# A two-dimensional semi-analytical model for multispecies transport of the contaminant and its degradation-related products subject to rate-limited sorption


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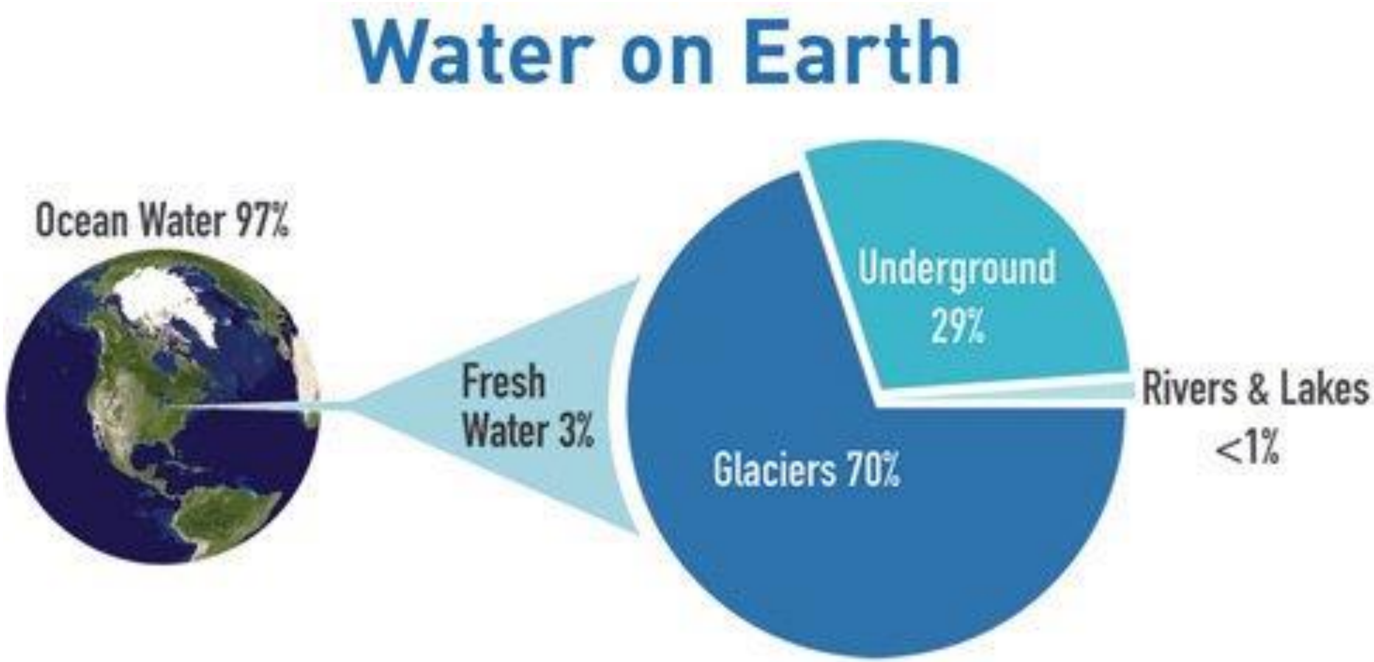
# OUTLINE:

# 1. Introduction

# The importance of groundwater:



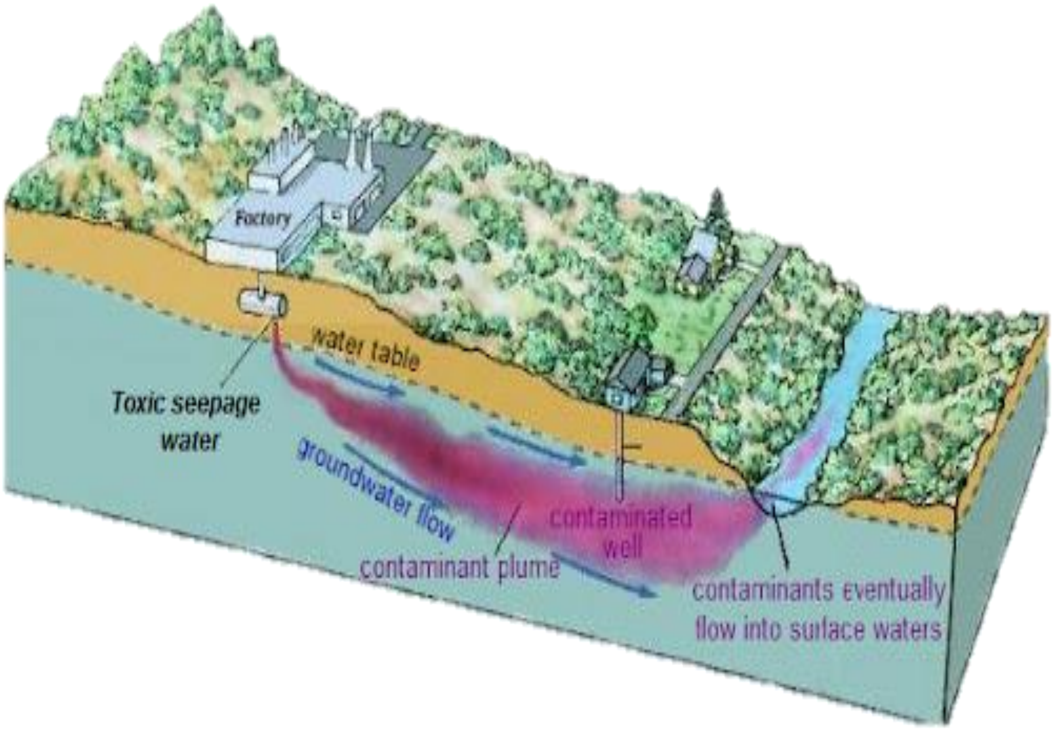

- World's aggregated groundwater abstraction is 1,000 km$^3$ per year.

- **22% of abstraction groundwater is used for domestic purposes (drinking water and sanitation).**

# Groundwater contamination

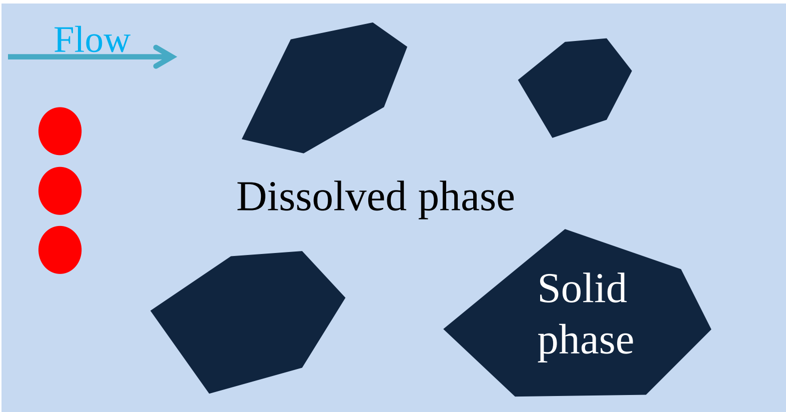
The sources of contamination in groundwater:

- Farming chemicals
- Septic waste
- Landfills
- Uncontrolled hazardous waste
- Storage tanks
- Atmospheric pollutants

