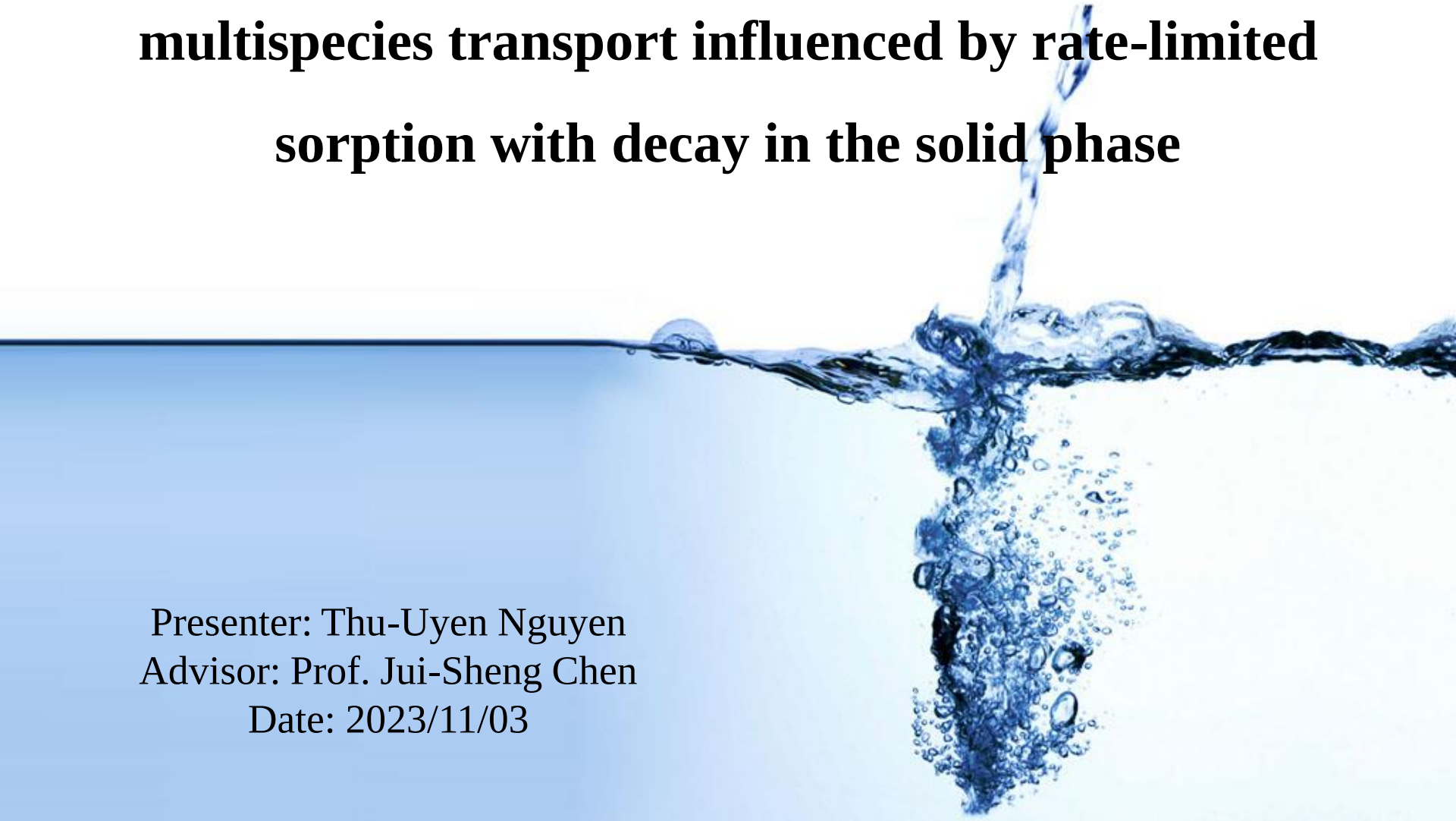
A two-dimensional semi-analytical model for multispecies transport influenced by rate-limited sorption with decay in the solid phase



