Semi-analytical model of non-equilibrium multi-species transport subject to multiple arbitrary time-dependent pollution sources

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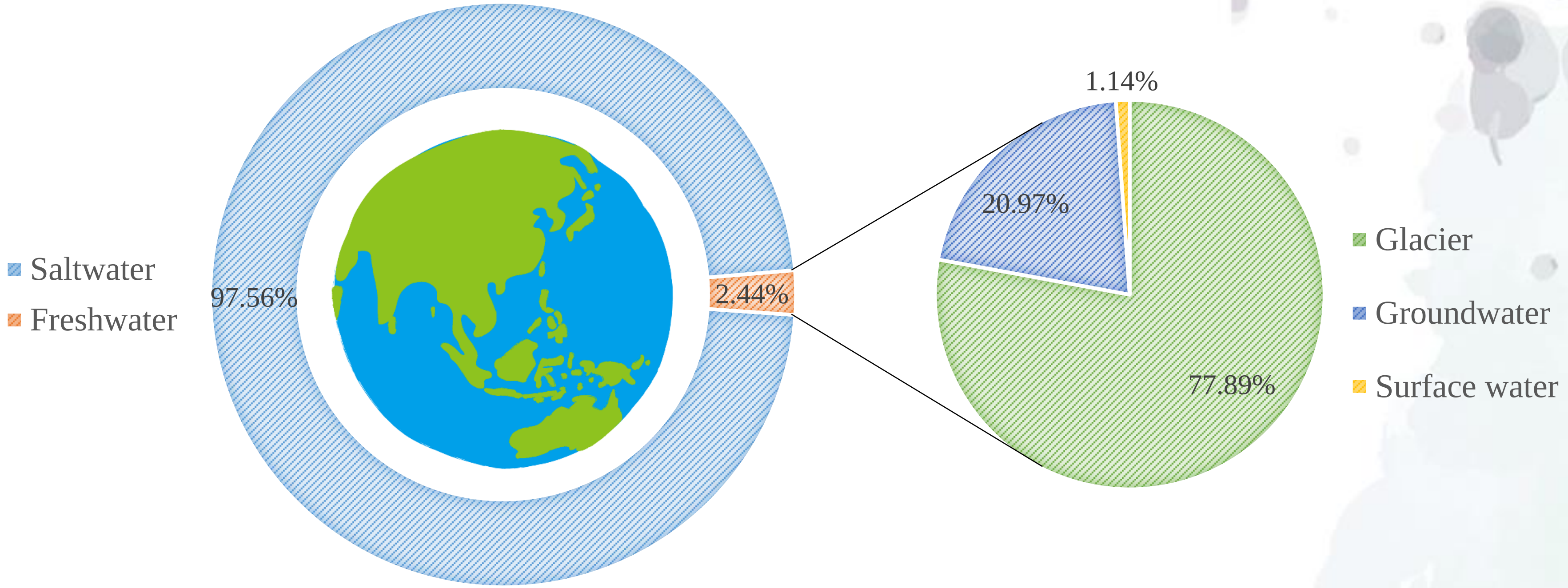
Outline

1. Introduction
2. Mathematical model
3. Results and Discussion
4. Conclusions

Introduction

Background

- "No water, no life. No blue, no green.“ – Sylvia Earle
- For those living on the land, freshwater resources are important and precious.

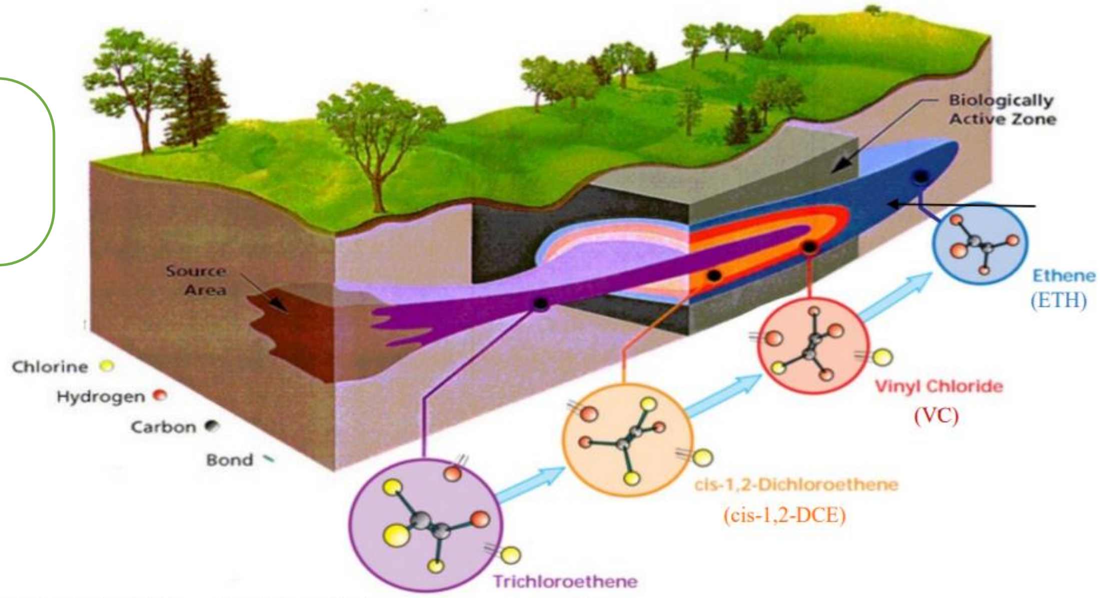


Introduction

Background

- Industrial waste dumping have caused lots of contaminated problems to environment and also health problems to human-beings after the extensive production since early 20th century.

Common contaminant:
Tetrachloroethylene, PCE
Trichloroethylene, TCE



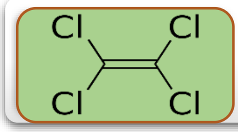
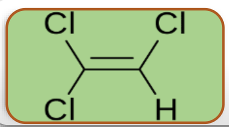
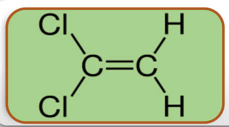
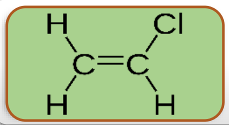
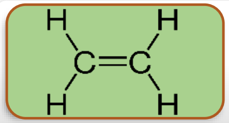
Sajeed Jamal, Beak International Inc, 1997

PCE → TCE → DCE → VC → ETH

Introduction

Relationship between health and chlorinated solvents

- Serious diseases as cancer could be caused by chlorinated solvents and also of their degradation products.

Structure	Compound	Control standard value (EPA) Drinking water	Others	
	PCE	0.005ppm	0.05ppm	Bladder Cancer
	TCE	0.005ppm	0.05ppm	Kidney and Liver Cancer
	DCE	0.007ppm	0.07ppm	
	VC	0.002ppm	0.02ppm	Liver and Lung Cancer
	ETH	-	-	

Introduction

Mathematical model

- To develop a proper remediation strategy for contaminated site, mathematical model can play an important role to simulate the contaminant transport in the aquifer.