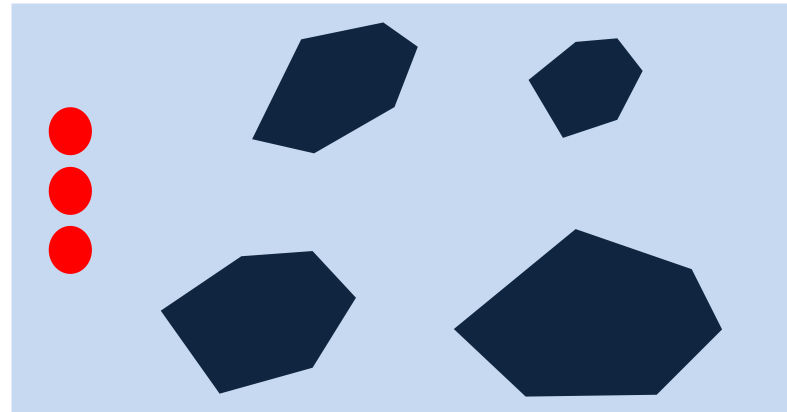


# Transport mechanism of contaminants

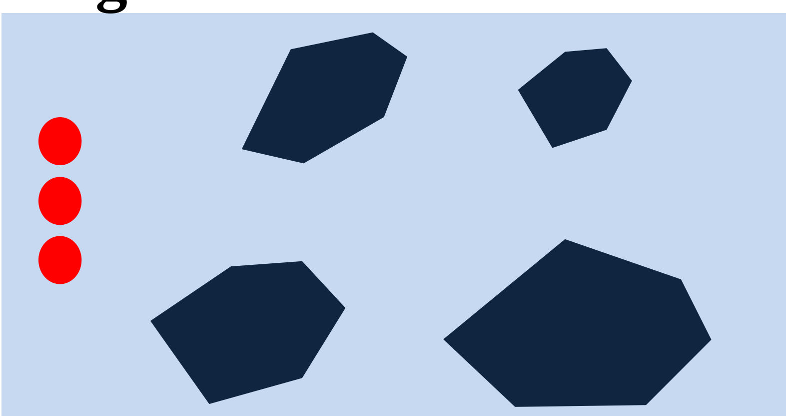
## Advection



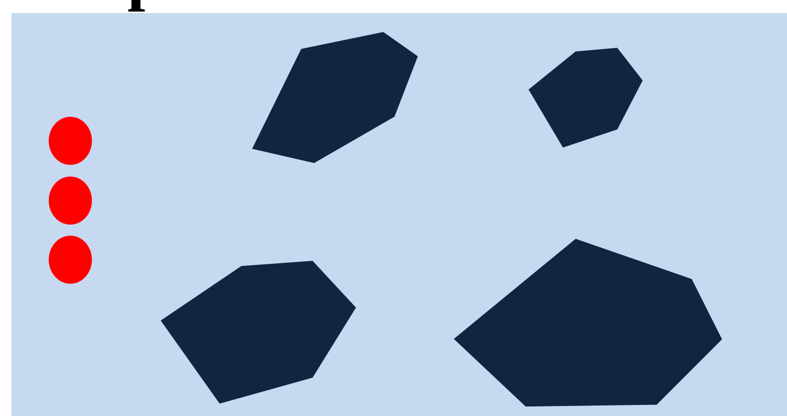

## Dispersion



## Degradation



## Sorption



# Advection-dispersion equations (ADEs)

- Using mathematical methods (numerical methods or **analytical methods**) to solve the advection-dispersion equations (ADEs).

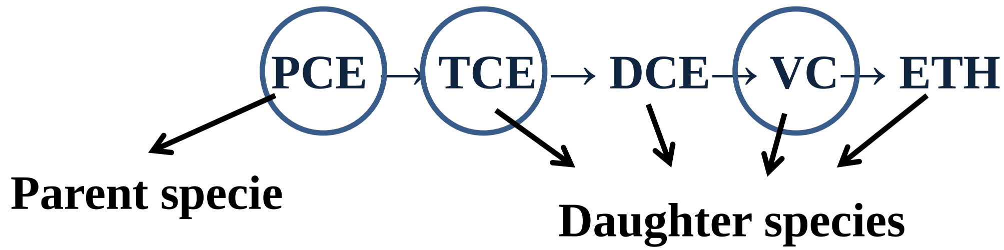
- **ADEs** can describe the transport of dissolved solutes in groundwater.

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} - \lambda C - \frac{\partial S}{\partial t}$$

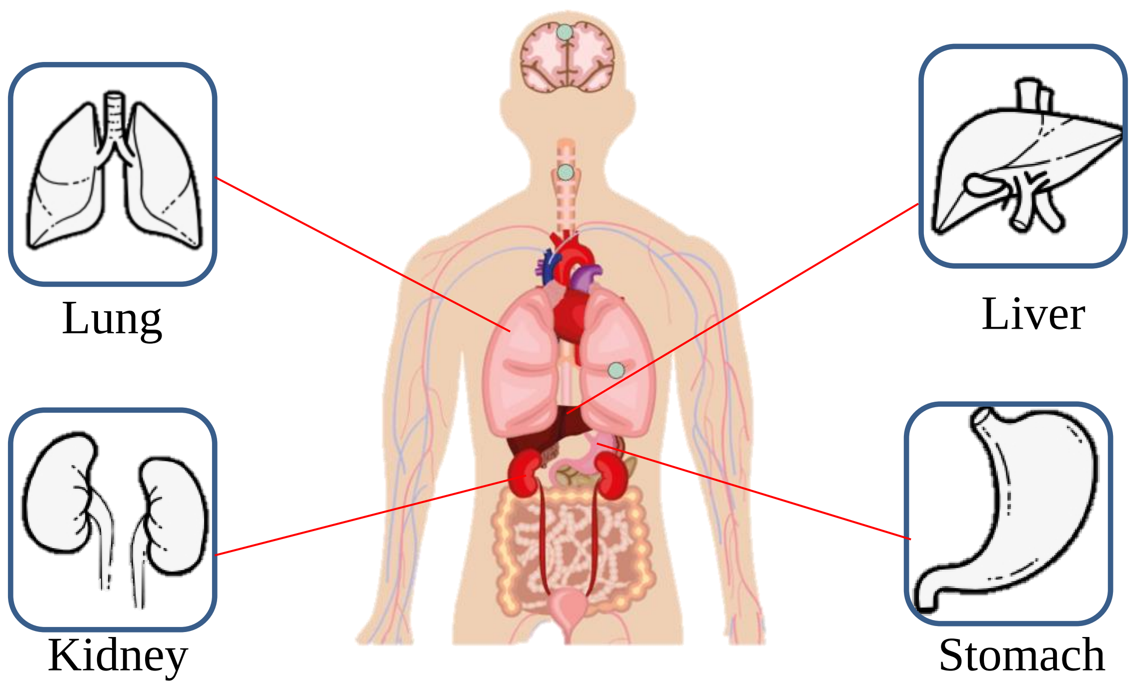
**Dispersion** **Advection** **Decay** **Sorption**

# Degradation Process

Multispecies contaminant




**How can estimate the concentration of each specie in the decay chain?**

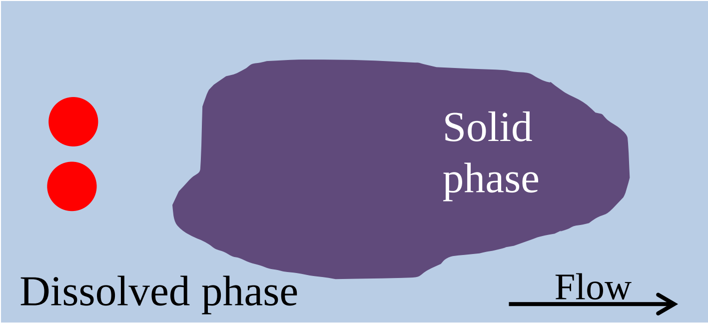


# Sorption process

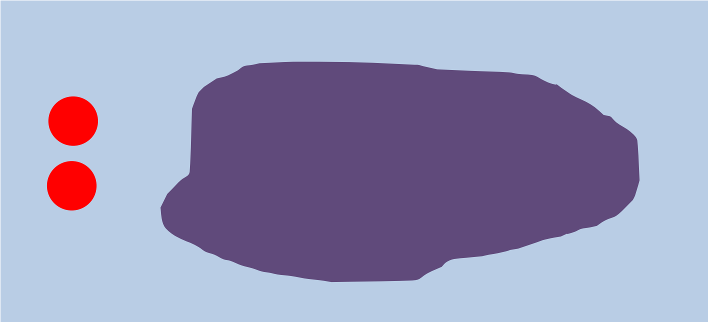
Control the rate at which the dissolved contaminants will partition on to the surrounding soil material.