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Date: 2023/11/03

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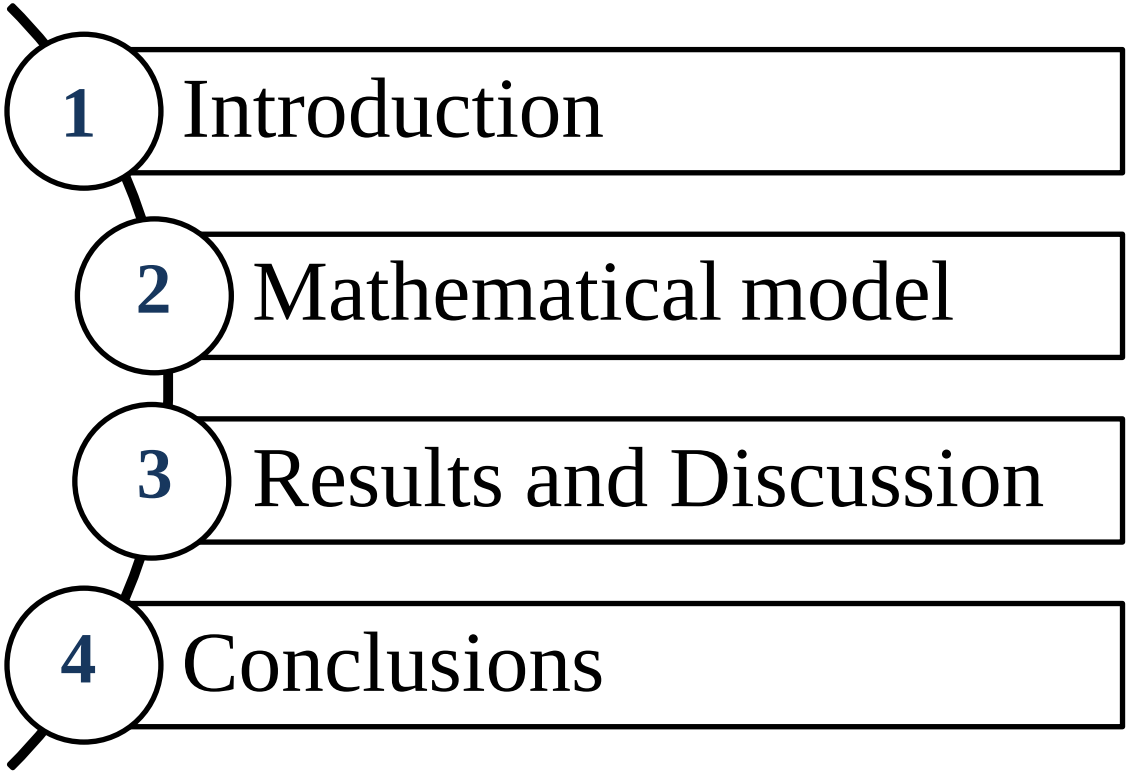
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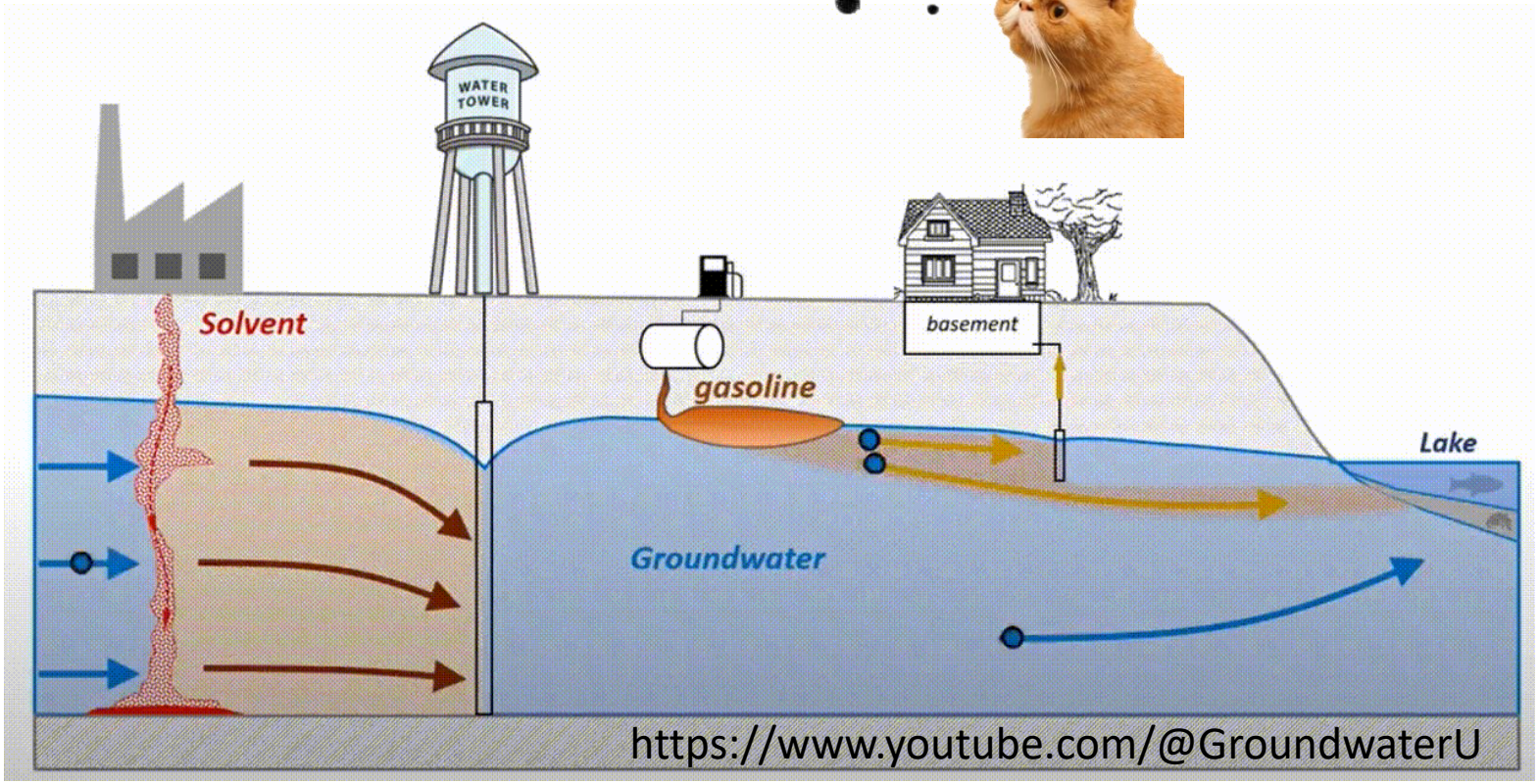
1. Introduction

Groundwater contamination

- 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.

How can we understand about **fate and transport of contaminant** in groundwater system?



Mathematical methods

- The advection-dispersion equations (ADEs) describe the transport of dissolved solutes in groundwater.

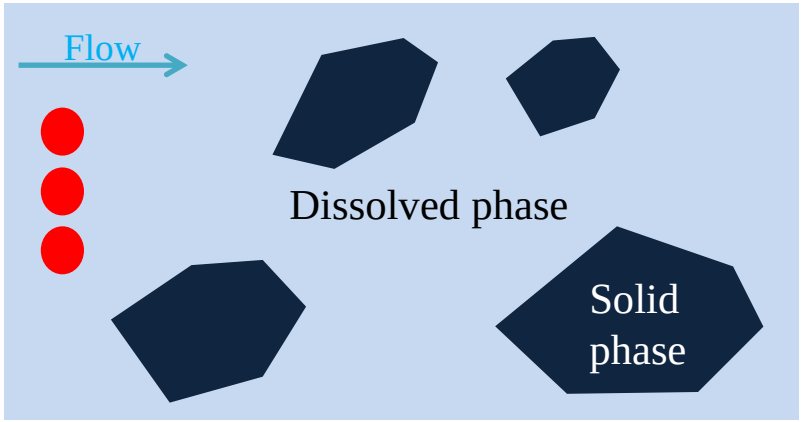
- Using mathematical methods (numerical methods or **analytical methods**) to solve ADEs.