- The pollutant transport models based on classical Advection–Dispersion Equation (ADE) are general tools to estimate the reactive migration in geological formations.

Dispersion **Advection**

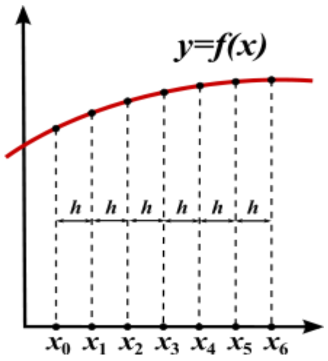
$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x}$$

Simple example for ADE

Introduction

How to solve ADE?

- Numerical solutions are commonly used to solve ADE as they considered more geological information to reproduce the real situation, however, there are some limitations that make them impossible to apply widely.



e.g. Finite difference method (FDM)

- Currently, analytical solutions are highly sought after as they provide greater insight into the governing transport processes, besides, they also make up for some shortcoming of numerical solutions. (Carr, 2021)

Introduction

Advantages of analytical solutions

- At sites where many key parameters are uncertain, analytical models can be run with a range of parameter values to screen or bracket the expected site behavior. (Falta and Kueper, 2014)

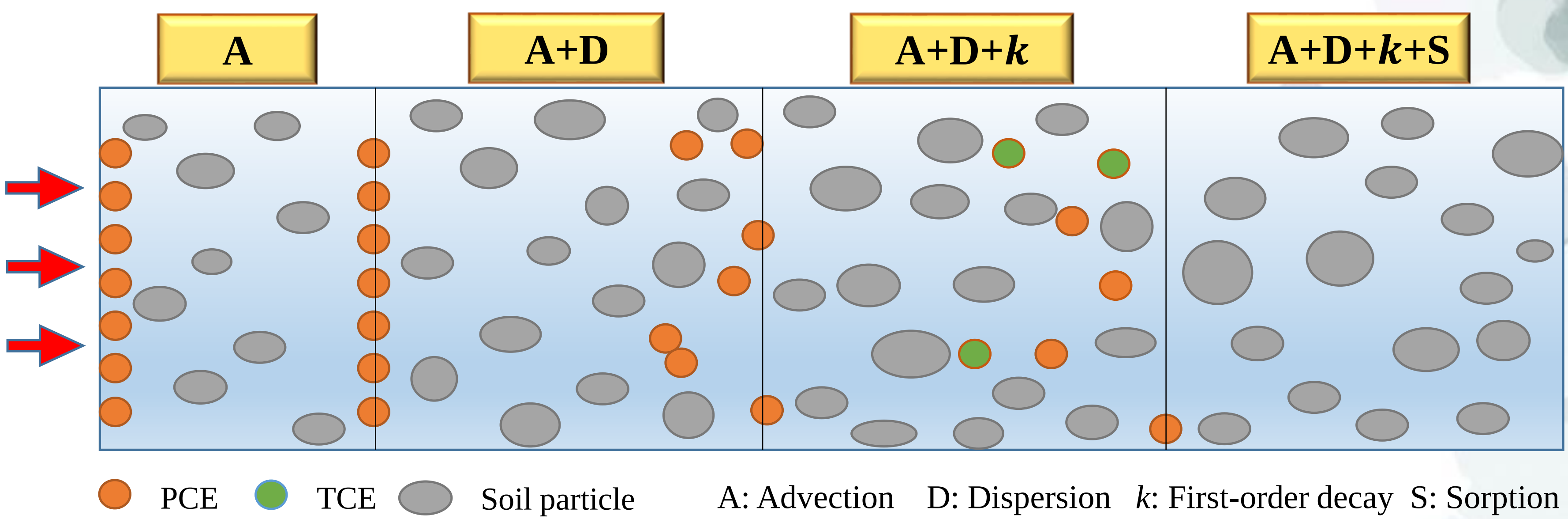
- Rapidly search for sensitive parameters of the model.

- Computing efficiently without the use of small temporal and spatial discretization step sizes.

- Provide important initial estimates of contaminated sites.

Introduction

Mechanisms of transportation



Introduction

Literature review

Analytical model

- Due to the high efficiency of analytical modeling, a number of analytical models has been derived for describing single-species transport of various contaminants.

Batu (1993)
Park and Zhan (2001)
Chen and Liu (2011)

- However, the transport processes for some contaminants of concern generally involve a more complicated series of chain degradation reactions.

Introduction

Literature review

Limitation of single-species model

- Single-species transport analytical models are unable to account for mass transformation from the parent species to the daughter species of degradable contaminants. (Chen et al., 2019)

Chen et al. (2012a, b)
Guerrero and Skaggs (2010)

Introduction

Literature review

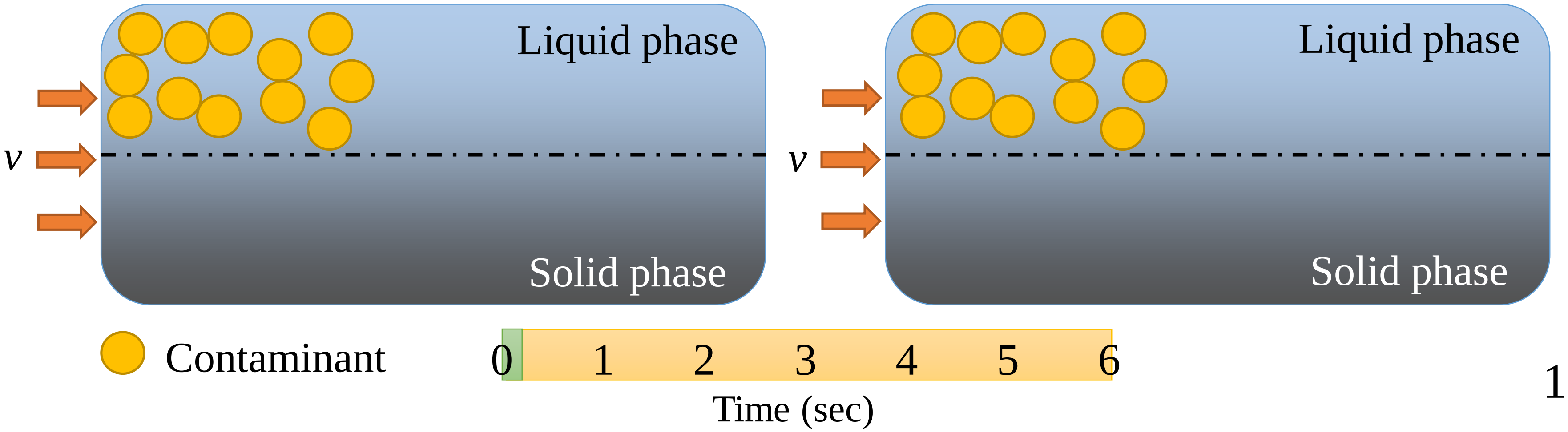
Limitation of equilibrium-controlled sorption

- Models considering equilibrium-controlled sorption often underestimate the concentration of degradable pollutants.

