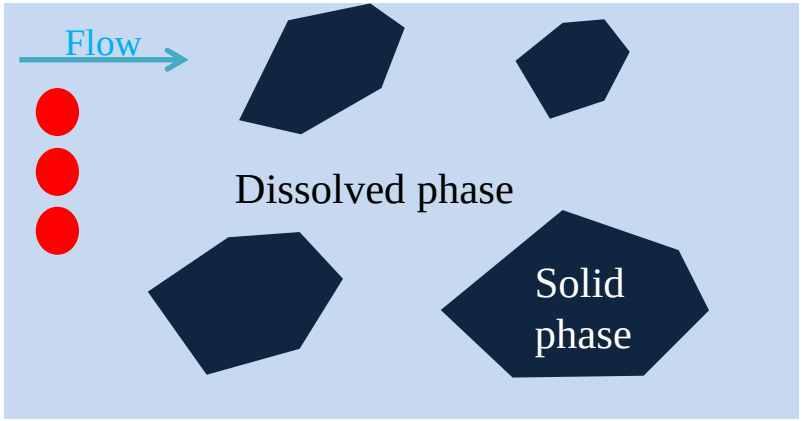
Dispersion



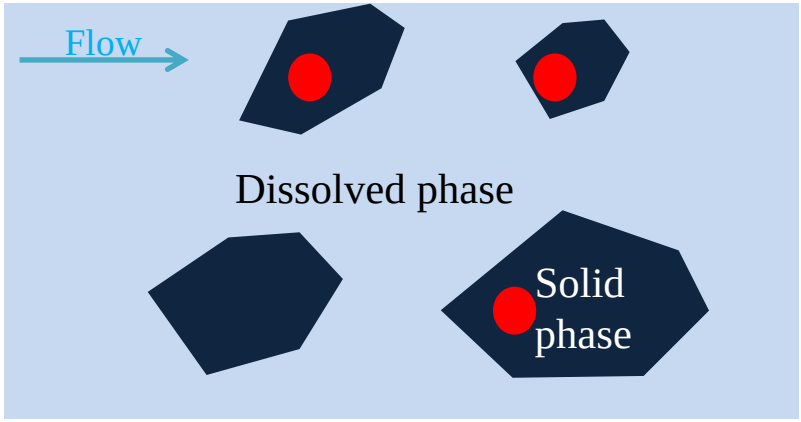
Sorption process

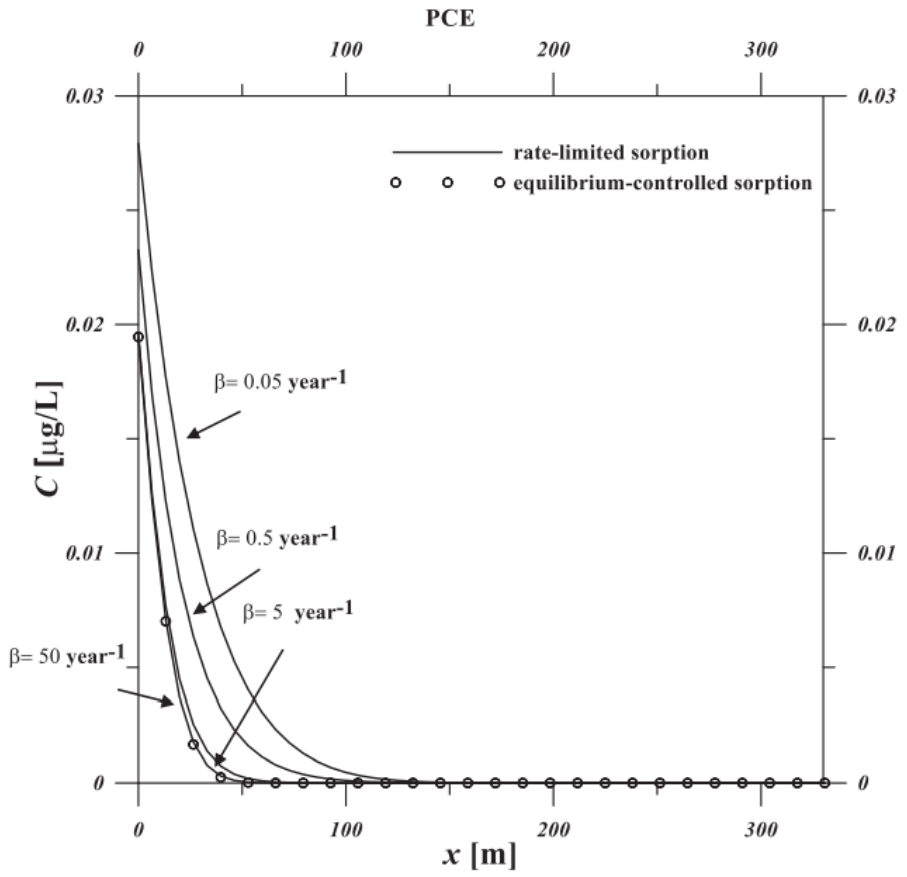


Sorption



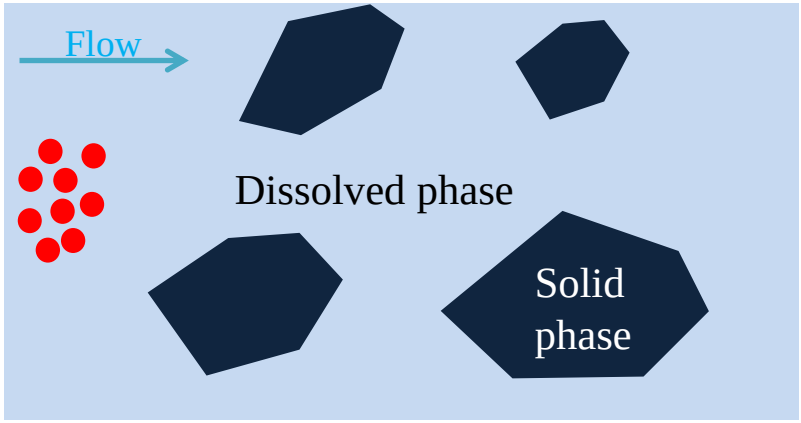
Desorption





(Chen et al., 2019)