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

F: all other physical, biological, chemical processes

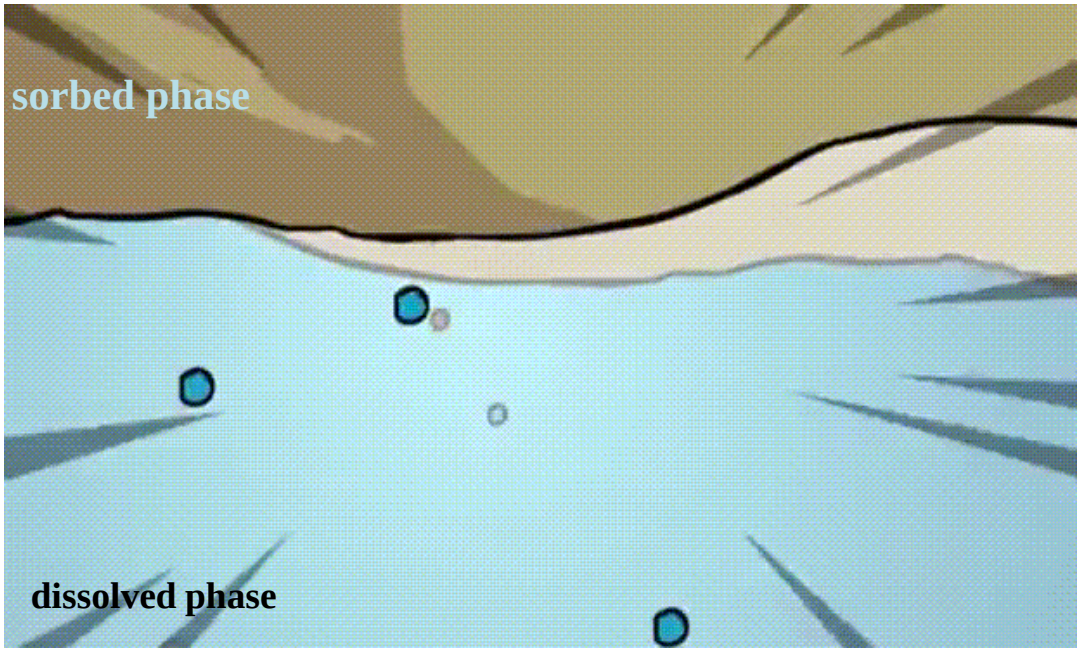
Advection

Dispersion

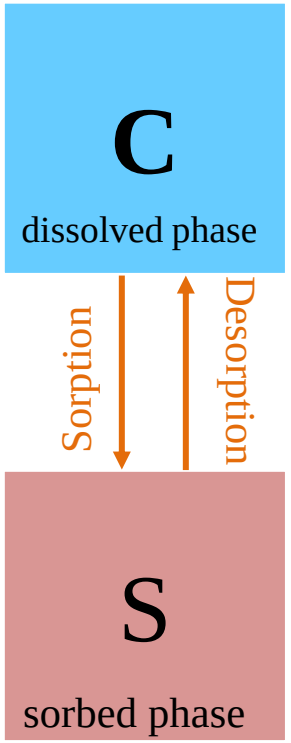


Sorption process

Control the rate at which the dissolved contaminants will partition on to the surrounding soil material.



Source: LearningGamesLab channel
https://www.youtube.com/watch?v=Az1h5qMfFQM

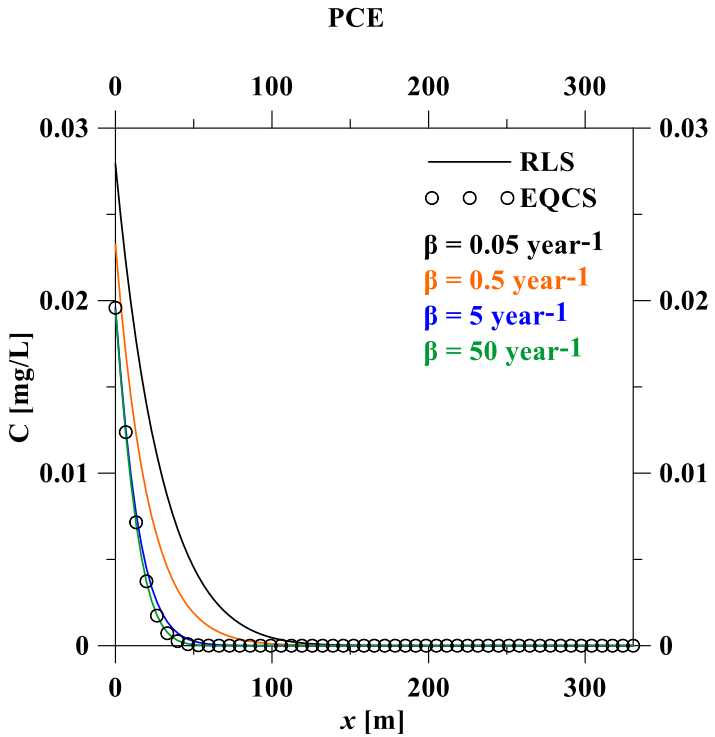


Effect of sorption rate

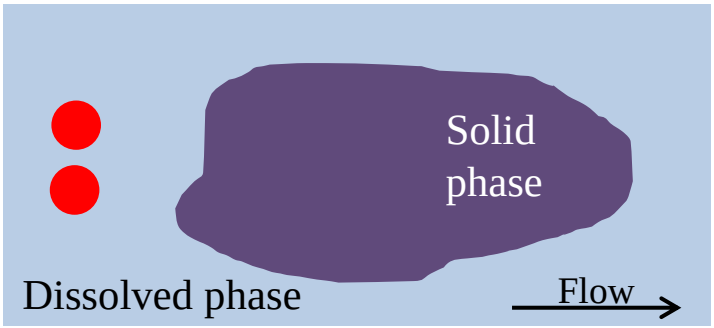
β: Sorption rate (time^{-1})

- When the sorption process is sufficiently fast compared to the time during which solutes and solid grains are in contact, sorption can be assumed as an equilibrium-controlled sorption.

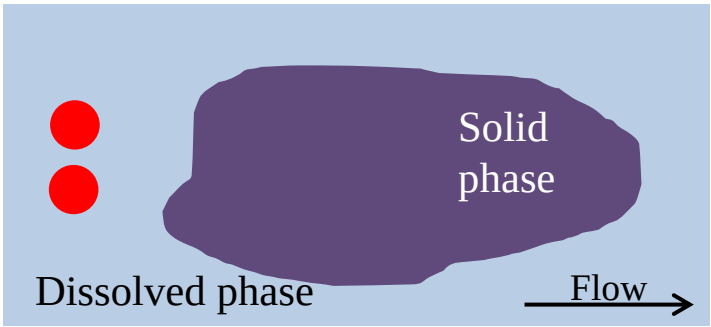
- **If not**, this process should be assumed as **rate-limited sorption**.