Chen et al. (2019)

β_i: sorption reaction rate constant $[T^{-1}]$

Equilibrium-controlled sorption, $\beta_i = \infty$ — Rate-limited sorption, $\beta_i = 0.1$



Introduction

Literature review

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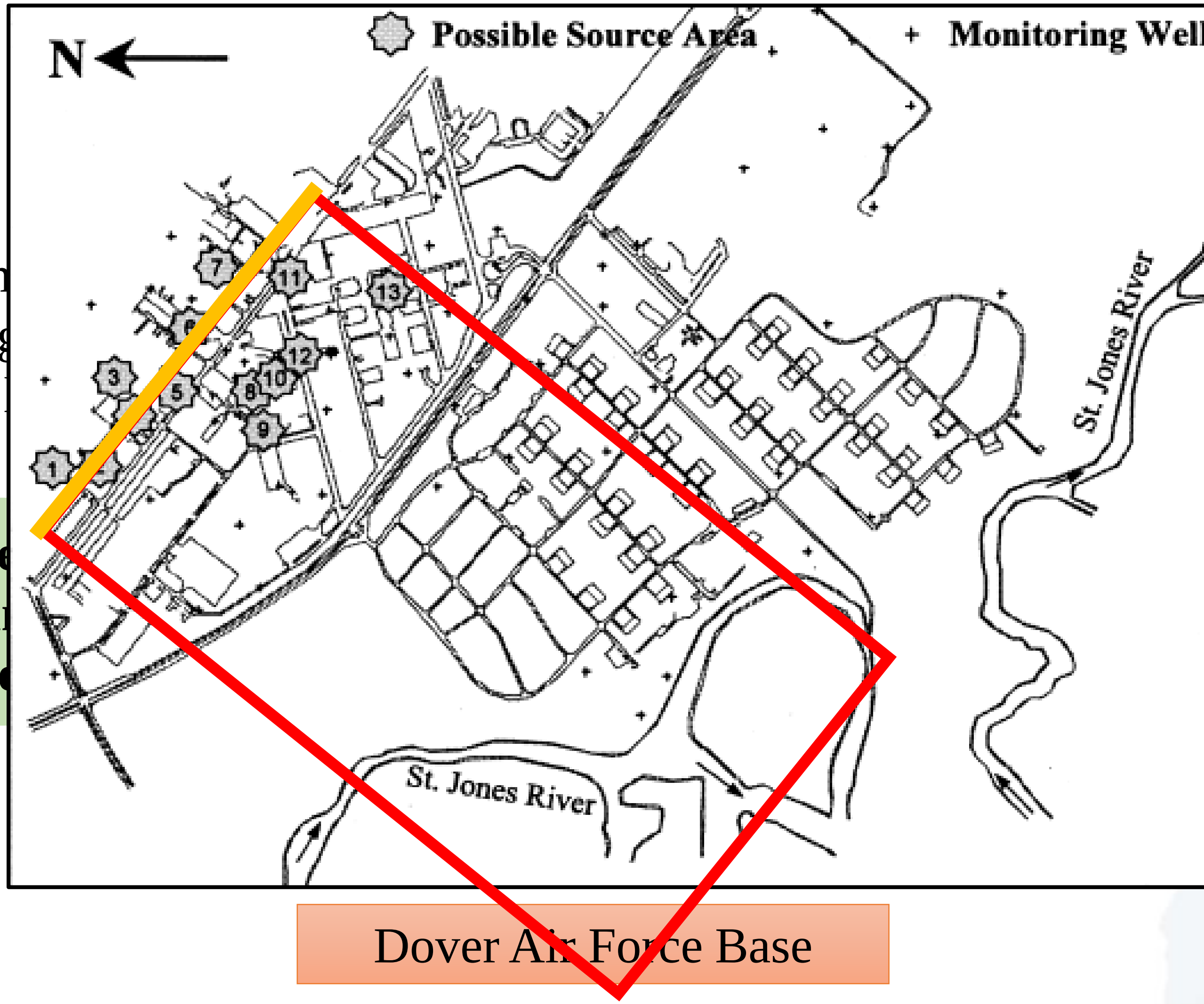