Degradation Process

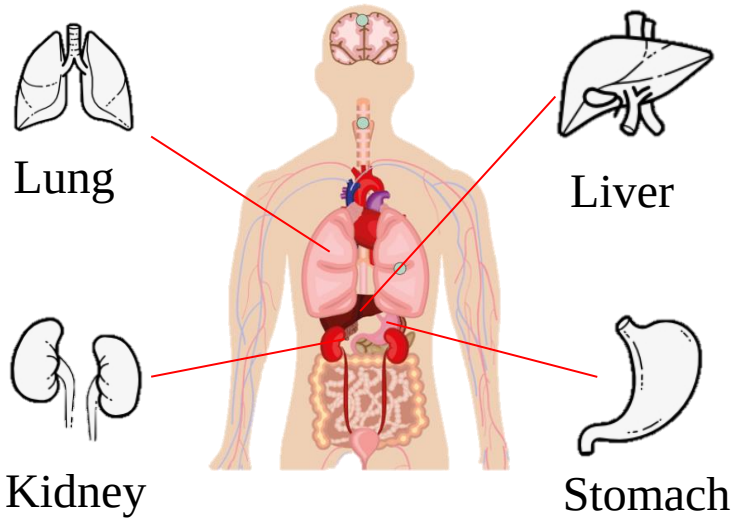


Multispecies contaminant

- **Parent species**
- **Daughter species**

PCE → TCE → DCE → VC → ETH

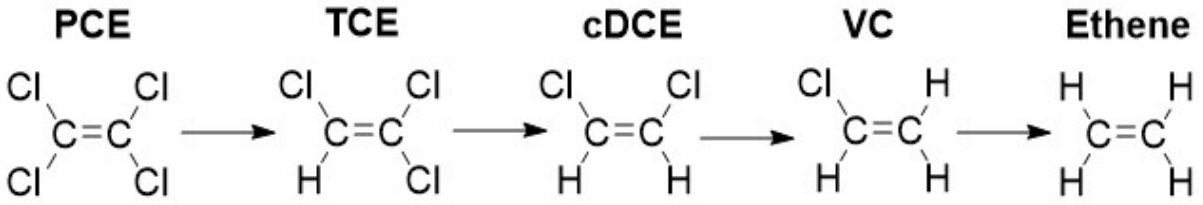
$Pu^{238} \rightarrow U^{234} \rightarrow Th^{230} \rightarrow Ra^{226}$



- Damage the DNA in our cells.
- High doses can cause Acute Radiation Syndrome (ARS) or Cutaneous Radiation Injuries (CRI).
- High doses can cause cancer, could harm fetuses, and can even lead to death.

Degradation/decay in sorbed phase

Degradation in the sorbed phase have a **negligible effect** on the concentrations of **organic contaminants**.



What about another multispecies contaminants?

Radioactive Waste

$$U^{238} \rightarrow U^{234} \rightarrow Th^{230} \rightarrow Ra^{226} \rightarrow Rn^{222} \rightarrow Pb$$

$$Pu^{238} \rightarrow U^{234} \rightarrow Th^{230} \rightarrow Ra^{226} \rightarrow Rn^{222} \rightarrow Pb$$

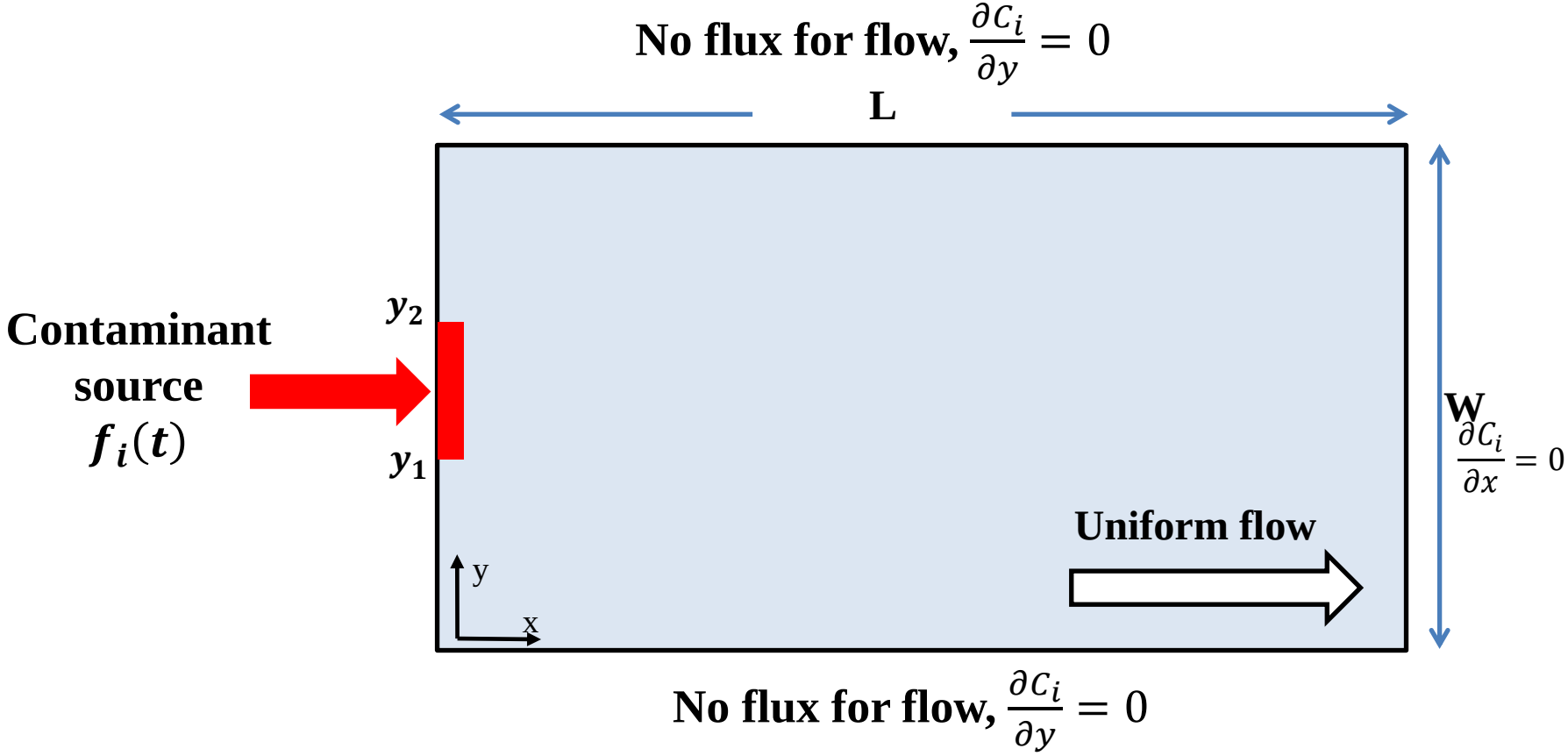
Objectives

- Develop a novel two-dimensional model to describe multi-species contaminant transport in groundwater considering decay/degradation process in the sorbed phase.