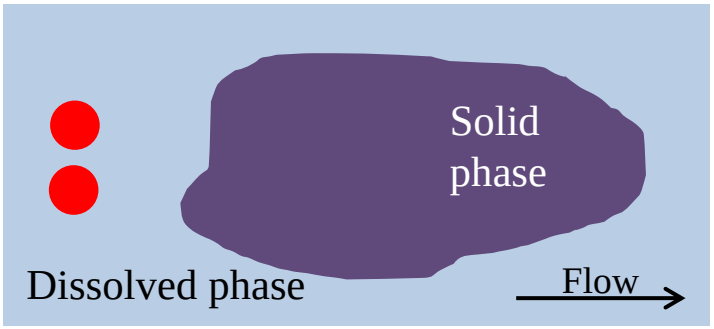
β = 0.5 year^{-1}



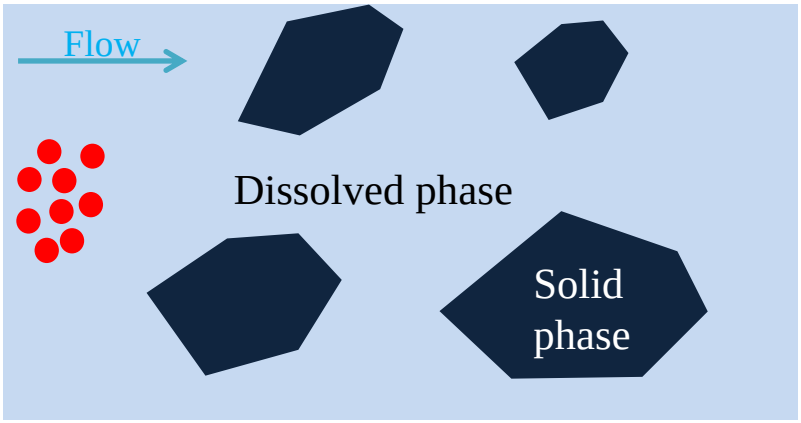
β = 5 year^{-1}



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



Decay/Degradation Process

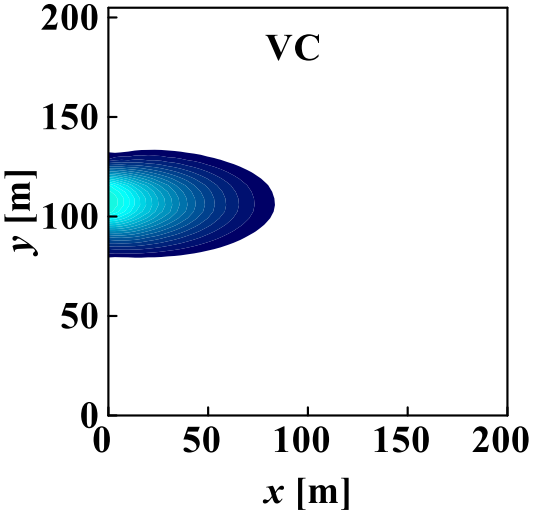


Multispecies contaminant

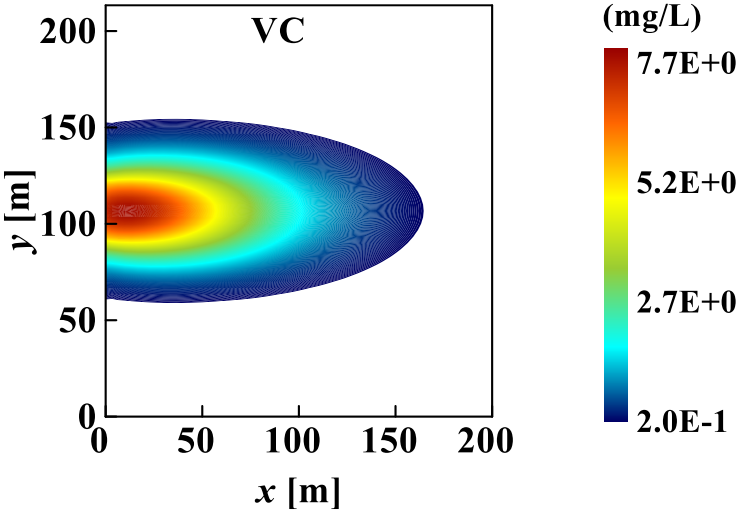
- **Parent species**
- **Daughter species**

PCE → TCE → DCE → VC → ETH

Without decay/degrade



With decay/degrade



Degradation/decay in solid phase

- Most models neglect the effect of this process on the organic contaminants transport.

- Guo et al. (2000) pointed out that degradation is inhibited for the sorbed chemicals, **it can still proceed slowly**

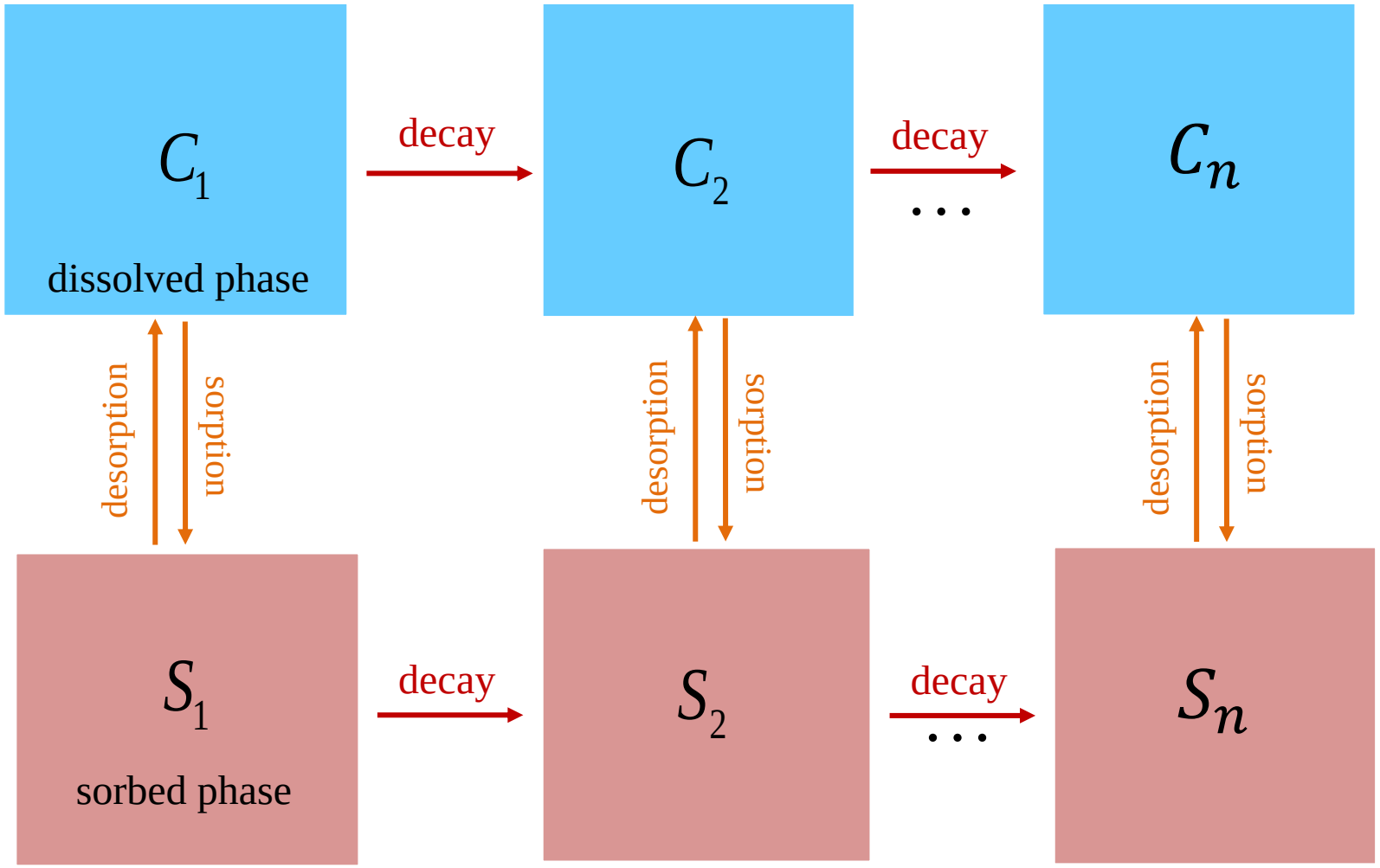
What about another multispecies contaminants?