Dover Air Force Base

Introduction

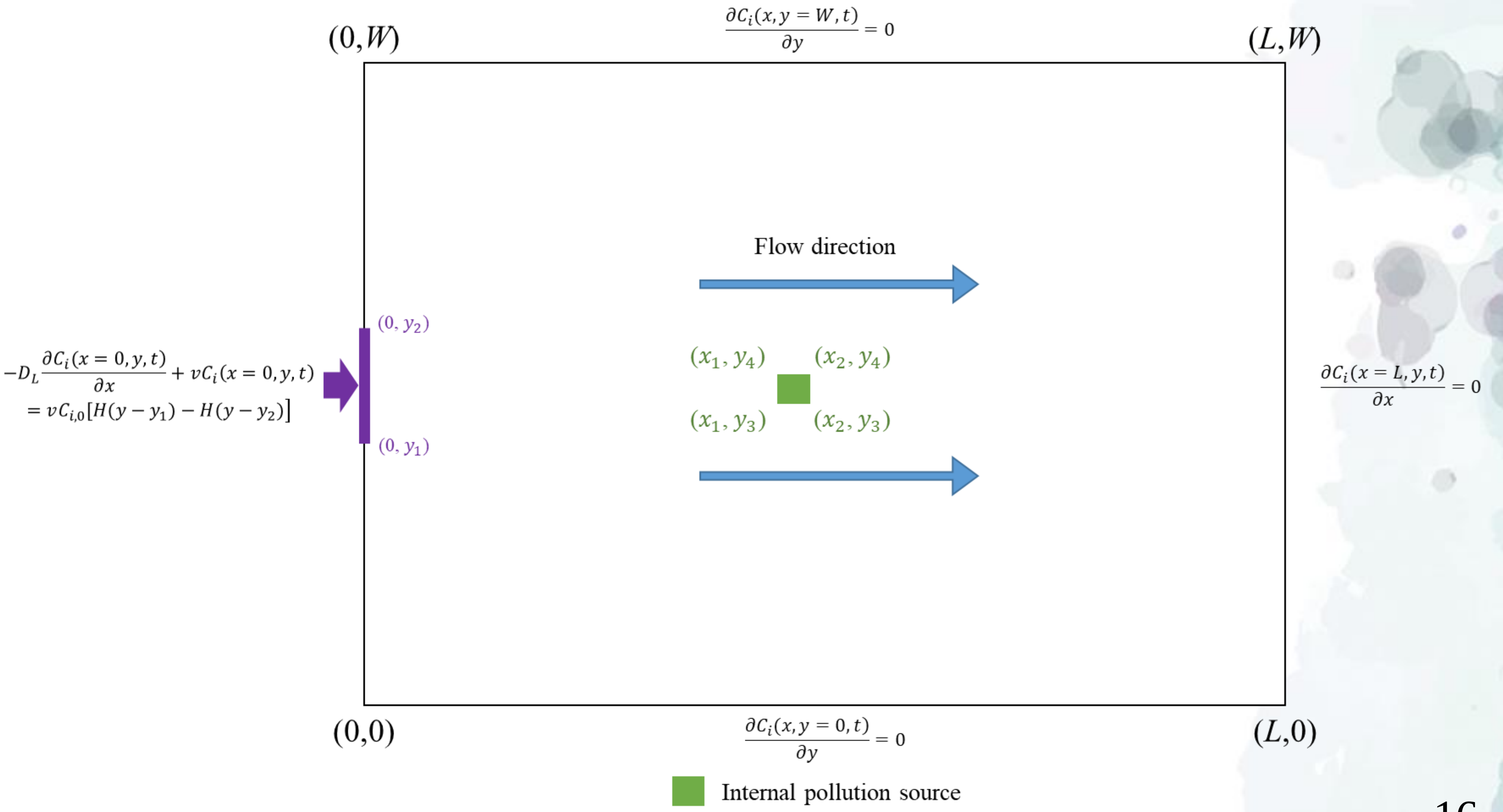
Objective

To develop a semi-analytical model for simulating multi-species advective-dispersive transport which considering rate-limited sorption and subject to multiple internal sources.

Outline

Mathematical model

Conceptual model



Mathematical model

Governing equation

$$D_L \frac{\partial^2 C_i(x,y,t)}{\partial x^2} - v\frac{\partial C_i(x,y,t)}{\partial x} + D_T \frac{\partial^2 C_i(x,y,t)}{\partial y^2} - k_i C_i(x,y,t) + k_{i-1}C_{i-1}(x,y,t) +$$

$$\sum_{m=1}^{NS} \frac{M_i^m}{\phi} p_{x,i}^m(x) p_{y,i}^m(y) q_i^m(t) - \frac{\beta_i}{\phi}[C_i(x,y,t) - \frac{S_i(x,y,t)}{K_{di}}] = \frac{\partial C_i(x,y,t)}{\partial t} \qquad i = 1,\ldots,\mathrm{N}$$

- First-order reversible kinetic sorption reaction between the dissolved and sorbed phases.

$$\rho_b \frac{\partial S_i(x,y,t)}{\partial t} = \beta_i [C_i(x,y,t) - \frac{S_i(x,y,t)}{K_{di}}] \qquad i = 1,\ldots,\mathrm{N}$$

$C_i(x,t)$: concentration of species i in the dissolved phase [ML^{-3}]
$S_i(x,t)$: concentration of species i in the sorbed phase [MM^{-1}]

Mathematical model

Governing equation

$$D_L \frac{\partial^2 C_i(x,y,t)}{\partial x^2} - v\frac{\partial C_i(x,y,t)}{\partial x} + D_T \frac{\partial^2 C_i(x,y,t)}{\partial y^2} - k_i C_i(x,y,t) + k_{i-1} C_{i-1}(x,y,t) +$$

$$\sum_{m=1}^{NS} \frac{M_i^m}{\phi} p_{x,i}^m(x) p_{y,i}^m(y) q_i^m(t) - \frac{\beta_i}{\phi}[C_i(x,y,t) - \frac{S_i(x,y,t)}{K_{di}}] = \frac{\partial C_i(x,y,t)}{\partial t} \qquad i = 1,\ldots,\mathrm{N}$$

Dispersion

- Due to the heterogeneity of the porous media at the micro scale, the flow path and the flow velocity of the solute in the pore water flow are different.

D: Dispersion coefficient $[\mathrm{L}^2\mathrm{T}^{-1}]$

Mathematical model

Governing equation

$$D_L \frac{\partial^2 C_i(x,y,t)}{\partial x^2} - v\frac{\partial C_i(x,y,t)}{\partial x} + D_T \frac{\partial^2 C_i(x,y,t)}{\partial y^2} - k_i C_i(x,y,t) + k_{i-1}C_{i-1}(x,y,t) +$$

$$\sum_{m=1}^{NS} \frac{M_i^m}{\phi} p_{x,i}^m(x) p_{y,i}^m(y) q_i^m(t) - \frac{\beta_i}{\phi}[C_i(x,y,t) - \frac{S_i(x,y,t)}{K_{di}}] = \frac{\partial C_i(x,y,t)}{\partial t} \qquad i = 1,\ldots,\mathrm{N}$$

Advection

- Flow velocity of the contaminated plume.

v: velocity $[\mathrm{LT}^{-1}]$

Mathematical model

Governing equation

$$D_L \frac{\partial^2 C_i(x,y,t)}{\partial x^2} - v\frac{\partial C_i(x,y,t)}{\partial x} + D_T \frac{\partial^2 C_i(x,y,t)}{\partial y^2} - \boxed{k_i C_i(x,y,t) + k_{i-1} C_{i-1}(x,y,t)} +$$

$$\sum_{m=1}^{NS} \frac{M_i^m}{\phi} p_{x,i}^m(x) p_{y,i}^m(y) q_i^m(t) - \frac{\beta_i}{\phi}[C_i(x,y,t) - \frac{S_i(x,y,t)}{K_{di}}] = \frac{\partial C_i(x,y,t)}{\partial t} \qquad i = 1,\ldots,\mathrm{N}$$

First-order degradation

- Describe the concentration change impact by the decay of parent species.

k_i: first order degradation rate constant $[\mathrm{T}^{-1}]$

Mathematical model

Governing equation

$$D_L \frac{\partial^2 C_i(x,y,t)}{\partial x^2} - v\frac{\partial C_i(x,y,t)}{\partial x} + D_T \frac{\partial^2 C_i(x,y,t)}{\partial y^2} - k_i C_i(x,y,t) + k_{i-1}C_{i-1}(x,y,t) +$$

$$\boxed{\sum_{m=1}^{NS} \frac{M_i^m}{\phi} p_{x,i}^m(x) p_{y,i}^m(y) q_i^m(t)} - \frac{\beta_i}{\phi}[C_i(x,y,t) - \frac{S_i(x,y,t)}{K_{di}}] = \frac{\partial C_i(x,y,t)}{\partial t} \qquad i = 1,\ldots,\mathrm{N}$$

Source

- Represent the sources that inject contaminants into the simulation area.

  NS: Total number of sources

  M_i^m: Mass of species i^{th} in source m^{th} [M]

  p_i^m: Function of species i^{th} changes with distance in source m^{th} [L^{-1}]

  q_i^m: Function of species i^{th} changes with time in source m^{th} [T^{-1}]

  ϕ : Porosity [-]

Mathematical model

Governing equation

$$D_L \frac{\partial^2 C_i(x,y,t)}{\partial x^2} - v\frac{\partial C_i(x,y,t)}{\partial x} + D_T \frac{\partial^2 C_i(x,y,t)}{\partial y^2} - k_i C_i(x,y,t) + k_{i-1}C_{i-1}(x,y,t) +$$

$$\sum_{m=1}^{NS} \frac{M_i^m}{\phi} p_{x,i}^m(x)\, p_{y,i}^m(y)\, q_i^m(t) - \boxed{\frac{\beta_i}{\phi}\left[C_i(x,y,t) - \frac{S_i(x,y,t)}{K_{di}}\right] = \frac{\partial C_i(x,y,t)}{\partial t}} \qquad i = 1,\ldots,\mathrm{N}$$

Retardation

- Including adsorption or other chemical reactions, which influence the concentration of dissolved contaminants.