$\beta$: Sorption rate

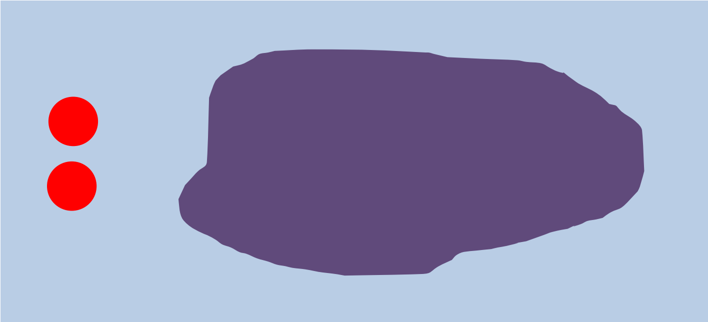
$\beta$ = 0.5 year$^{-1}$



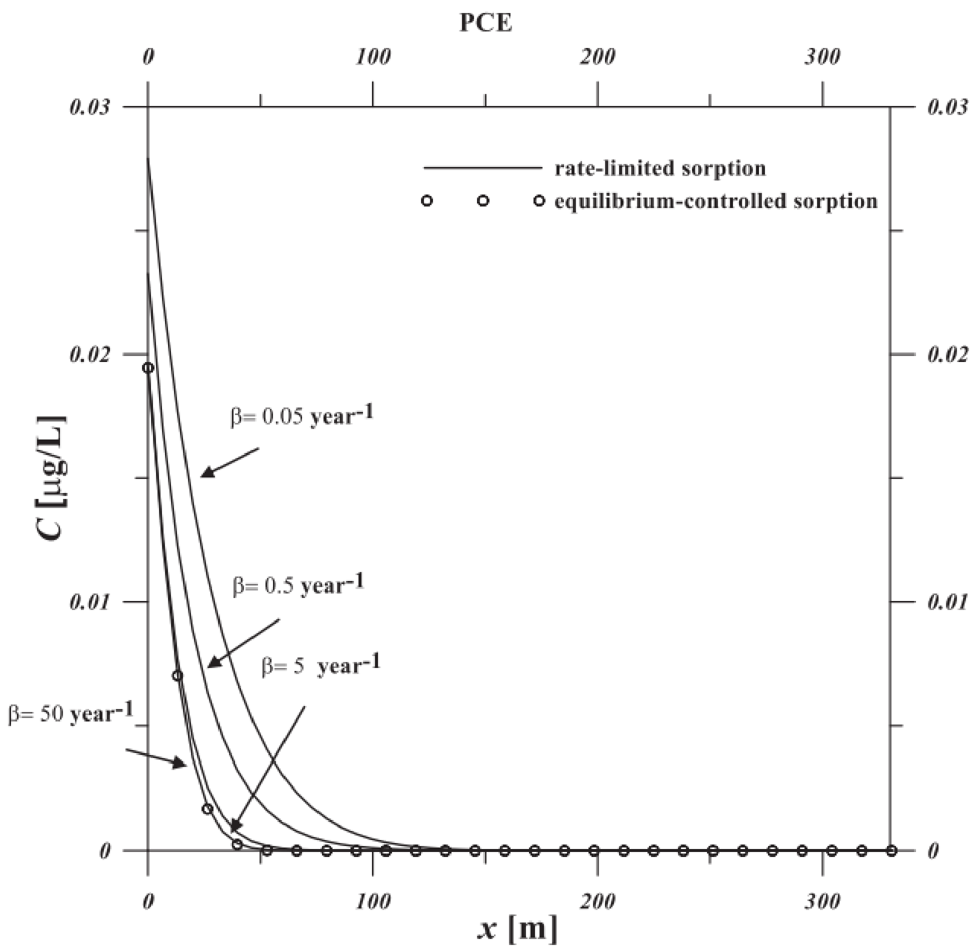

$\beta$ = 5 year$^{-1}$



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



# Comparison between Equilibrium-controlled sorption and Rate-limited sorption




**Chen et al. (2019):**

- The equilibrium-controlled sorption model will **agrees well** with the rate-limited sorption model when the sorption rate **greater than 50 year$^{-1}$**.

# Limitations of previous studies

- Most models of multispecies transport assume the sorption process to be equilibrium-controlled sorption.

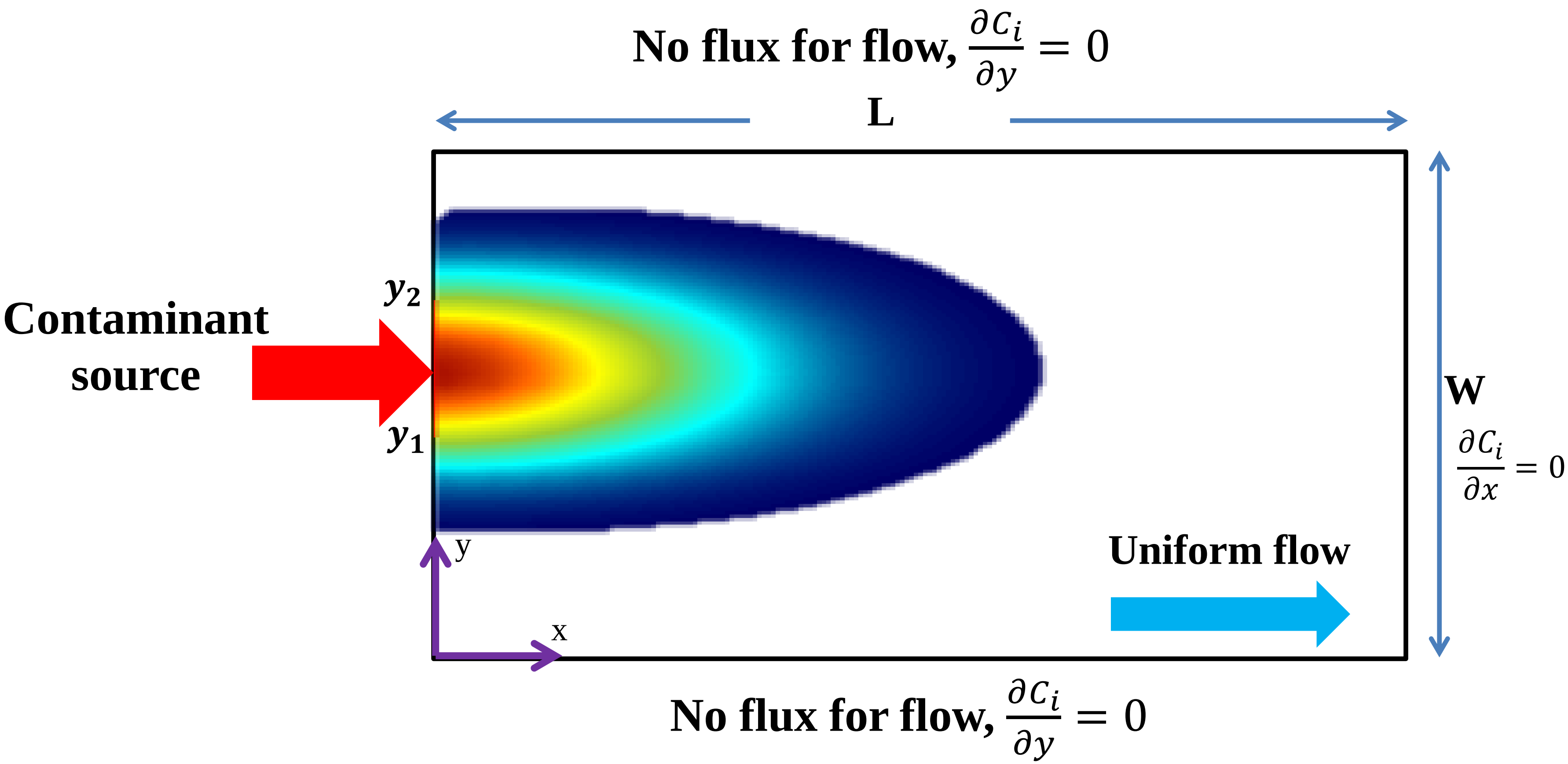
- The rate-limited sorption models for multispecies transport currently reported are limited to one-dimensional advective – dispersive transport.

# Objective:

To develop a multidimensional analytical model for describing multispecies reactive transport subject to rate-limited sorption.