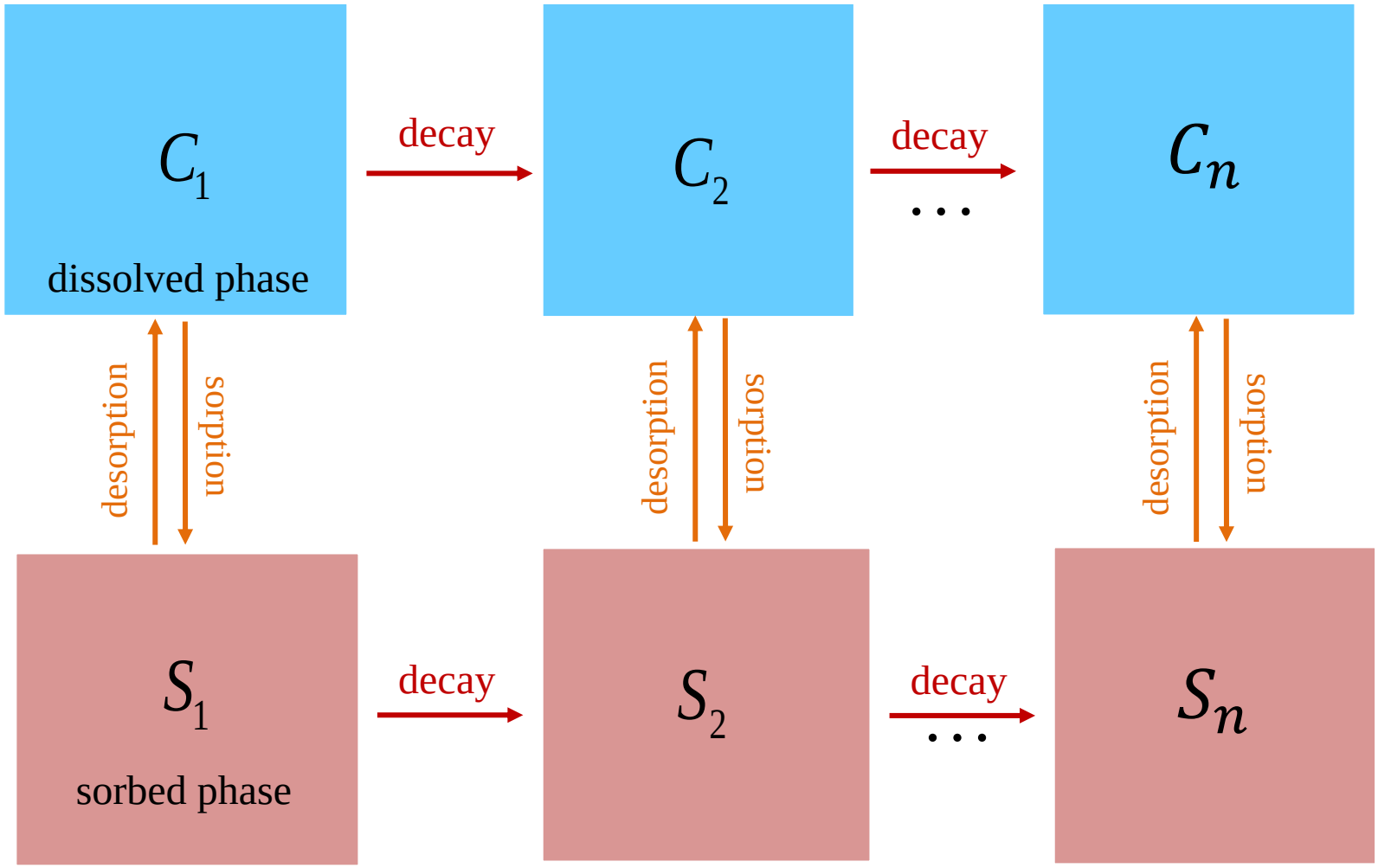
- In this study, the multispecies contaminants used to predict concentrations were chlorinated solvents and radionuclide. The sorption process is assumed to be rate-limited sorption with constant sorption rate.

2. Mathematical model

Conceptual model



Schematic diagram for multispecies transport



Governing equation

Dissolved phase:

Dispersion | Advection | Decay

$$D_L \frac{\partial^2 C_i(x,y,t)}{\partial x^2} + D_T \frac{\partial^2 C_i(x,y,t)}{\partial y^2} - v \frac{\partial C_i(x,y,t)}{\partial x} - \lambda_i C_i(x,y,t) + \lambda_{i-1} C_{i-1}(x,y,t) - \frac{\beta}{\theta}\left(C_i(x,y,t) - \frac{S_i(x,y,t)}{K_i}\right) = \frac{\partial C_i(x,y,t)}{\partial t}$$

Sorption

$$i = 1, 2, 3, \ldots$$

Sorbed Phase:

Decay

$$\rho_b \frac{\partial S_i(x,y,t)}{\partial t} = \beta_i\left(C_i(x,y,z,t) - \frac{S_i(x,y,t)}{K_i}\right) - \rho_b \gamma_i S_i(x,y,z,t) + \rho_b \gamma_{i-1} S_{i-1}(x,y,z,t)$$

$\boldsymbol{C_i(x,y,t)}$: Concentration in dissolved phase (M/L^3)

$\boldsymbol{S_i(x,y,t)}$: Concentration in sorbed phase (M/L^3)

$\boldsymbol{D_L}$: Longitudinal Dispersion coefficient (M^2/T)

$\boldsymbol{D_T}$: Transverse Dispersion coefficient (M^2/T)

$\boldsymbol{v}$: The flow velocity (L/T)

γ_i: Decay rate of specie i^{th} in sorbed phase(T^{-1})

$\boldsymbol{\lambda_i}$: Decay rate of specie i^{th} (T^{-1})

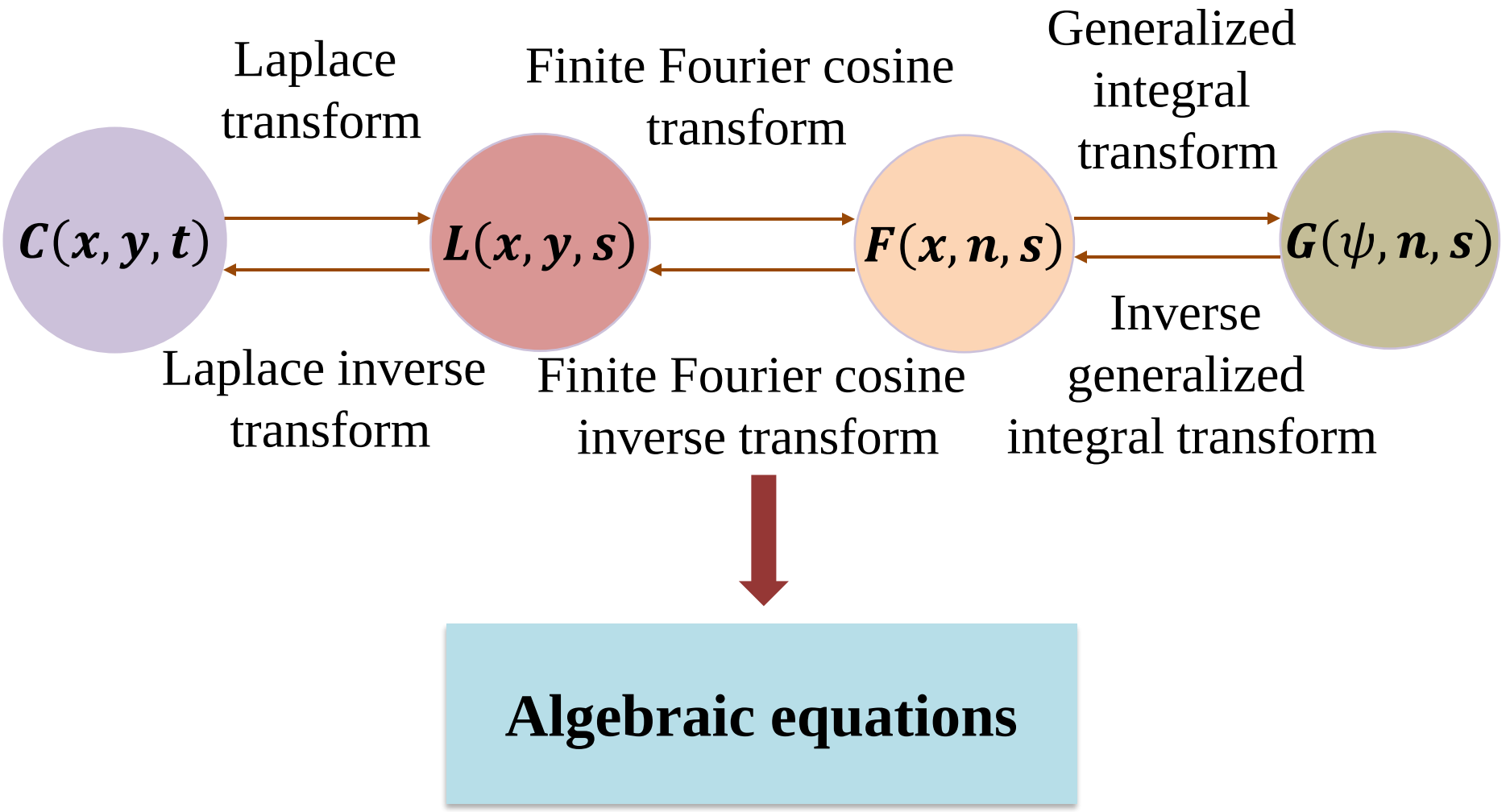
$\boldsymbol{\beta}$: Kinetic sorption rate (T^{-1})