K_{di}: Distribution coefficient of species i^{th} $[\mathrm{M}^{-1}\mathrm{L}^3]$

β_i: First-order sorption rate constant of species i^{th} between the dissolved and sorbed phases $[\mathrm{T}^{-1}]$

Mathematical model

Solving process

$C_i(x,y,t)$

↓ **Laplace transform**

$$\bar{C}_i(x,y,s) = \int_0^\infty e^{-st}\, C_i(x,y,t)dt$$

$\bar{C}_i(x,y,s)$

↓ **Fourier cosine transform**

$$H_i(x,n,s) = \int_0^1 C_i(x,y,s)\cos(n\pi y)dy$$

$H_i(x,n,s)$

↓ **Changes-of-variables**

$$\varphi_i(x,n,s) = e^{-\frac{Pe_L}{2}x}\left[H_i(x,n,s) - \frac{C_{i,0}}{s}\Phi(n)\right]$$

$\varphi_i(x,y,t)$

↓ **Generalized integral transform**

$$\overline{\varphi_i}(\xi_l,n,s) = \int_0^1 K(\xi_l,x)\varphi_i(x,n,s)\,dx$$

$\bar{\varphi}_i(\xi_l,y,t)$

→ A series of inverse transform

Algebraic equations

Outline

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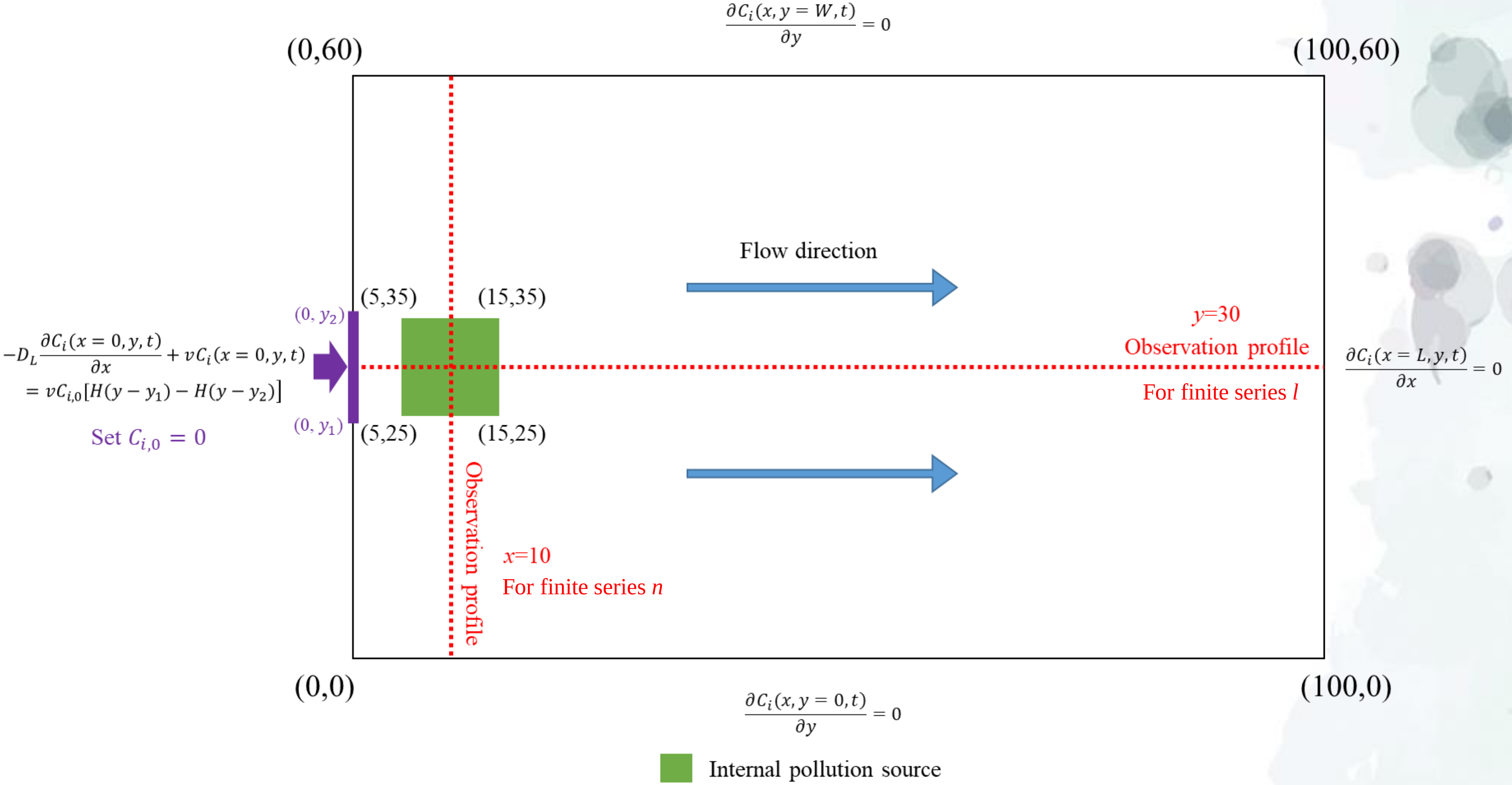
2. Mathematical model
3. Results and Discussion
4. Conclusions

Results and Discussion

Convergence test



Results and Discussion

Convergence test

Contaminant parameters	PCE	TCE	DCE	VC	ETH
Distribution coefficient [kg m^{-3}]	0.784	0.239	0.230	0.0545	0.556
Sorption reaction rate constant [$year^{-1}$]	0.5	0.5	0.5	0.5	0.5
Decay constant [$year^{-1}$]	2.0	1.0	0.7	0.4	0

(Chen et al., 2019)

Geological parameters	Value
Domain length [m]	100
Domain width [m]	60
Velocity [m $year^{-1}$]	1 / 10 / 25
Longitudinal dispersion coefficient [m^2 $year^{-1}$]	100
Transverse dispersion coefficient [m^2 $year^{-1}$]	10
Bulk dry density of the solid grain [kg m^{-3}]	1.6
Effective porosity [-]	0.2
Peclet number	**1 / 10 /25**

Source parameters	Value	
Mass release [kg]	100	
Release duration [year]	0~1	
Simulation time [year]	10	
Source domain [m]	x: 5~15	y: 25~35