# 2. Mathematical model

# Conceptual model



# Governing equation

## Dissolved phase:

Dispersion / Advection / Decay

$$D_L \frac{\partial^2 C_i(x,y,t)}{\partial x^2} + D_T \frac{\partial^2 C_i(x,y,t)}{\partial y^2} - v \frac{\partial C_i(x,y,t)}{\partial x} - \lambda_i C_i(x,y,t) + \lambda_{i-1} C_{i-1}(x,y,t) - \frac{\beta}{\theta}\left(C_i(x,y,t) - \frac{S_i(x,y,t)}{K_i}\right) = \frac{\partial C_i(x,y,t)}{\partial t} \qquad \boldsymbol{i = 1, 2, 3, \ldots}$$

Sorption

## Sorbed Phase:

$$\rho_b \frac{\partial S_i(x,y,t)}{\partial t} = \beta\left(C_i(x,y,t) - \frac{S_i(x,y,t)}{K_i}\right)$$

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

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

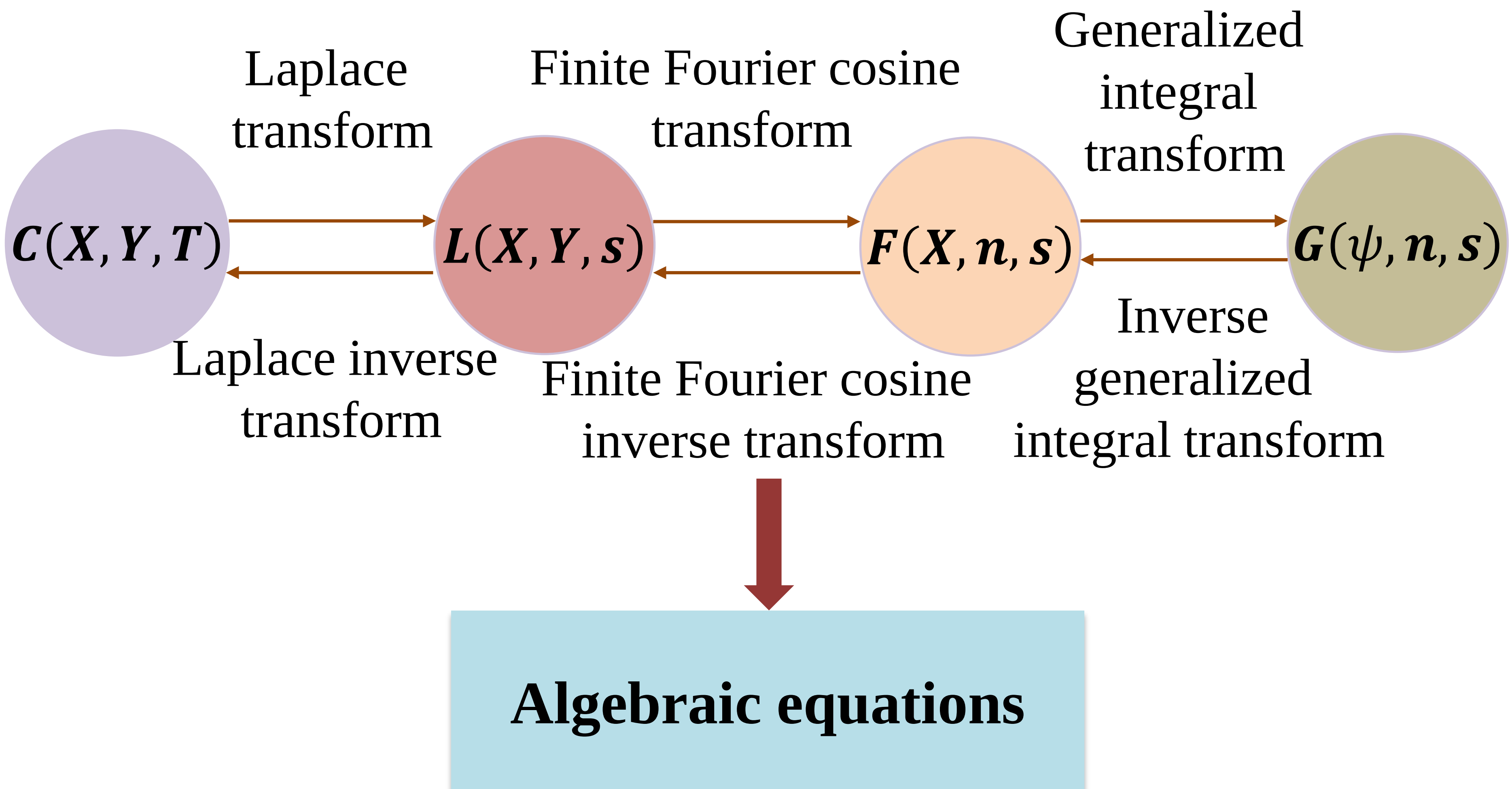
$\boldsymbol{\beta}$: Kinetic sorption rate of specie $i^{th}$ ($T^{-1}$)