Radioactive Waste

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

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

Schematic diagram for multispecies transport



Objectives

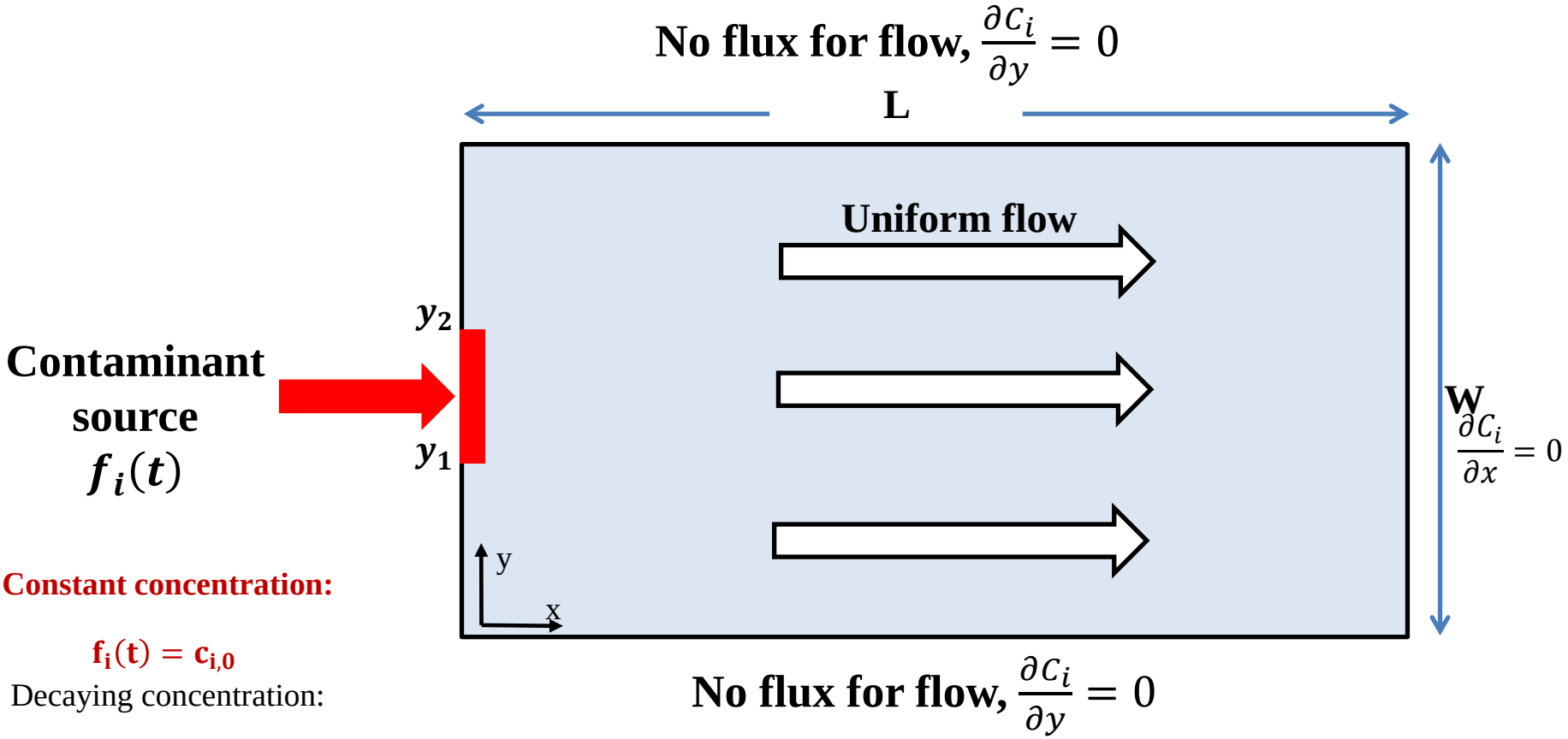
- Develop a novel two-dimensional model to describe multi-species contaminant transport in groundwater considering decay/degradation process in the sorbed phase.

- In this study, the multispecies contaminant used to predict concentrations is radionuclide decay chain. The sorption process is assumed to be rate-limited sorption with a constant sorption rate.

- The effects of decay in sorbed phase on contaminant transport in groundwater are discussed in this study.

2. Mathematical model

Conceptual model



Constant concentration:

$\mathbf{f_i(t) = c_{i,0}}$

Decaying concentration:

$$f_i(t) = c_{i,0} e^{-\lambda_{m,i} t}$$

Pulse loading:

$$f_i(t) = \begin{cases} c_{i,0} & 0 < t < t_0 \\ 0 & t > t_0 \end{cases}$$

Governing equation

Dissolved phase:

Dispersion | Advection | Decay

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

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

Sorption

Sorbed Phase:

Decay

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

$\boldsymbol{C_i(x,y,t)}$: 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})