Peclet number (Pe) = $\frac{vL}{D_L}$

Results and Discussion

Convergence test

PCE

	l=25	l=50	l=75	l=100	l=125
x=0	1.591E+00	1.591E+00	1.591E+00	[illegible]	1.591E+00
x=20	1.000E+00	1.000E+00	1.000E+00	[illegible]	1.000E+00
x=40	1.069E-01	1.069E-01	1.069E-01	[illegible]	1.069E-01
x=60	6.253E-03	6.273E-03	6.270E-03	6.270E-03	[illegible]
x=80	2.855E-04	2.767E-04	2.730E-04	2.731E-04	[illegible]
x=100	6.810E-06	2.292E-05	1.906E-05	1.900E-05	[illegible]

TCE

	l=10	l=20	l=30	l=40	l=50
x=0	3.731E+00	3.726E+00	3.726E+00	[illegible]	3.726E+00
x=20	2.782E+00	2.778E+00	2.778E+00	[illegible]	2.778E+00
x=40	8.036E-01	8.007E-01	8.007E-01	[illegible]	8.007E-01
x=60	1.431E-01	1.404E-01	1.404E-01	1.404E-01	[illegible]
x=80	2.095E-02	1.828E-02	1.828E-02	1.828E-02	[illegible]
x=100	6.440E-03	3.549E-03	3.549E-03	3.550E-03	[illegible]

DCE

	l=5	l=10	l=15	l=20	l=25
x=0	5.399E+00	5.393E+00	5.392E+00	[illegible]	5.392E+00
x=20	4.509E+00	4.511E+00	4.510E+00	[illegible]	4.510E+00
x=40	1.892E+00	1.896E+00	1.895E+00	[illegible]	1.895E+00
x=60	4.871E-01	4.827E-01	4.824E-01	4.824E-01	[illegible]
x=80	8.057E-02	8.594E-02	8.564E-02	8.564E-02	[illegible]
x=100	2.675E-02	2.158E-02	2.126E-02	2.126E-02	[illegible]

VC

	l=5	l=10	l=15	l=20	l=25
x=0	6.578E+00	6.577E+00	6.577E+00	[illegible]	6.577E+00
x=20	6.067E+00	6.067E+00	6.067E+00	[illegible]	6.067E+00
x=40	3.391E+00	3.392E+00	3.392E+00	[illegible]	3.392E+00
x=60	1.278E+00	1.278E+00	1.278E+00	1.278E+00	[illegible]
x=80	3.612E-01	3.624E-01	3.624E-01	3.624E-01	[illegible]
x=100	1.449E-01	1.436E-01	1.436E-01	1.436E-01	[illegible]

ETH

	l=4	l=6	l=8	l=10	l=12
x=0	3.626E+00	3.633E+00	3.633E+00	[illegible]	3.633E+00
x=20	3.386E+00	3.380E+00	3.380E+00	[illegible]	3.380E+00
x=40	1.918E+00	1.921E+00	1.921E+00	[illegible]	1.921E+00
x=60	7.221E-01	7.248E-01	7.247E-01	7.247E-01	[illegible]
x=80	2.090E-01	2.008E-01	2.010E-01	2.010E-01	[illegible]
x=100	6.566E-02	7.707E-02	7.692E-02	7.690E-02	[illegible]

PCE

	n=100	n=150	n=200	n=250	[illegible]
y=0	2.305E-05	2.201E-05	2.215E-05	2.213E-05	[illegible]
y=10	2.118E-03	2.119E-03	2.119E-03	2.119E-03	[illegible]
y=20	1.964E-01	1.964E-01	1.964E-01	1.964E-01	1.964E-01
y=30	1.690E+00	1.690E+00	1.690E+00	[illegible]	1.690E+00

TCE

	n=50	n=80	n=110	n=140	[illegible]
y=0	3.376E-03	3.377E-03	3.377E-03	3.377E-03	[illegible]
y=10	6.123E-02	6.123E-02	6.123E-02	6.123E-02	[illegible]
y=20	1.054E+00	1.054E+00	1.054E+00	1.054E+00	1.054E+00
y=30	3.691E+00	3.691E+00	3.691E+00	[illegible]	3.691E+00

DCE

	n=15	n=20	n=25	n=30	[illegible]
y=0	1.957E-02	1.936E-02	1.937E-02	1.937E-02	[illegible]
y=10	2.280E-01	2.281E-01	2.281E-01	2.281E-01	[illegible]
y=20	2.220E+00	2.221E+00	2.221E+00	2.221E+00	2.221E+00
y=30	5.420E+00	5.420E+00	5.420E+00	[illegible]	5.420E+00

VC

	n=8	n=16	n=24	n=33	[illegible]
y=0	1.211E-01	1.198E-01	1.198E-01	1.198E-01	[illegible]
y=10	6.739E-01	6.732E-01	6.732E-01	6.732E-01	[illegible]
y=20	3.598E+00	3.599E+00	3.599E+00	3.599E+00	3.599E+00
y=30	6.763E+00	6.765E+00	6.765E+00	[illegible]	6.765E+00

ETH

	n=6	n=12	n=18	n=24	[illegible]
y=0	5.907E-02	6.459E-02	6.460E-02	6.460E-02	[illegible]
y=10	3.839E-01	3.807E-01	3.807E-01	3.807E-01	[illegible]
y=20	2.033E+00	2.030E+00	2.030E+00	2.030E+00	2.030E+00
y=30	3.738E+00	3.744E+00	3.744E+00	[illegible]	3.744E+00

Pe=1

l=100 *n*=250

The farther away from the source, the greater the required *l* and *n*

Results and Discussion

Convergence test

l=200 *n*=300

PCE	l=50	l=100	l=150	l=200	l=250
x=0	6.260E-01	6.260E-01	6.260E-01	6.260E-01	6.260E-01
x=20	1.213E+00	1.213E+00	1.213E+00	1.213E+00	1.213E+00
x=40	2.862E-01	2.862E-01	2.862E-01	2.862E-01	2.862E-01
x=60	3.674E-02	3.671E-02	3.671E-02	3.671E-02	3.671E-02
x=80	3.584E-03	3.500E-03	3.500E-03	3.500E-03	3.500E-03
x=100	6.615E-04	4.320E-04	4.313E-04	4.322E-04	4.322E-04

l=40 *n*=100

TCE	l=10	l=20	l=30	l=40	l=50
x=0	9.888E-01	9.858E-01	9.858E-01	9.858E-01	9.858E-01
x=20	2.512E+00	2.506E+00	2.506E+00	2.506E+00	2.506E+00
x=40	1.660E+00	1.650E+00	1.650E+00	1.650E+00	1.650E+00
x=60	6.507E-01	6.305E-01	6.305E-01	6.305E-01	6.305E-01
x=80	2.283E-01	1.782E-01	1.782E-01	1.782E-01	1.782E-01
x=100	1.925E-01	5.762E-02	5.754E-02	5.761E-02	5.761E-02

l=20 *n*=35

DCE	l=5	l=10	l=15	l=20	l=25
x=0	9.917E-01	9.947E-01	9.944E-01	9.944E-01	9.944E-01
x=20	3.054E+00	3.041E+00	3.040E+00	3.040E+00	3.040E+00
x=40	3.148E+00	3.190E+00	3.189E+00	3.189E+00	3.189E+00
x=60	1.967E+00	1.867E+00	1.865E+00	1.865E+00	1.865E+00
x=80	4.873E-01	7.462E-01	7.409E-01	7.409E-01	7.409E-01
x=100	9.631E-01	3.203E-01	3.059E-01	3.061E-01	3.061E-01