$\boldsymbol{\theta}$: The porosity (-)

$\boldsymbol{\rho_b}$: Bulk density of material (M/L^3)

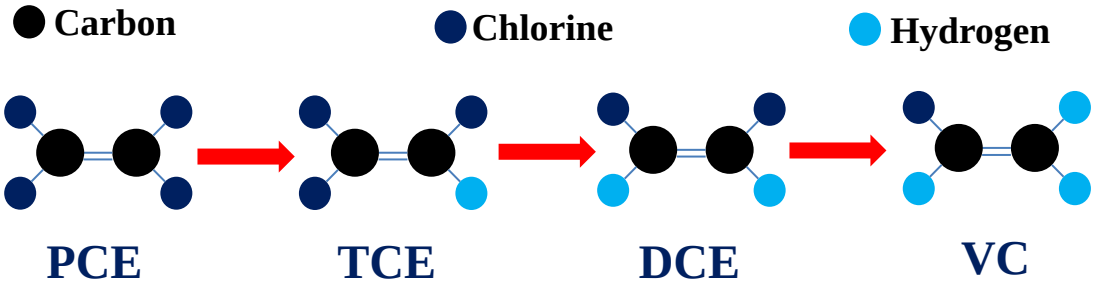
$\boldsymbol{K_i}$: The distribution coefficient (L^3/M)

Solving procedure

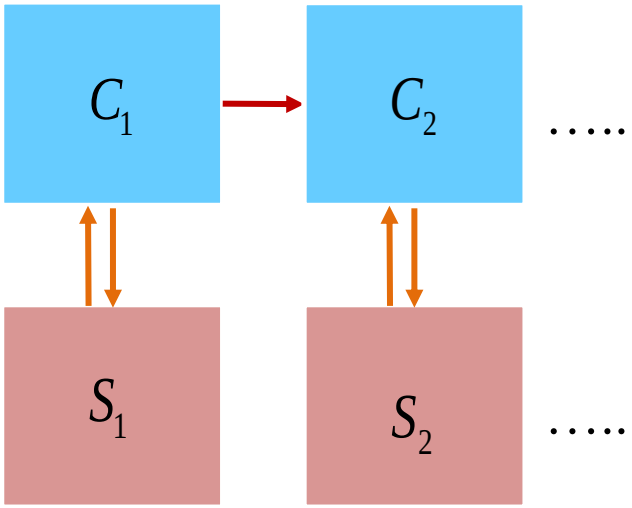


3. Preliminary results

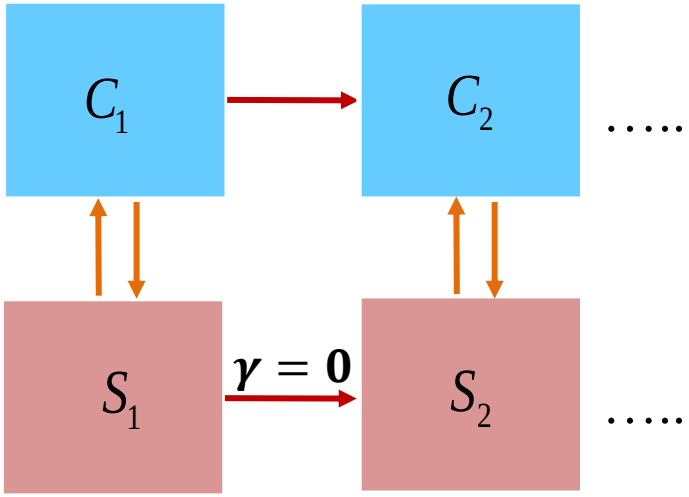
Verification example



Laplace transform finite different (LTFD)



Current study



Parameters for verification

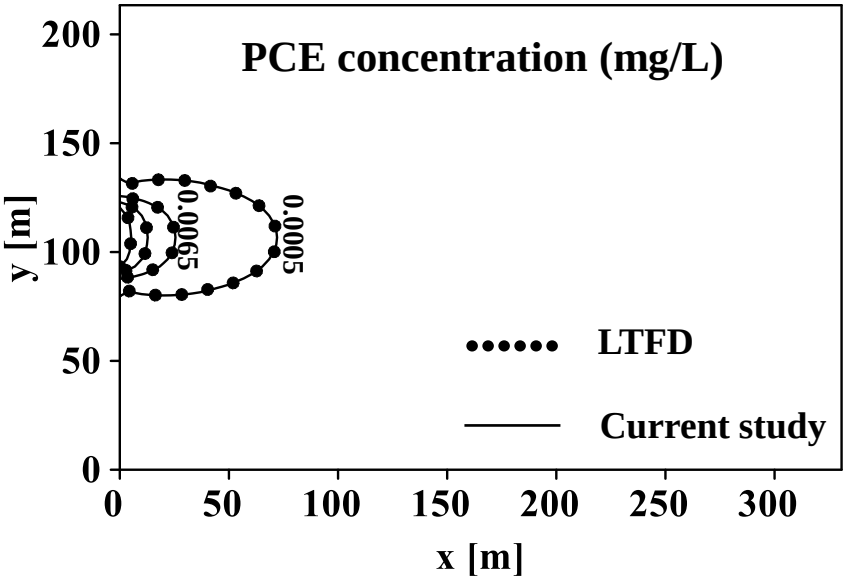
Domain length, L [m]	330.7
Domain width, W [m]	213.4
Seepage velocity, v [m/year]	34
Longitudinal dispersivity, α_L [m]	29.4
Longitudinal Dispersion coefficient, D_L [m^2/year]	1000
Transverse Dispersion coefficient, D_T [m^2/year]	100
Bulk density, ρ_b [kg/L]	1.6
Effective porosity, θ [-]	0.2
Sorption reaction rate constant, β [$year^{-1}$]	**0.5**