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

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

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

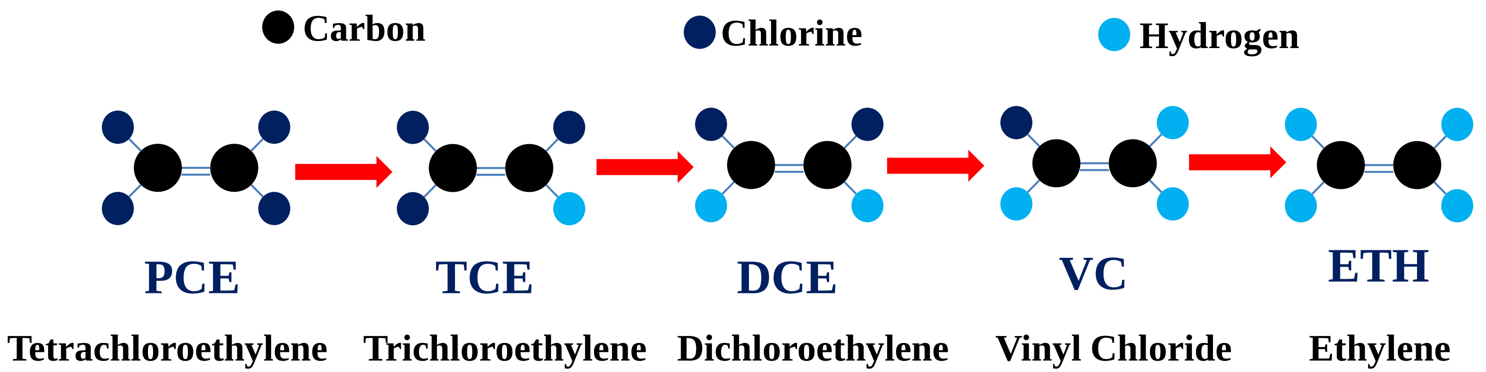
# Solving procedure



# 3. Results and Discussion

# Verification example

## The biodegradation pathway of the chlorinated solvent



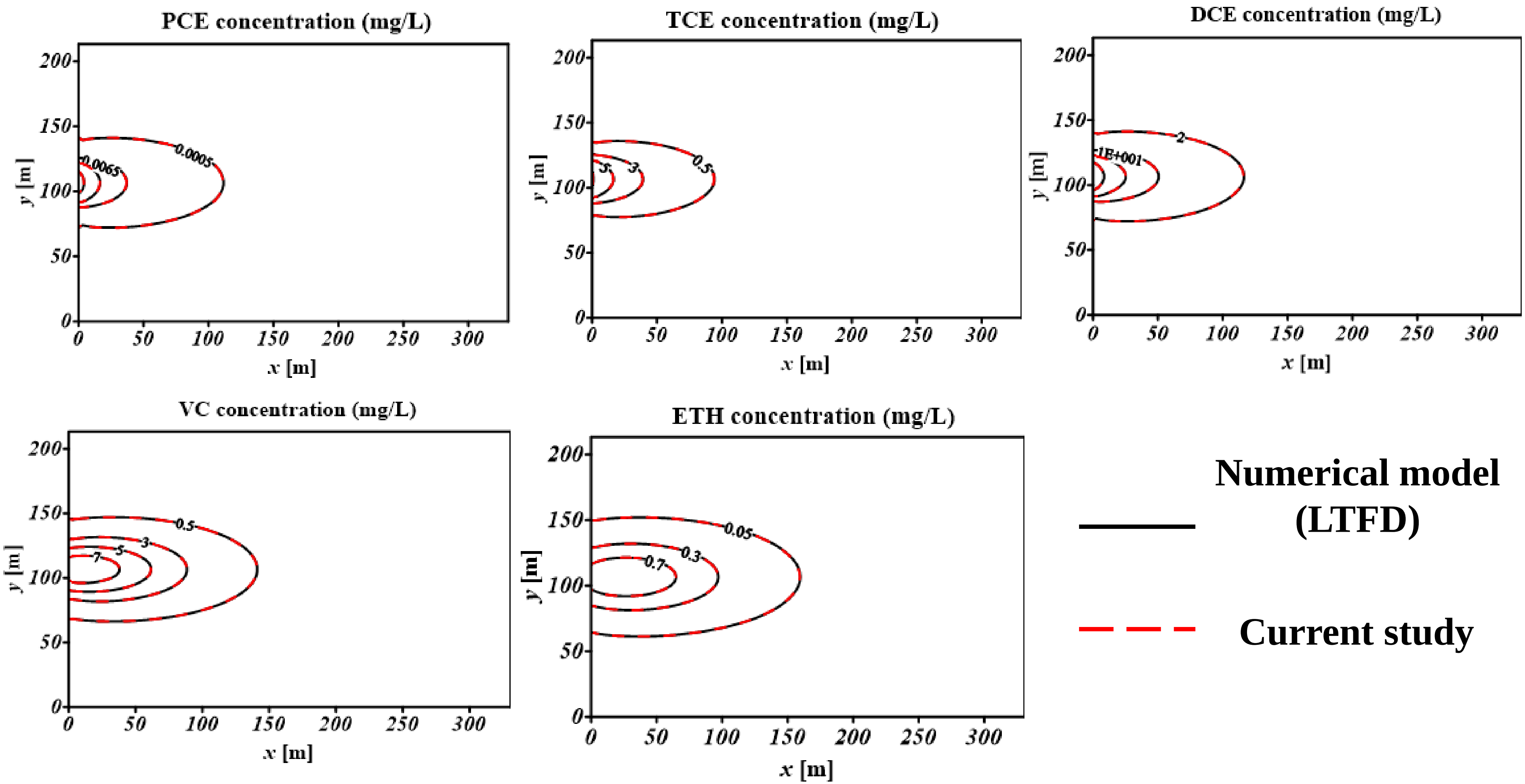
# Parameters for verification

| Parameter | Value | | | | |
|---|---|---|---|---|---|
| Domain length, L [m] | 330.7 | | | | |
| Domain width, W [m] | 213.4 | | | | |
| Seepage velocity, v [m/year] | 34.0 | | | | |
| Longitudinal Dispersion coefficient, $D_L$ [$m^2$/year] | 2000 | | | | |
| Transverse Dispersion coefficient, $D_T$ [$m^2$/year] | 200 | | | | |
| Bulk density, $\rho_b$ [kg/L] | 1.6 | | | | |
| Effective porosity, θ [-] | 0.2 | | | | |
| Sorption reaction rate constant,β [$year^{-1}$] | 0.05 0.5 5 50 | | | | |
| | **PCE** | **TCE** | **DCE** | **VC** | **ETH** |
| Distribution coefficient, $K_i$ [L/kg] | 0.784 | 0.239 | 0.230 | 0.0545 | 0.556 |
| Decay constant, $\lambda_i$ [$year^{-1}$] | 2 | 1 | 0.7 | 0.4 | 0 |
| Source concentration, $c_{i,0}$ [mg/L] | 0.056 | 15.8 | 98.5 | 3.08 | 0.03 |