l=13 *n*=26

VC	l=4	l=7	l=10	l=13	l=16
x=0	7.639E-01	7.731E-01	7.729E-01	7.729E-01	7.729E-01
x=20	2.734E+00	2.715E+00	2.715E+00	2.715E+00	2.715E+00
x=40	3.954E+00	3.978E+00	3.979E+00	3.979E+00	3.979E+00
x=60	3.500E+00	3.521E+00	3.520E+00	3.520E+00	3.520E+00
x=80	2.486E+00	2.226E+00	2.224E+00	2.224E+00	2.224E+00
x=100	3.200E-01	1.386E+00	1.396E+00	1.395E+00	1.395E+00

l=10 *n*=18

ETH	l=4	l=6	l=8	l=10	l=12
x=0	4.003E-01	4.034E-01	4.034E-01	4.034E-01	4.034E-01
x=20	1.462E+00	1.456E+00	1.456E+00	1.456E+00	1.456E+00
x=40	2.229E+00	2.236E+00	2.236E+00	2.236E+00	2.236E+00
x=60	2.021E+00	2.030E+00	2.030E+00	2.030E+00	2.030E+00
x=80	1.371E+00	1.274E+00	1.274E+00	1.274E+00	1.274E+00
x=100	3.922E-01	7.800E-01	7.813E-01	7.807E-01	7.807E-01

PCE	n=100	n=200	n=300	n=400	n=500
y=0	8.860E-06	7.960E-06	7.937E-06	7.937E-06	7.937E-06
y=10	1.018E-03	1.019E-03	1.019E-03	1.019E-03	1.019E-03
y=20	1.299E-01	1.299E-01	1.299E-01	1.299E-01	1.299E-01
y=30	1.320E+00	1.320E+00	1.320E+00	1.320E+00	1.320E+00

TCE	n=25	n=50	n=75	n=100	n=125
y=0	8.307E-04	8.062E-04	8.067E-04	8.068E-04	8.068E-04
y=10	1.969E-02	1.966E-02	1.966E-02	1.966E-02	1.966E-02
y=20	4.765E-01	4.764E-01	4.764E-01	4.764E-01	4.764E-01
y=30	2.005E+00	2.005E+00	2.005E+00	2.005E+00	2.005E+00

DCE	n=15	n=25	n=35	n=45	n=55
y=0	4.187E-03	4.024E-03	4.023E-03	4.023E-03	4.023E-03
y=10	6.031E-02	6.034E-02	6.034E-02	6.034E-02	6.034E-02
y=20	7.542E-01	7.544E-01	7.544E-01	7.544E-01	7.544E-01
y=30	2.093E+00	2.092E+00	2.092E+00	2.092E+00	2.092E+00

VC	n=10	n=18	n=26	n=34	n=42
y=0	1.637E-02	1.640E-02	1.639E-02	1.639E-02	1.639E-02
y=10	1.182E-01	1.182E-01	1.182E-01	1.182E-01	1.182E-01
y=20	8.033E-01	8.033E-01	8.033E-01	8.033E-01	8.033E-01
y=30	1.687E+00	1.687E+00	1.687E+00	1.687E+00	1.687E+00

ETH	n=6	n=12	n=18	n=24	n=30
y=0	6.951E-03	9.237E-03	9.241E-03	9.241E-03	9.241E-03
y=10	6.960E-02	6.826E-02	6.826E-02	6.826E-02	6.826E-02
y=20	4.442E-01	4.430E-01	4.430E-01	4.430E-01	4.430E-01
y=30	8.844E-01	8.871E-01	8.871E-01	8.871E-01	8.871E-01

Pe=10

l=200 *n*=300

As the degradation of species, the required *l* and *n* are lower

Results and Discussion

Convergence test

PCE					
	l=100	l=200	l=300	l=400	l=500
x=0	1.062E-01	1.062E-01	1.062E-01	1.062E-01	1.062E-01
x=20	1.034E+00	1.034E+00	1.034E+00	1.034E+00	1.034E+00
x=40	6.143E-01	6.143E-01	6.143E-01	6.143E-01	6.143E-01
x=60	1.959E-01	1.959E-01	1.959E-01	1.959E-01	1.959E-01
x=80	4.696E-02	4.693E-02	4.693E-02	4.693E-02	4.693E-02
x=100	1.194E-02	1.158E-02	1.159E-02	1.159E-02	1.159E-02

TCE					
	l=25	l=50	l=75	l=100	l=125
x=0	7.650E-02	7.651E-02	7.651E-02	7.651E-02	7.651E-02
x=20	1.032E+00	1.032E+00	1.032E+00	1.032E+00	1.032E+00
x=40	1.617E+00	1.617E+00	1.617E+00	1.617E+00	1.617E+00
x=60	1.349E+00	1.349E+00	1.349E+00	1.349E+00	1.349E+00
x=80	8.515E-01	8.533E-01	8.531E-01	8.531E-01	8.531E-01
x=100	5.288E-01	5.085E-01	5.068E-01	5.067E-01	5.067E-01

DCE					
	l=15	l=25	l=35	l=45	l=55
x=0	3.160E-02	3.159E-02	3.159E-02	3.159E-02	3.159E-02
x=20	5.489E-01	5.490E-01	5.490E-01	5.490E-01	5.490E-01
x=40	1.561E+00	1.561E+00	1.561E+00	1.561E+00	1.561E+00
x=60	2.215E+00	2.217E+00	2.217E+00	2.217E+00	2.217E+00
x=80	2.170E+00	2.151E+00	2.151E+00	2.151E+00	2.151E+00
x=100	1.496E+00	1.722E+00	1.722E+00	1.722E+00	1.722E+00

VC					
	l=8	l=14	l=20	l=26	l=32
x=0	8.924E-03	2.969E-03	2.969E-03	2.969E-03	2.969E-03
x=20	1.846E-01	6.812E-02	6.812E-02	6.812E-02	6.812E-02
x=40	7.694E-01	3.443E-01	3.443E-01	3.443E-01	3.443E-01
x=60	1.625E+00	8.511E-01	8.511E-01	8.511E-01	8.511E-01
x=80	2.335E+00	1.346E+00	1.346E+00	1.346E+00	1.346E+00
x=100	3.184E+00	1.566E+00	1.565E+00	1.565E+00	1.565E+00

ETH					
	l=6	l=10	l=14	l=18	l=22
x=0	2.965E-03	2.969E-03	2.969E-03	2.969E-03	2.969E-03
x=20	6.818E-02	6.812E-02	6.812E-02	6.812E-02	6.812E-02
x=40	3.440E-01	3.443E-01	3.443E-01	3.443E-01	3.443E-01
x=60	8.465E-01	8.512E-01	8.511E-01	8.511E-01	8.511E-01
x=80	1.453E+00	1.347E+00	1.346E+00	1.346E+00	1.346E+00
x=100	4.584E-01	1.585E+00	1.566E+00	1.565E+00	1.565E+00