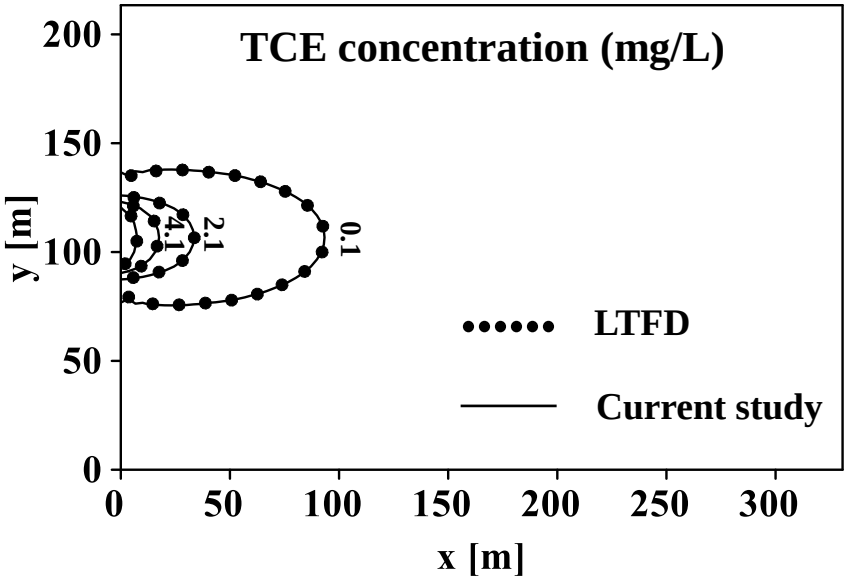
(United States Environmental Protection Agency, USEPA)

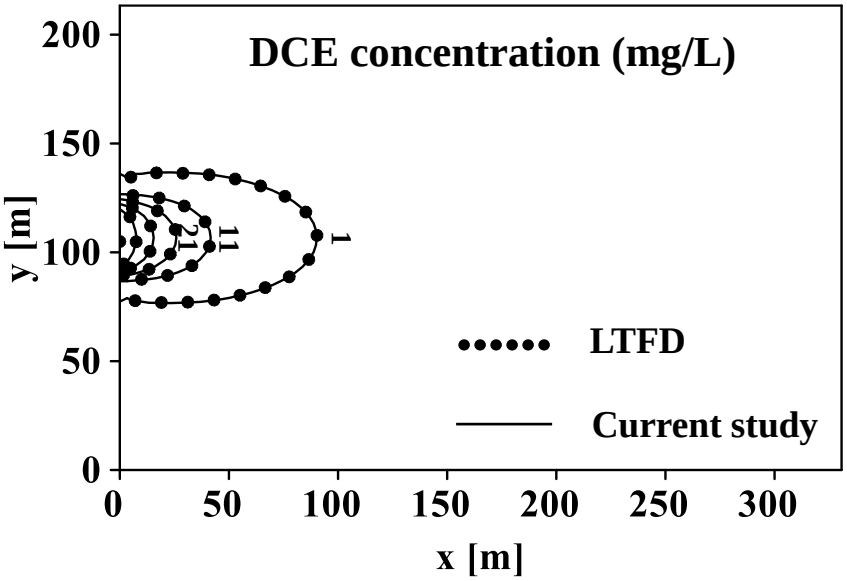
Decay constant rate in solid phase, γ_i[$year^{-1}$]	
PCE	0
TCE	0
DCE	0
VC	0

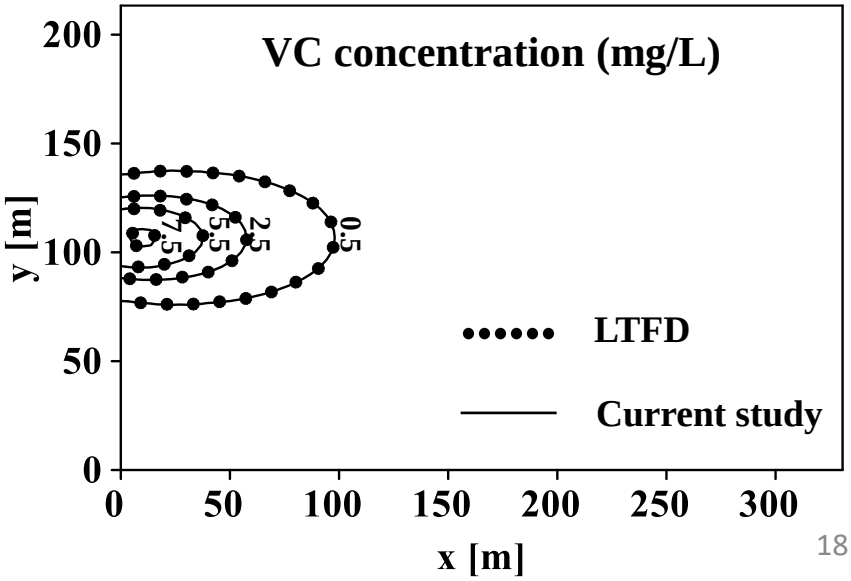
Distribution coefficient, K_i [L/kg]	
PCE	0.784
TCE	0.239
DCE	0.23
VC	0.0545
Decay constant rate in dissolve phase, λ_i [$year^{-1}$]	
PCE	2
TCE	1
DCE	0.7
VC	0.4
Source concentration, $c_{i,0}$ [mg/L]	
PCE	0.056
TCE	15.8
DCE	98.5
VC	3.08
Retardation factor, R_i [-]	
PCE	7.1
TCE	2.9
DCE	2.8
VC	1.4