***(United States Environmental Protection Agency, USEPA)***

# Verification of the derived analytical solution

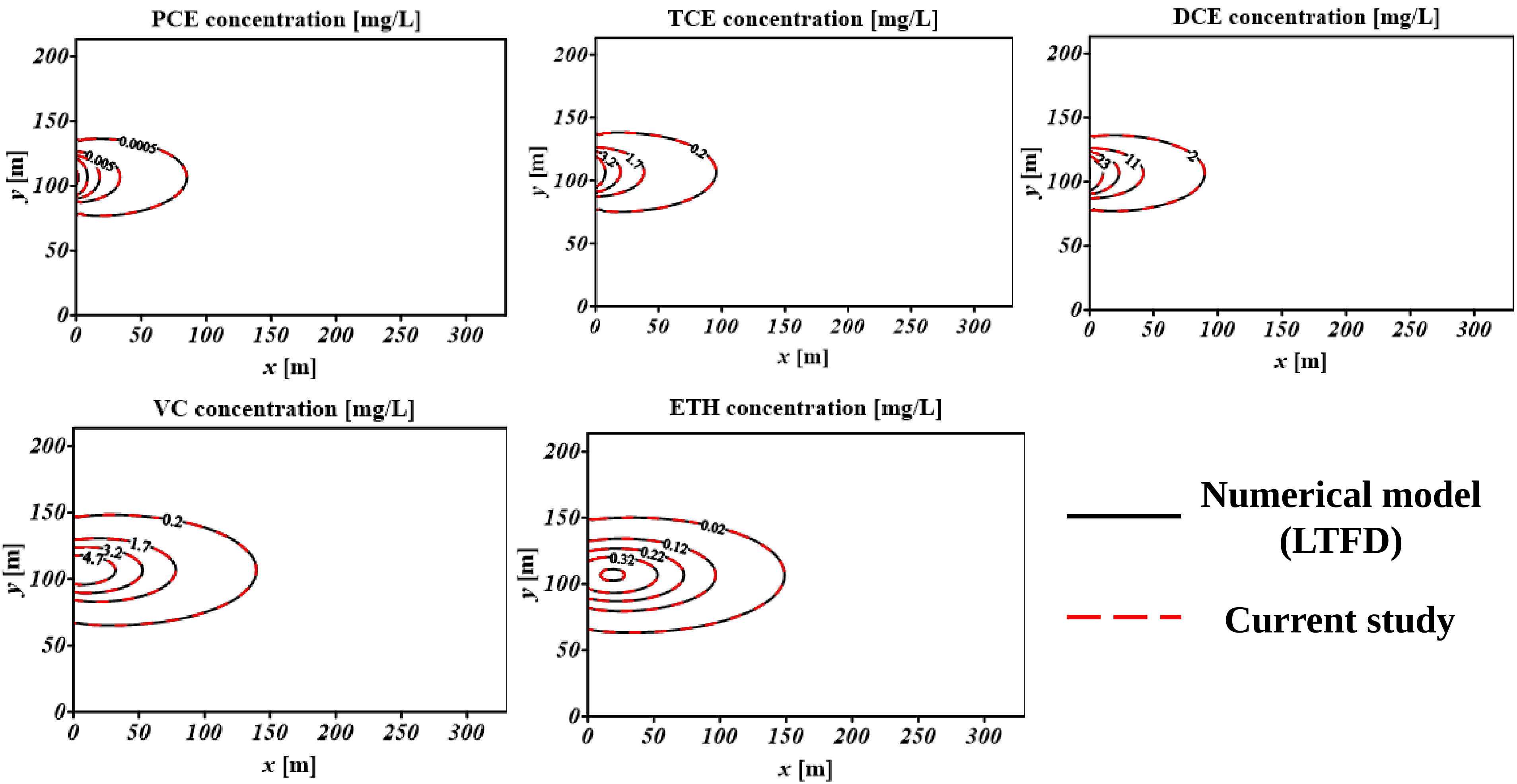
$$\beta = 0.05\ \text{year}^{-1}$$




**LTFD: Laplace transform finite difference method (Moridis and Reddell, 1991)**

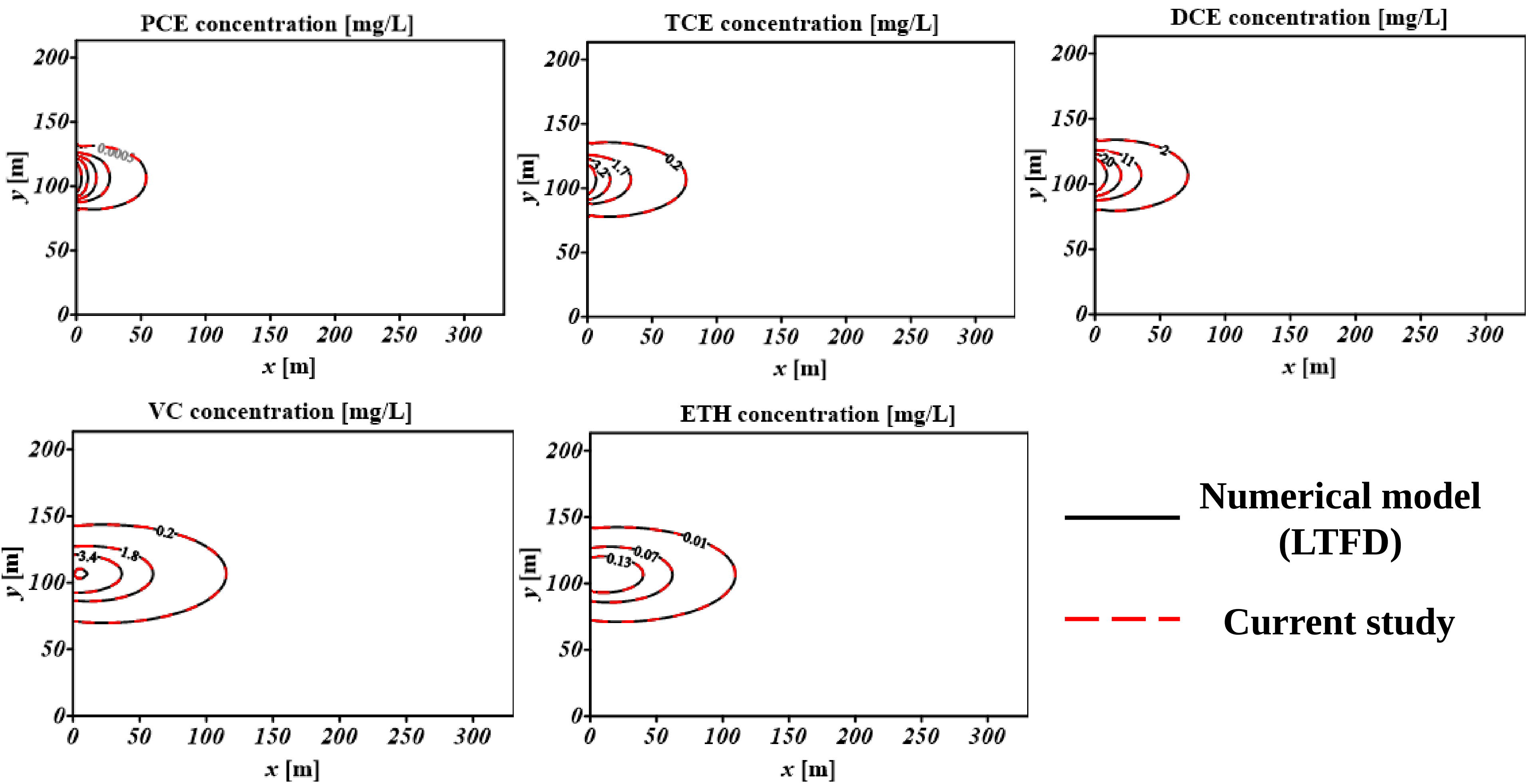
# Verification of the derived analytical solution

## $\beta = 0.5\ \text{year}^{-1}$



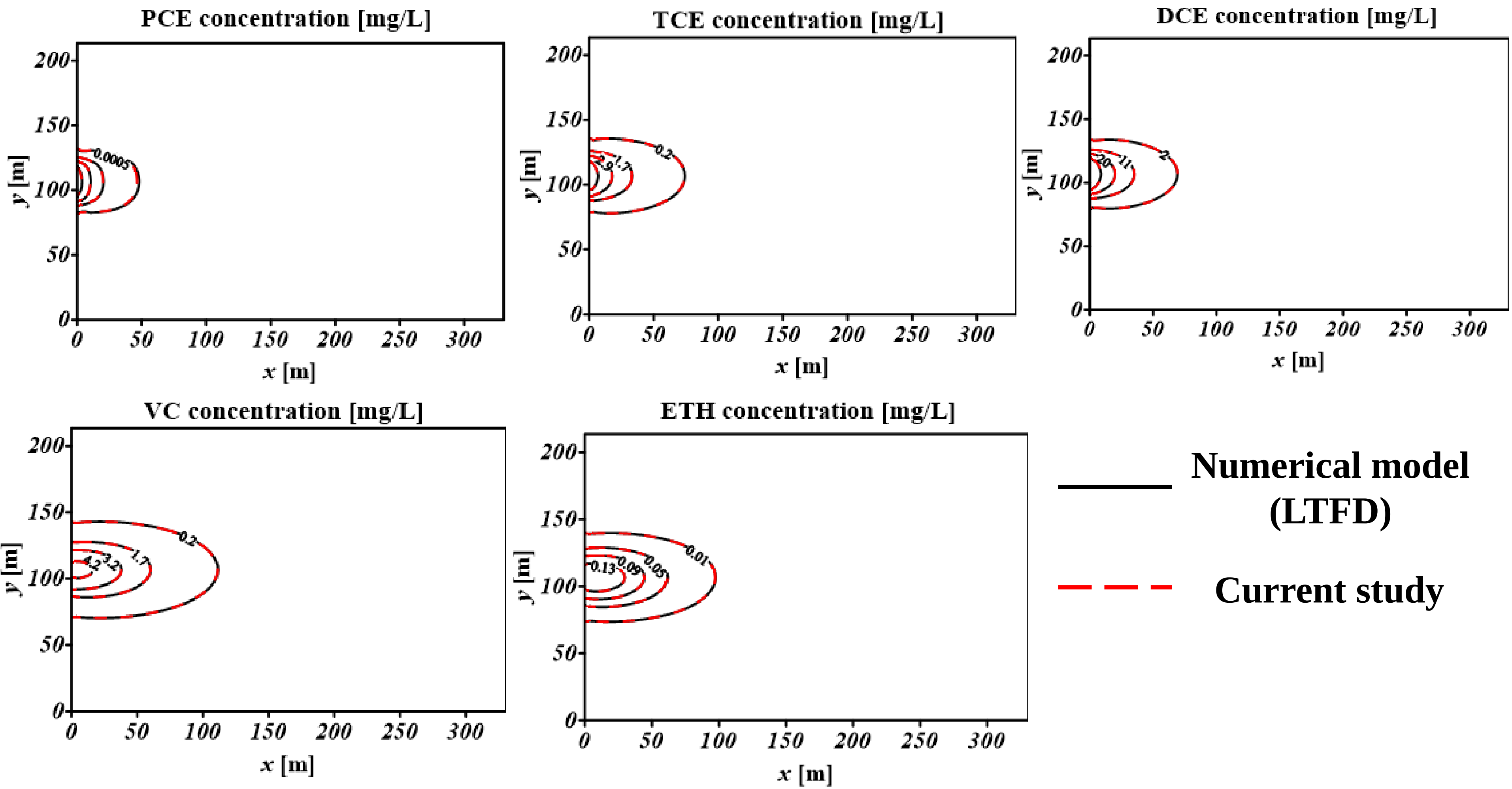
# Verification of the derived analytical solution