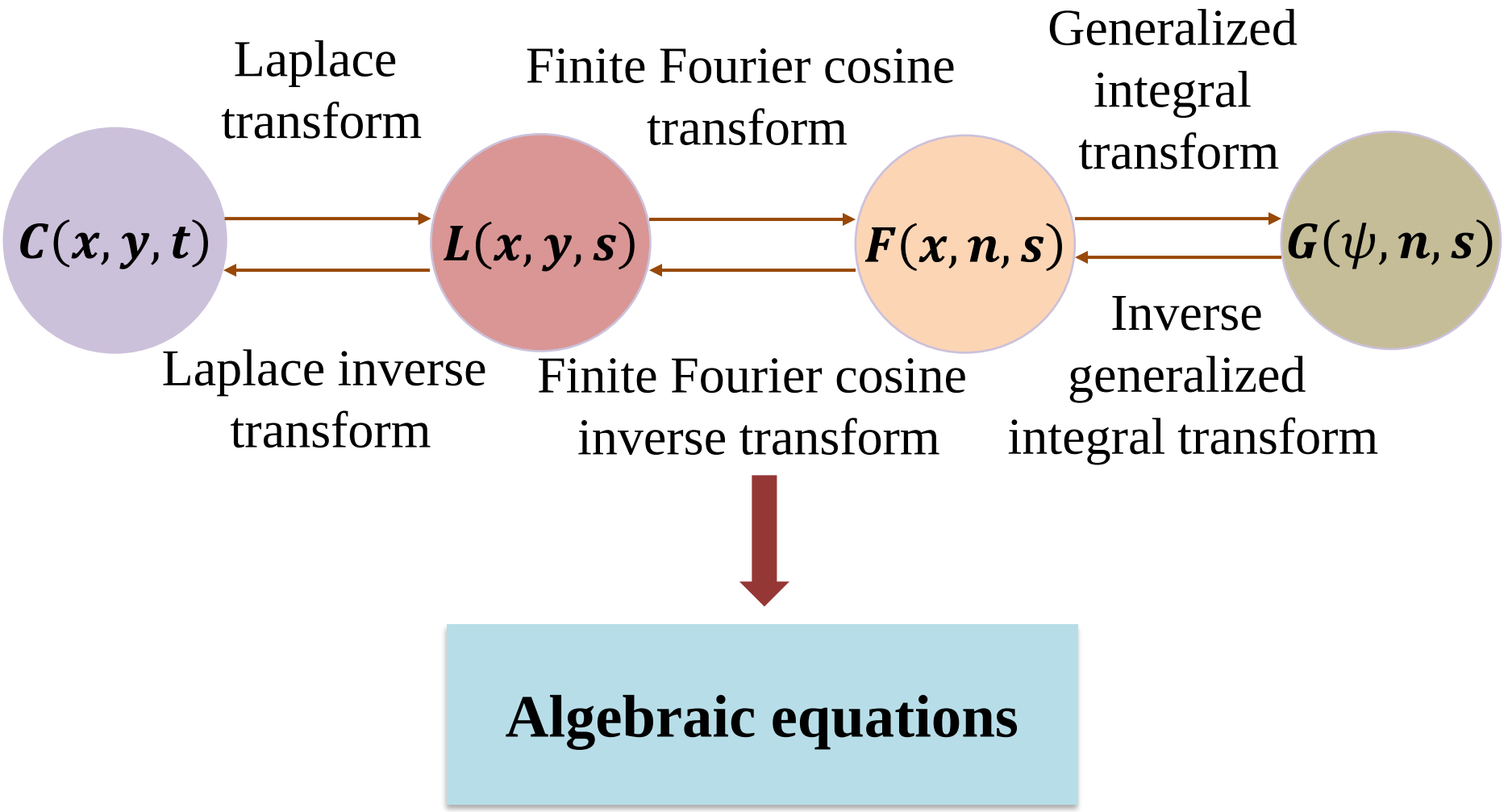
$\boldsymbol{\beta}$: Kinetic sorption rate (T^{-1})

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

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

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

Solving procedure

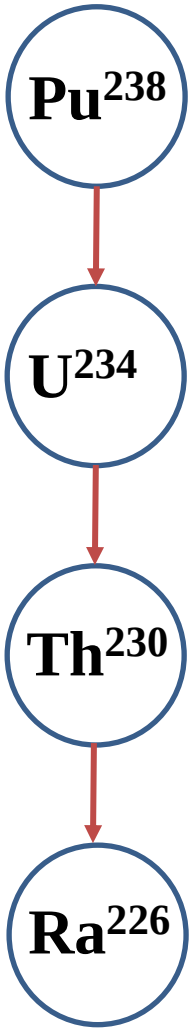


3. Results and Discussion

Verification example

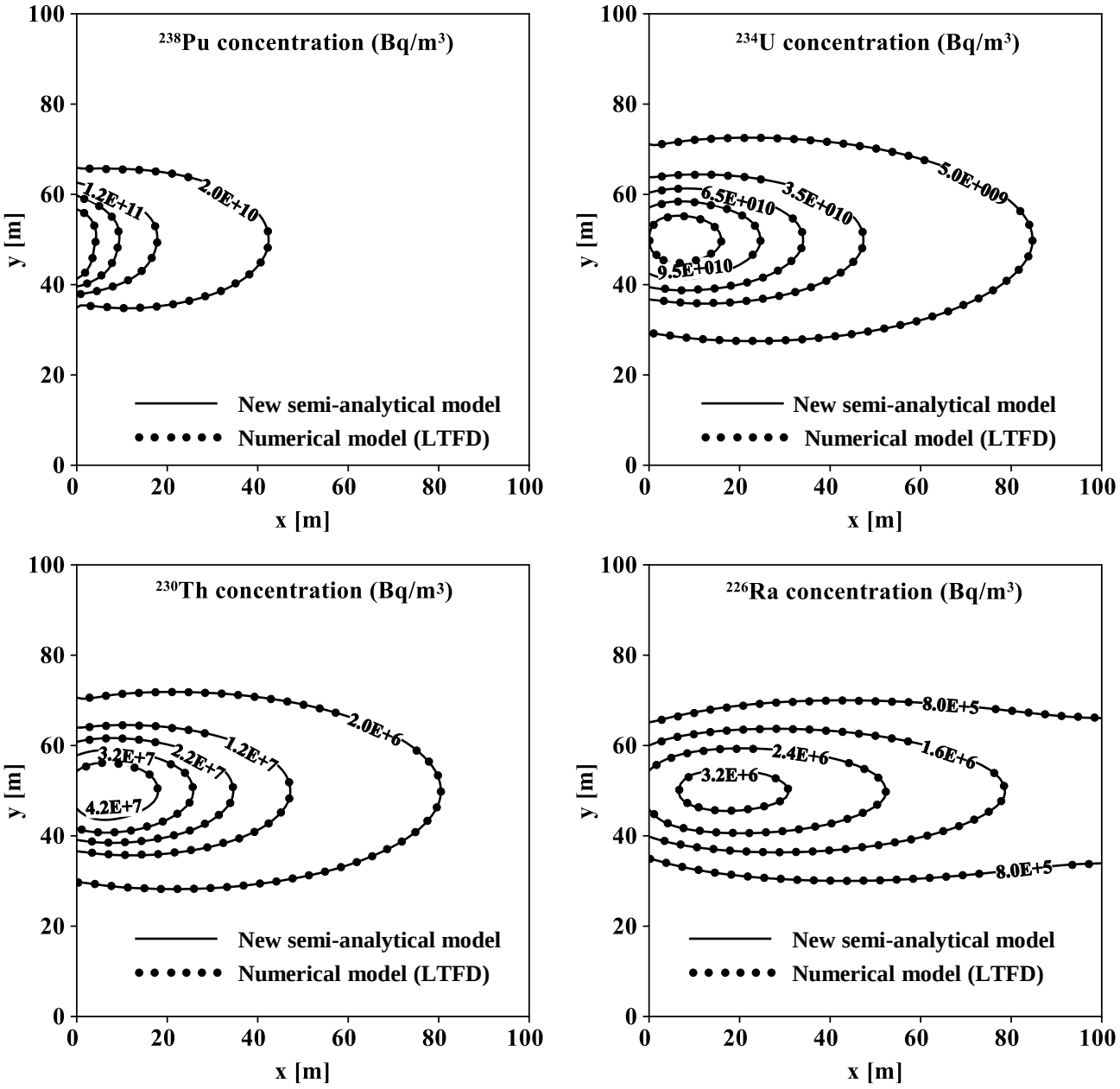
(van Genuchten, 1985)