Verification









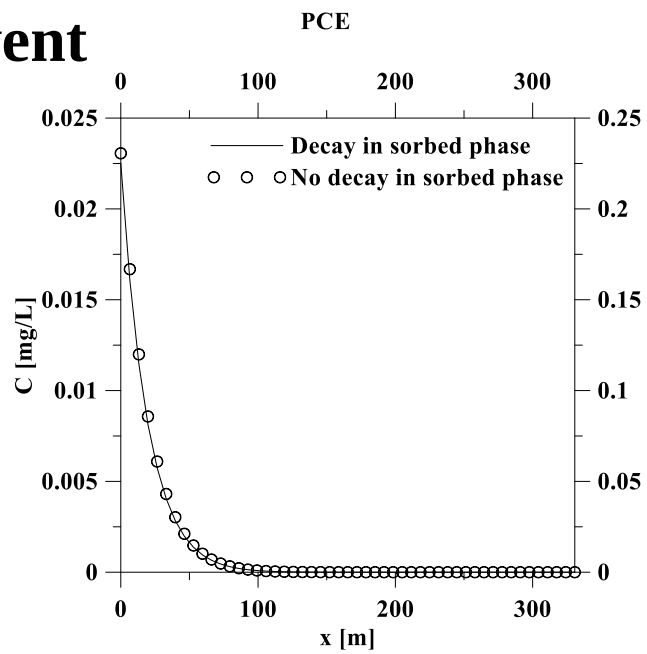
Effect of decay rate in sorbed phase

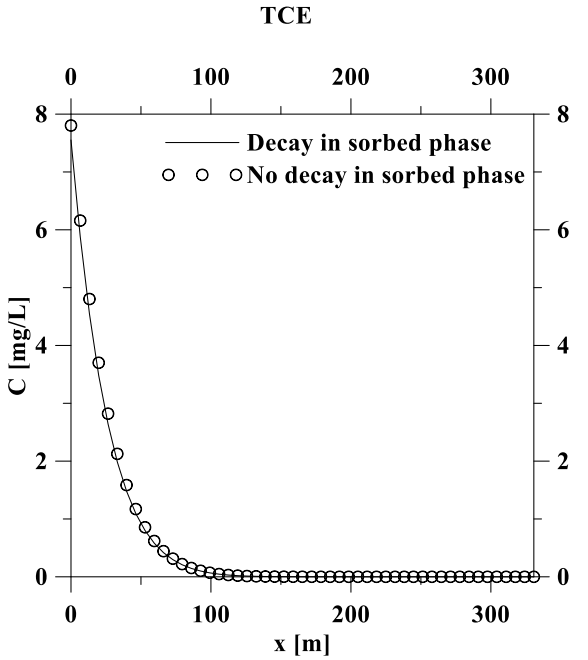
For chlorinated solvent

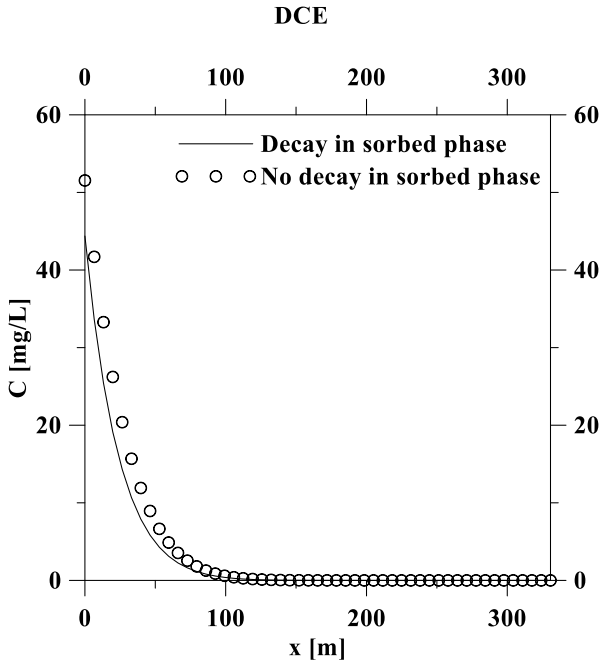
Time: 1 year

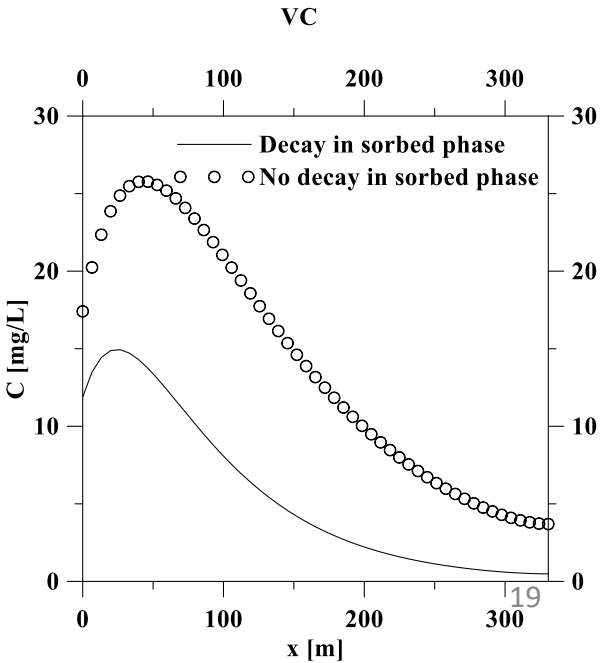
λ_i [year^{-1}]	
PCE	2
TCE	1
DCE	0.7
VC	0.4

γ_i [year^{-1}]	
PCE	2
TCE	1
DCE	0.7
VC	0.4









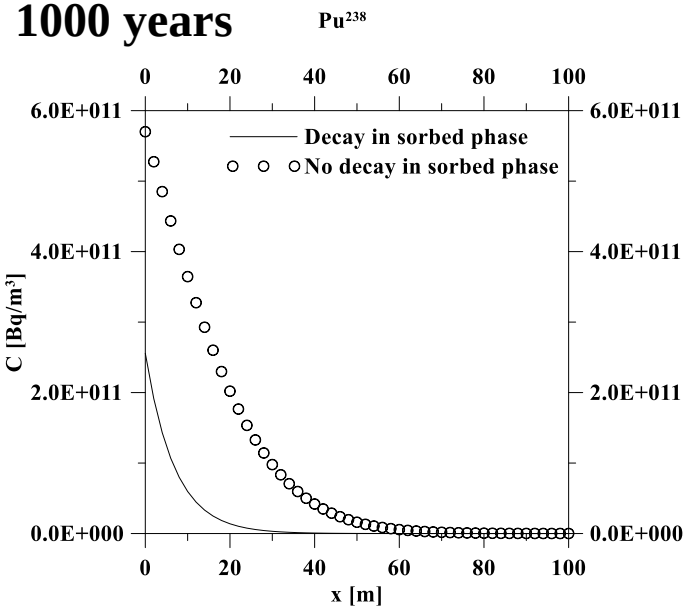
Parameter for radionuclide decay chain

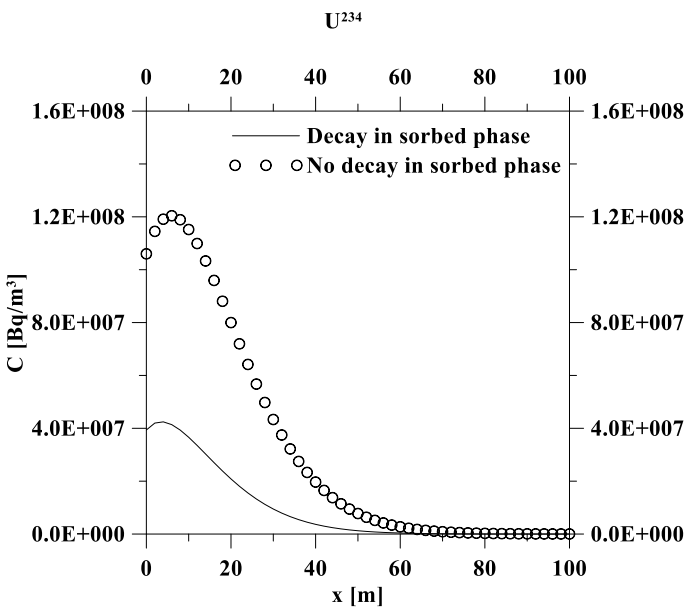
Parameter	Value
Domain length, L [m]	100
Domain width, W [m]	50
Seepage velocity, v [m/year]	100
Longitudinal Dispersion coefficient, D_L [m^2/year]	2000
Transverse Dispersion coefficient, D_T [m^2/year]	200
Bulk density, ρ_b [kg/L]	1.5
Effective porosity, θ [-]	0.25
Sorption reaction rate constant, β [$year^{-1}$]	0.5
Distribution coefficient, K_i [L/kg]	
Pu^{238}	1667
U^{234}	2333
Th^{230}	8333
Ra^{226}	83.2
Decay constant rate in dissolved phase, λ_i [$year^{-1}$]	
Pu^{238}	0.0079
U^{234}	0.0000028
Th^{230}	0.0000087
Ra^{226}	0.00043
Decay constant rate in sorbed phase, γ_i [$year^{-1}$]	
Pu^{238}	0.0079
U^{234}	0.0000028
Th^{230}	0.0000087
Ra^{226}	0.00043
Source concentration, $c_{i,0}$ [Bq/m^3]	
Pu^{238}	$1x10^{12}$
U^{234}	0
Th^{230}	0
Ra^{226}	0