## $\beta = 5\ \text{year}^{-1}$

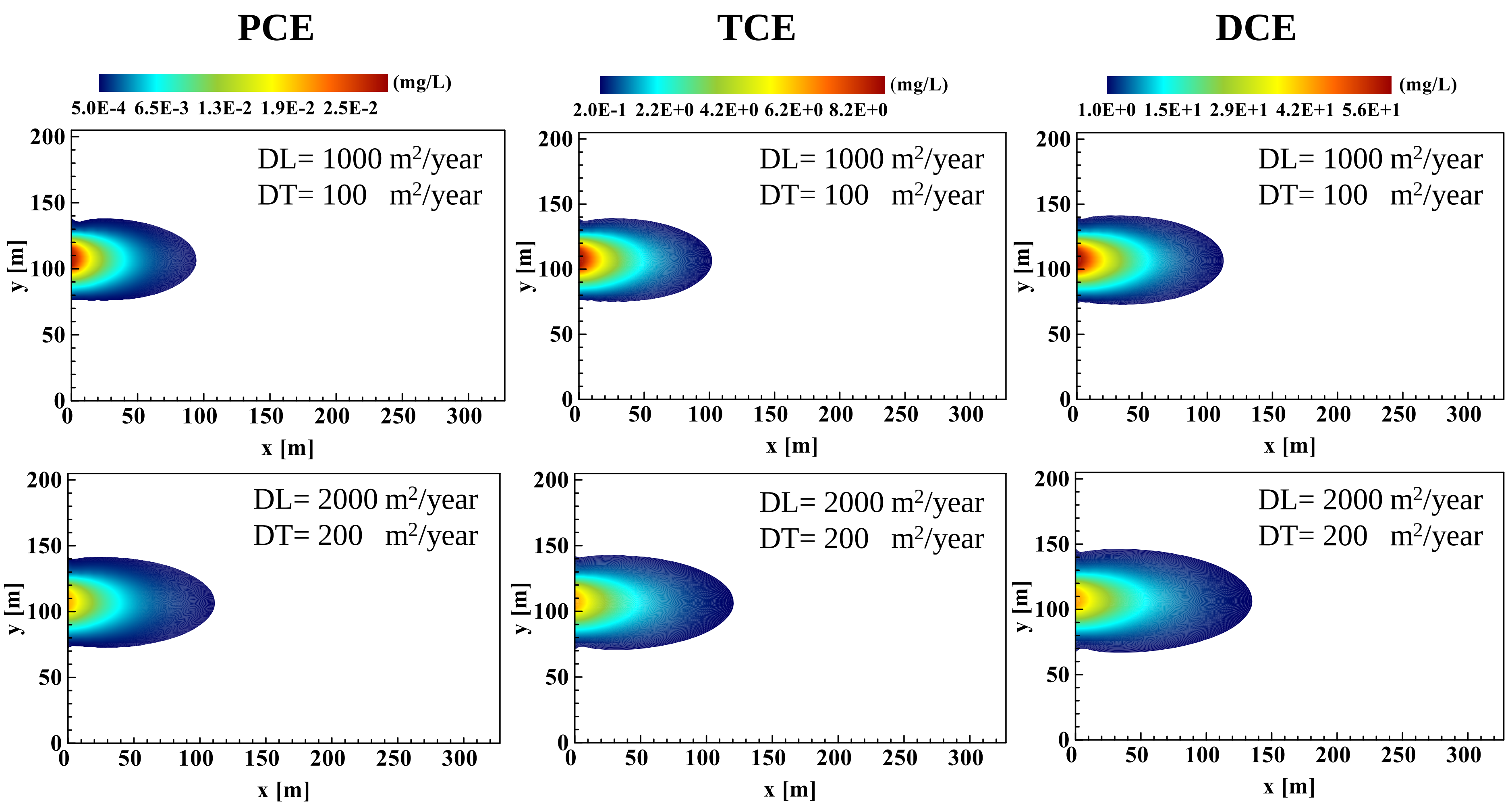


# Verification of the derived analytical solution

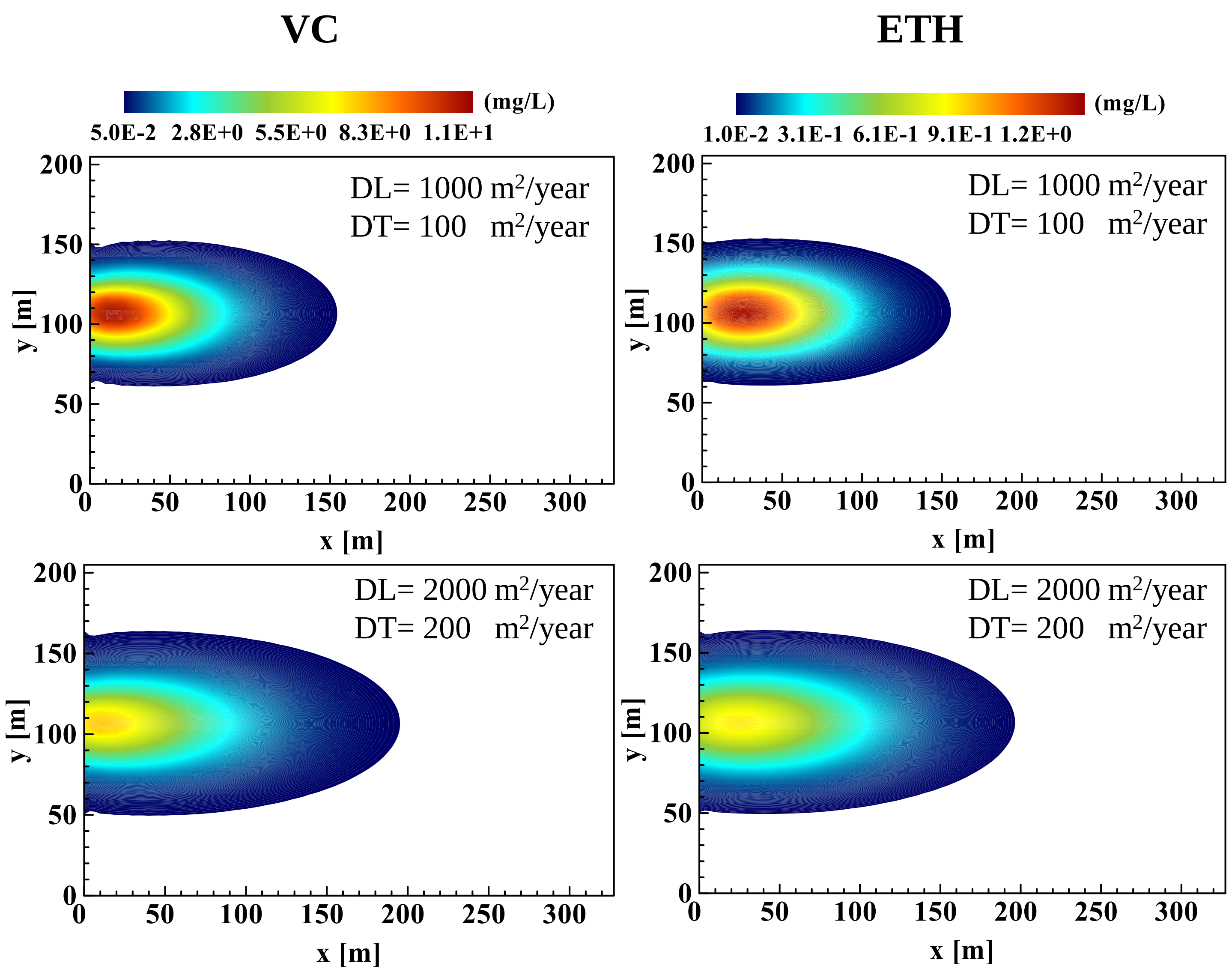
$$\beta = 50\ \text{year}^{-1}$$



# Assessing Dispersion coefficient on the plume migration

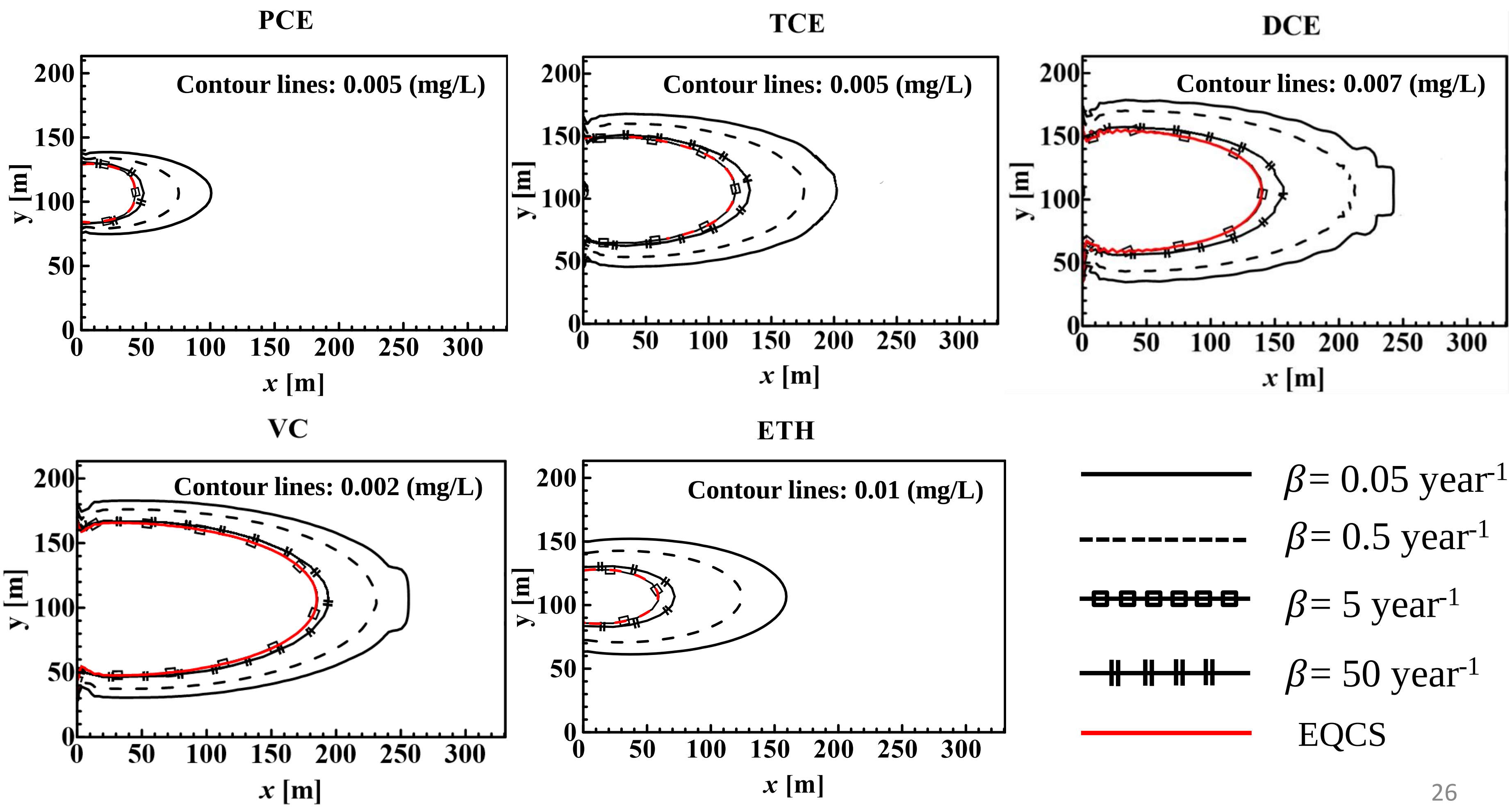


# Assessing Dispersion coefficient on the plume migration



# Effect of sorption rate with the plume extent

| | PCE | TCE | DCE | VC | ETH |
|---|---|---|---|---|---|
| Standard *(Source: EPA)* | 0.005 mg/L | 0.005 mg/L | 0.002 mg/L | 0.007 mg/L | - |



# 4. Conclusions

- Increase of the longitudinal and transverse dispersion coefficients enhances the spreading of the plume extensively along the longitudinal and transverse directions, thereby lowering the plume concentration level.

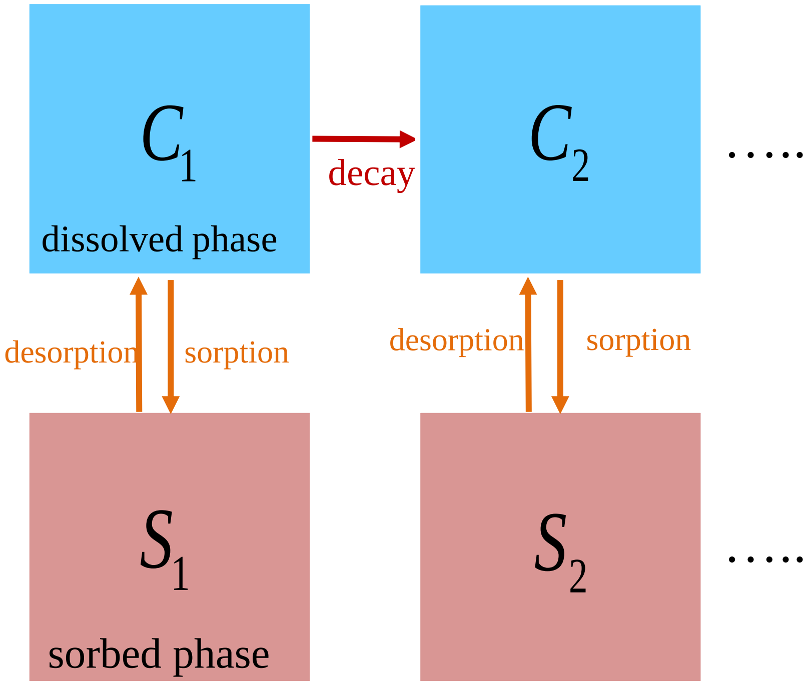
- Concentration levels and extent of contamination plumes are affected by rate-limited sorption. If the sorption rate increases, the plume extension is restricted, and concentration levels are reduced.

- The rate-limited sorption model with low sorption rate may give a wider plume zone for contaminant and its degradation products than the equilibrium-controlled sorption model. The use of a equilibrium-controlled sorption model in most of cases may not accurately assess contamination in groundwater.