Radionuclide decay chain



Parameter	Value
Domain length, L [m]	100
Domain width, W [m]	100
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

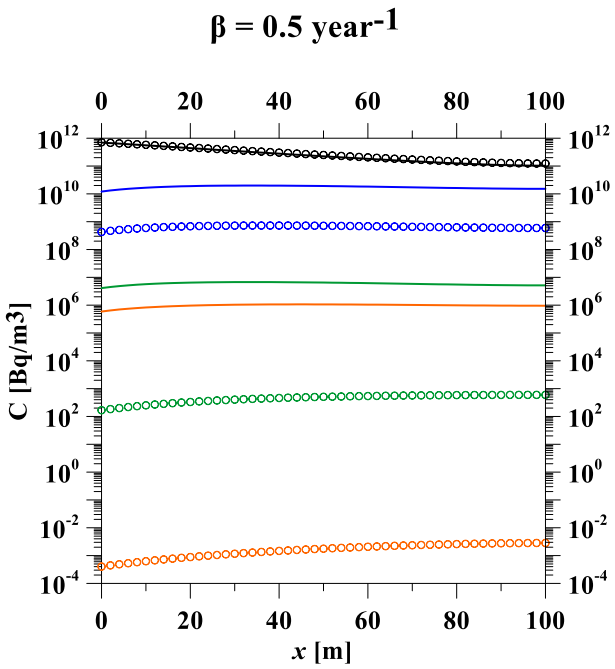
Verification results

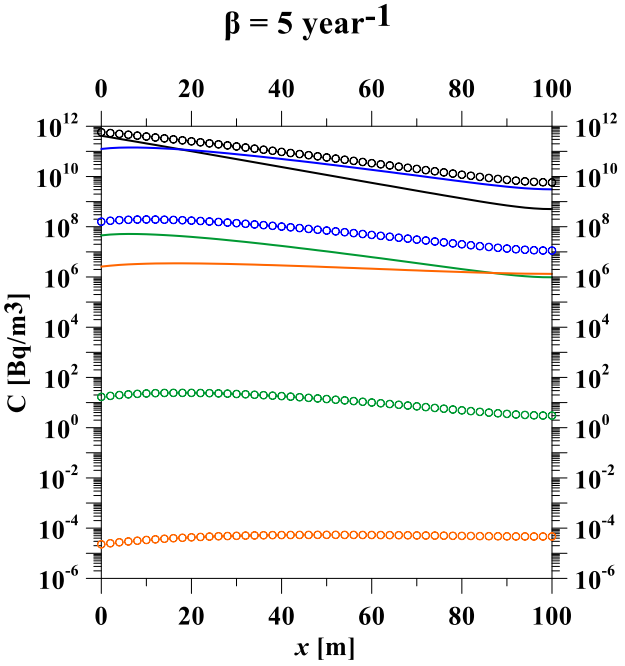


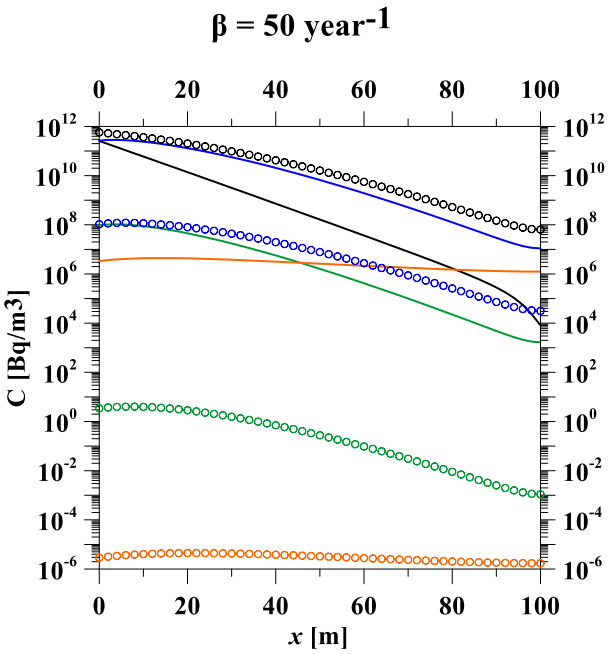
Effect of decay rate on solid phase

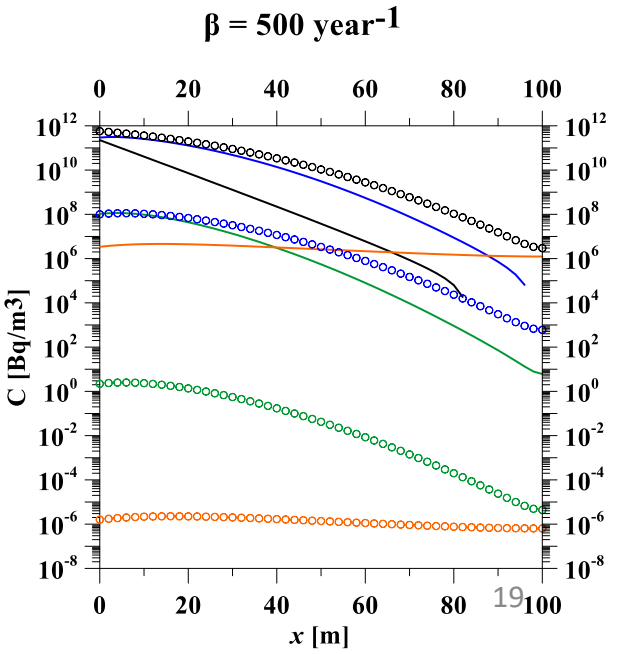
Time: 1000 years

- The concentration of the first contaminant in the decay chain (Pu^{238}) tends to decrease.
- With daughter species (U^{234}, Th^{230}, and Ra^{226}), their concentration significantly increases when decay occurs in both phases.