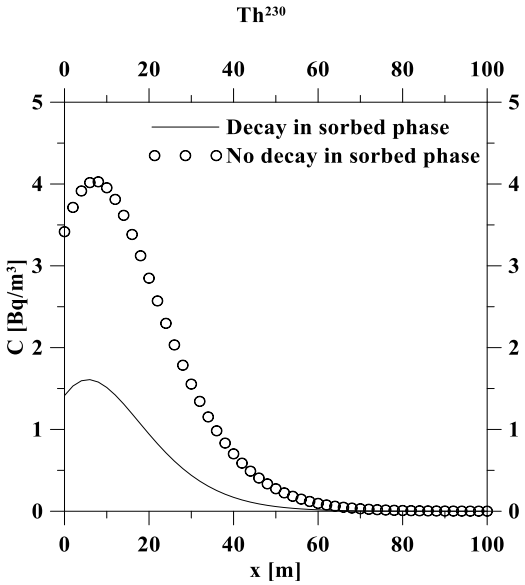
Effect of decay rate in sorbed phase

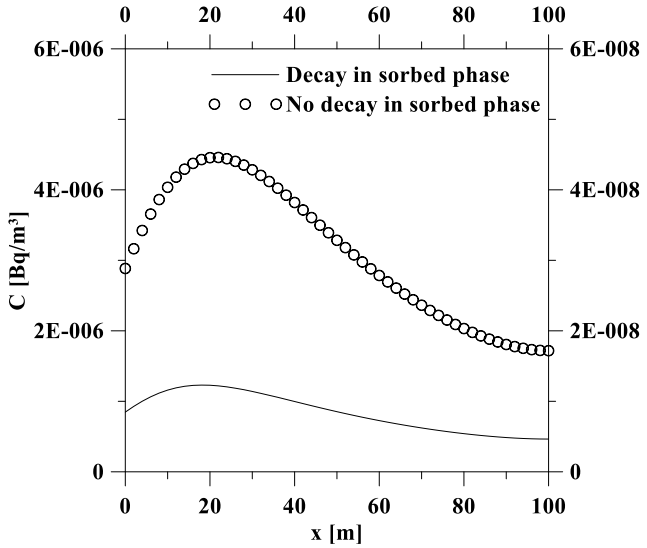
for radionuclide decay chain

Time: 1000 years









4. Conclusions

→ In this study, two examples with and without degradation in the sorbed phase were considered. Predicting the concentrations of multispecies contaminants is obviously affected by the decay/degradation process in the sorbed phase.

→ When compared to the situation without decay/degradation in the sorbed phase, the concentrations of species with decay/degradation in the sorbed phase tend to decrease.

→ For chlorinated solvents, degradation in the sorbed phase did not significantly change the predicted concentrations of species such as PCE and TCE, but the difference was gradually more pronounced in daughter species such as DCE and VC.

→ When decay in the sorbed phase is taken into account, the concentrations of all species on the radionuclide decay chain significantly decrease.

(Note that the decay rate in sorbed phase is assumed to be equal to in the dissolved phase. The given results are only consistent with the parameters mentioned in this study.)

5. Future work

- Verify the model by comparison with other models that take into account decay in sorbed phase.

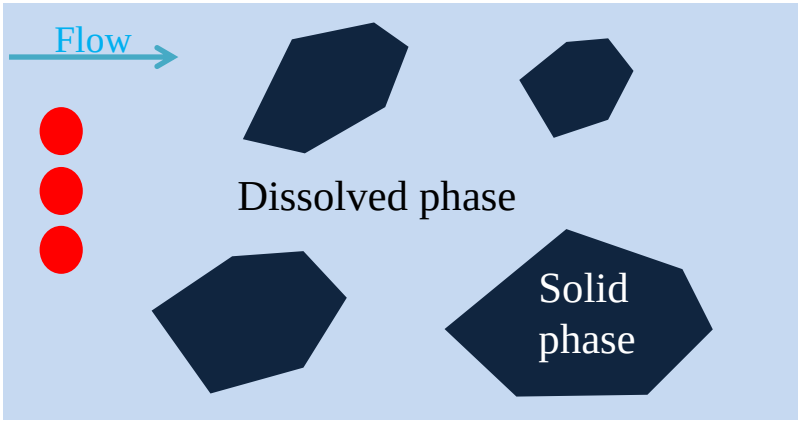
- Use different sorption rate values and compare with equilibrium-controlled sorption.

- Apply different inlet boundary conditions such as exponentially decaying or pulse loading.

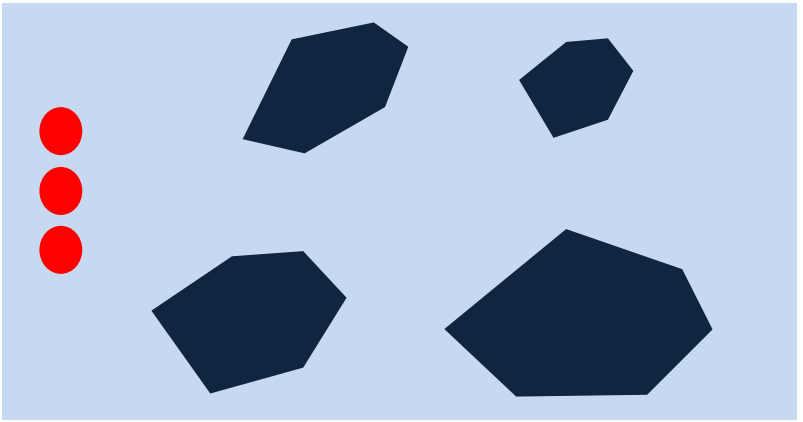
Thank you for your attention!