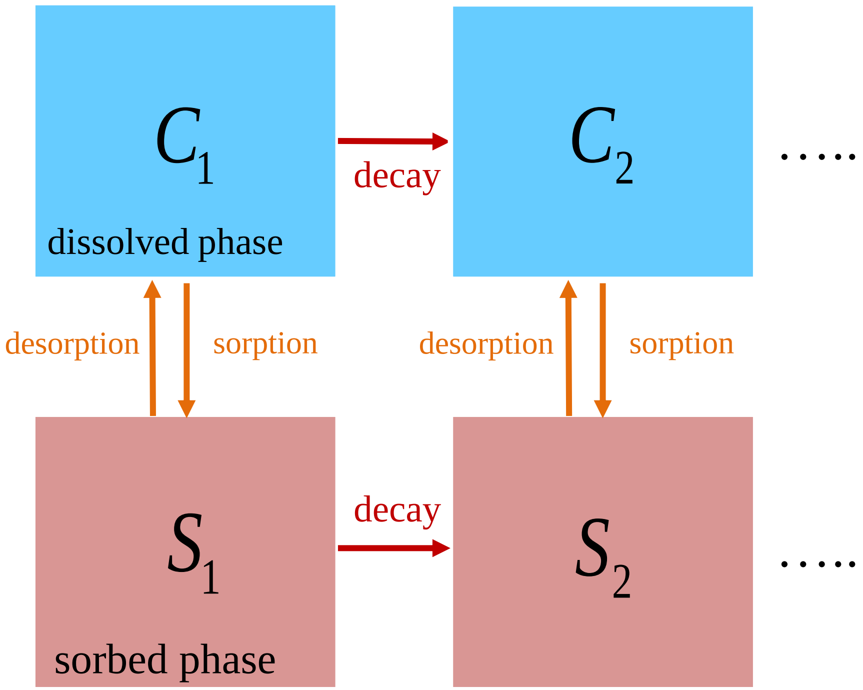
# 5. Future works

# Schematic diagram for multispecies transport

## Current study



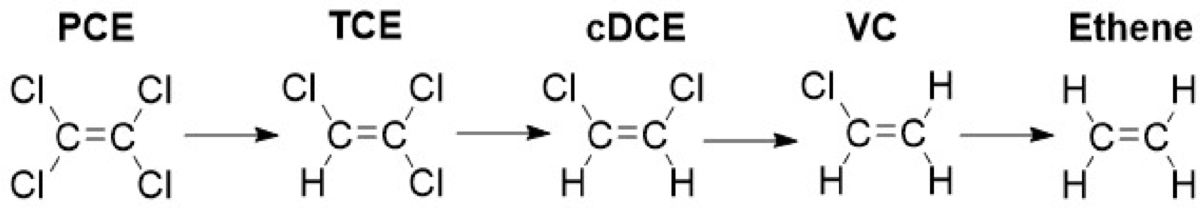

## Future work




Considering degradation reaction in sorbed phase

# 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**

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

# Governing equation

## Dissolved phase:

Decay

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

## Sorbed phase:

**Without decay:**

$$\rho_b \frac{\partial S_i(x,y,t)}{\partial t} = \beta\left(C_i(x,y,t) - \frac{S_i(x,y,t)}{K_i}\right)$$

**With decay:**

Decay

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

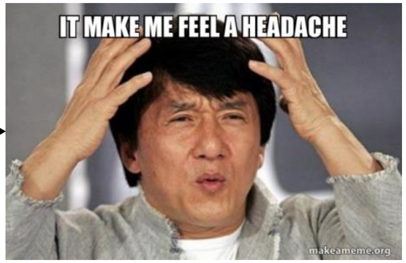
$\gamma_i$: Decay rate of specie $i^{th}$ in sorbed phase($T^{-1}$)

# Workflow

**Solve governing equation**

Analytical solution

**Transfer to computer code**




**Verify model accuracy**

Compare with some previously developed models, or compare with real datas **if possible**!!!

**Evaluation of the effect of degradation/decay in the sorbed phase.**

# THANK YOU FOR YOUR ATTENTION!