^{238}Pu

^{234}U

^{230}Th

^{226}Ra

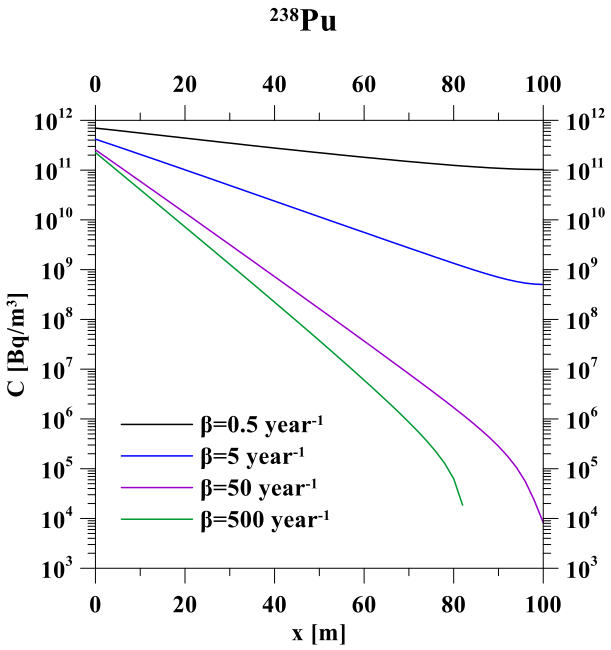
Decay in sorbed phase

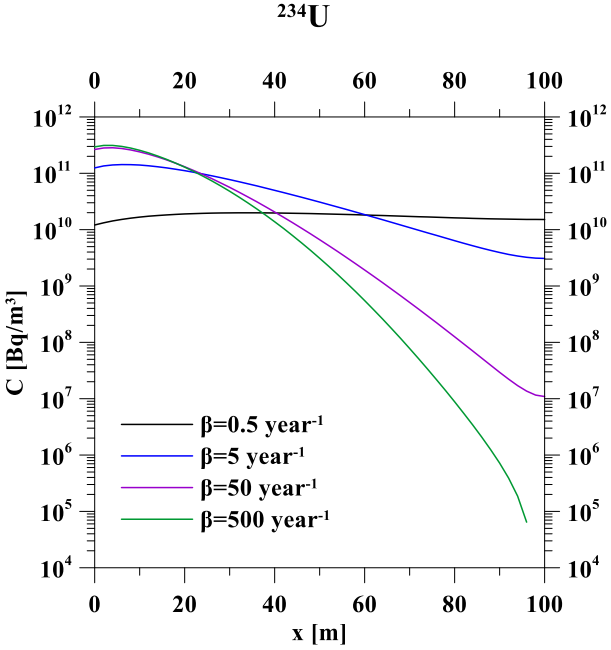
No decay in sorbed phase

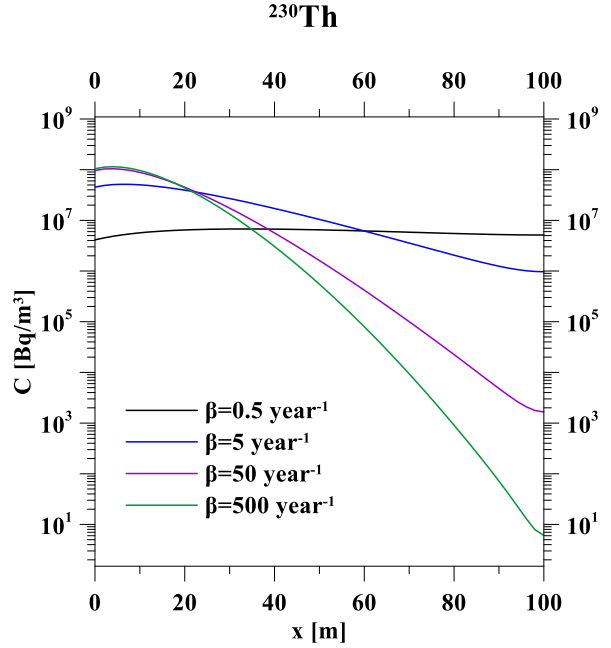
Effect of sorption rate on the concentration of contaminants

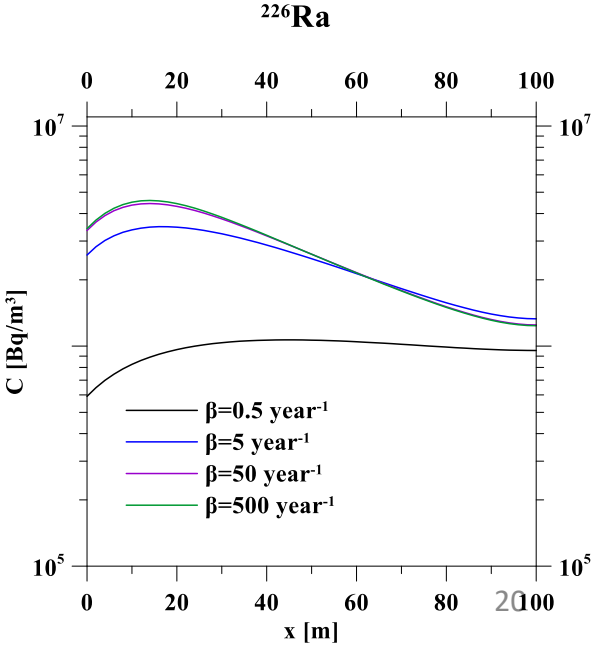
Time: 1000 years

- The concentration of the first contaminant (Pu^{238}) tends to decrease as the sorption rate increases.
- U^{234}, Th^{230}, and Ra^{226} have the opposite trend, especially in areas near the pollution source.









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.

→ The concentration of the first contaminant (Pu^{238}) tends to decrease as the sorption rate increases. However, daughter species (U^{234}, Th^{230}, and Ra^{226}) tend to increase in concentration as sorption rate increases, especially in areas near the pollution source.

→ The concentration of the first contaminant in the decay chain (Pu^{238}) tends to decrease when considering the decay process in the solid phase. Meanwhile, with the contaminants formed through the decay process (U^{234}, Th^{230}, and Ra^{226}), their concentration significantly increases when decay occurs in both phases.

→ This demonstrates that not considering the decay process in the solid phase can lead to an erroneous assessment of contaminant concentrations in groundwater, especially for hazardous contaminants such as radioactive waste.

Thank you for your attention!