Transport mechanism of contaminants

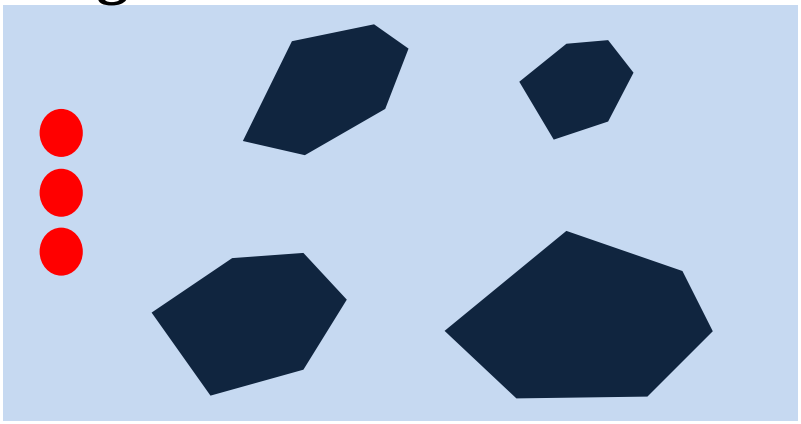
Advection



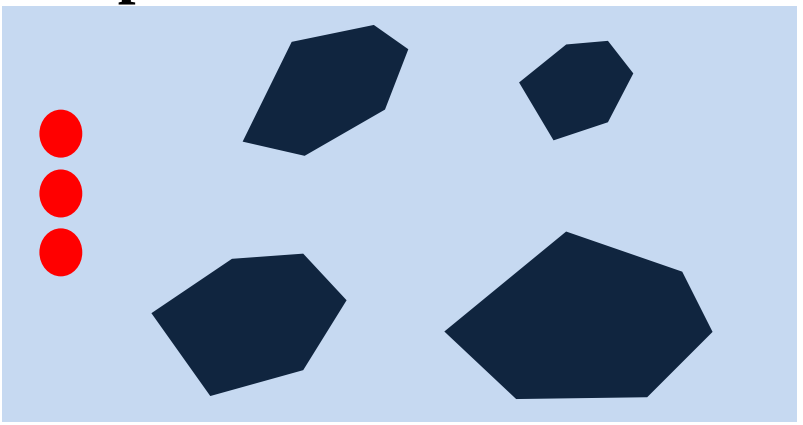
Dispersion



Degradation



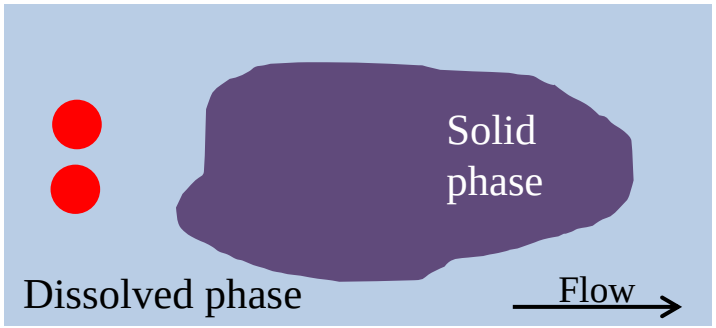
Sorption



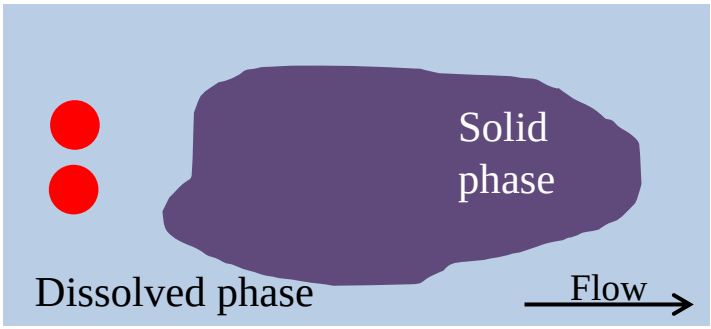
Effect of sorption rate

β: Sorption rate (time^{-1})

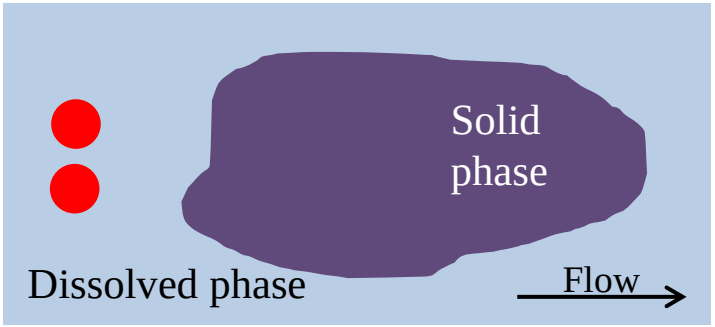
β = 0.5 year^{-1}



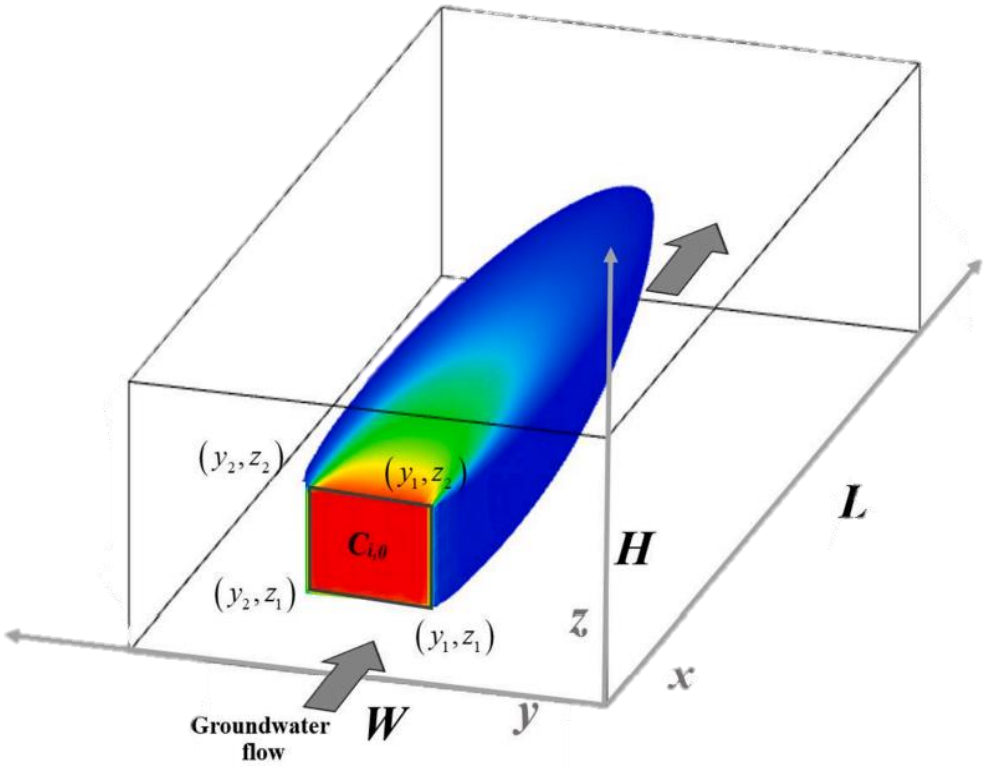
β = 5 year^{-1}



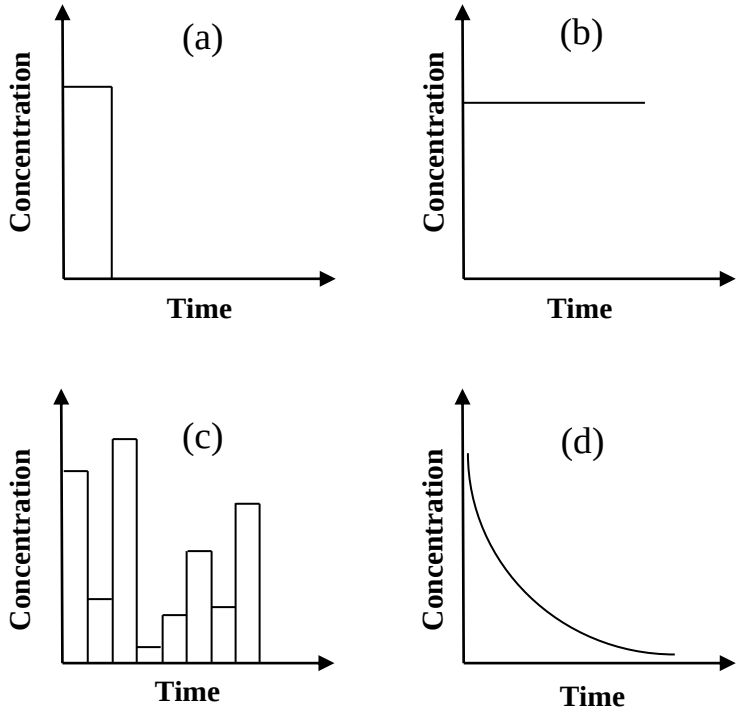
$\beta \rightarrow \infty$ **(Equilibrium-controlled sorption)**



Effect of different inlet boundary conditions



(*Liao et al., 2021*)



Concentration - time functions are used to characterize contaminant loadings from various types of source (*Zheng and Bennett, 2002*)

(a) Pulse loading
(b) Constant concentration
(c) Variable concentration
(d) Decaying concentration