PCE					
	n=200	n=300	n=400	n=500	n=600
y=0	3.262E-07	3.043E-07	3.044E-07	3.051E-07	3.053E-07
y=10	1.053E-04	1.053E-04	1.053E-04	1.053E-04	1.053E-04
y=20	3.755E-02	3.755E-02	3.755E-02	3.755E-02	3.755E-02
y=30	6.407E-01	6.407E-01	6.407E-01	6.407E-01	6.407E-01

TCE					
	n=50	n=100	n=150	n=200	n=250
y=0	9.193E-06	9.734E-06	9.727E-06	9.727E-06	9.727E-06
y=10	7.362E-04	7.362E-04	7.362E-04	7.362E-04	7.362E-04
y=20	5.963E-02	5.962E-02	5.962E-02	5.962E-02	5.962E-02
y=30	4.452E-01	4.452E-01	4.452E-01	4.452E-01	4.452E-01

DCE					
	n=30	n=40	n=50	n=60	n=70
y=0	2.940E-05	2.989E-05	2.994E-05	2.995E-05	2.995E-05
y=10	1.215E-03	1.214E-03	1.214E-03	1.214E-03	1.214E-03
y=20	4.220E-02	4.220E-02	4.220E-02	4.220E-02	4.220E-02
y=30	1.915E-01	1.915E-01	1.915E-01	1.915E-01	1.915E-01

VC					
	n=10	n=20	n=30	n=40	n=50
y=0	3.097E-05	4.062E-05	4.093E-05	4.095E-05	4.095E-05
y=10	8.831E-04	8.930E-04	8.932E-04	8.932E-04	8.932E-04
y=20	1.695E-02	1.696E-02	1.696E-02	1.696E-02	1.696E-02
y=30	5.652E-02	5.648E-02	5.648E-02	5.648E-02	5.648E-02

ETH					
	n=10	n=15	n=20	n=25	n=30
y=0	2.301E-05	2.468E-05	2.409E-05	2.410E-05	2.410E-05
y=10	4.651E-04	4.659E-04	4.661E-04	4.661E-04	4.661E-04
y=20	6.875E-03	6.874E-03	6.874E-03	6.874E-03	6.874E-03
y=30	1.938E-02	1.938E-02	1.938E-02	1.938E-02	1.938E-02

The greater the Pe, the greater the required *l* and *n*

Pe=25

l=300 *n*=500

Pe=10

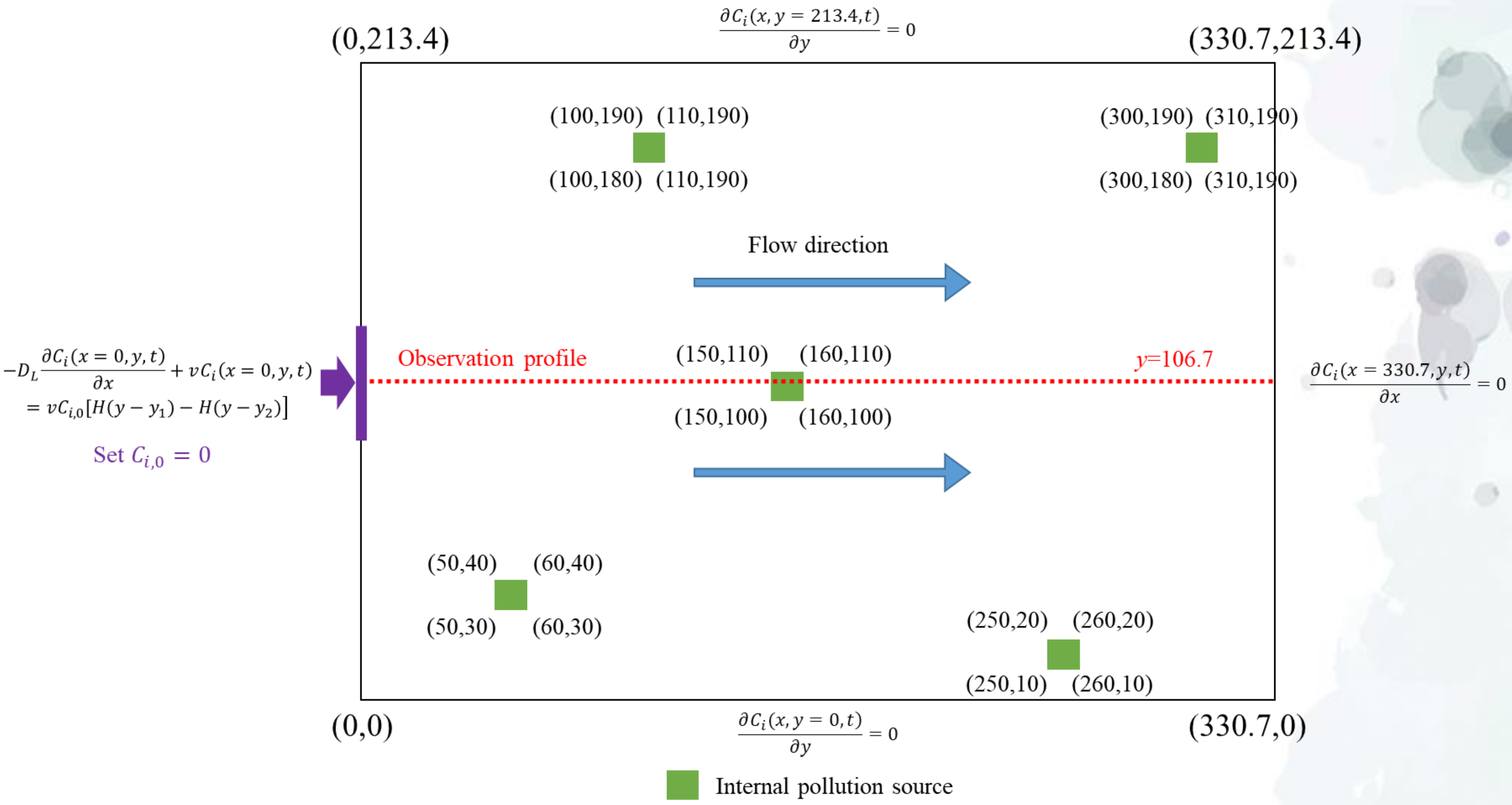
l=200 *n*=300

Pe=1

l=100 *n*=250

Results and Discussion

Verification



Results and Discussion

Verification

Contaminant parameters	PCE	TCE	DCE	VC	ETH
Distribution coefficient [kg m^{-3}]	0.784	0.239	0.230	0.0545	0.556
Sorption reaction rate constant [$year^{-1}$]	0.5	0.5	0.5	0.5	0.5
Decay constant [$year^{-1}$]	2.0	1.0	0.7	0.4	0

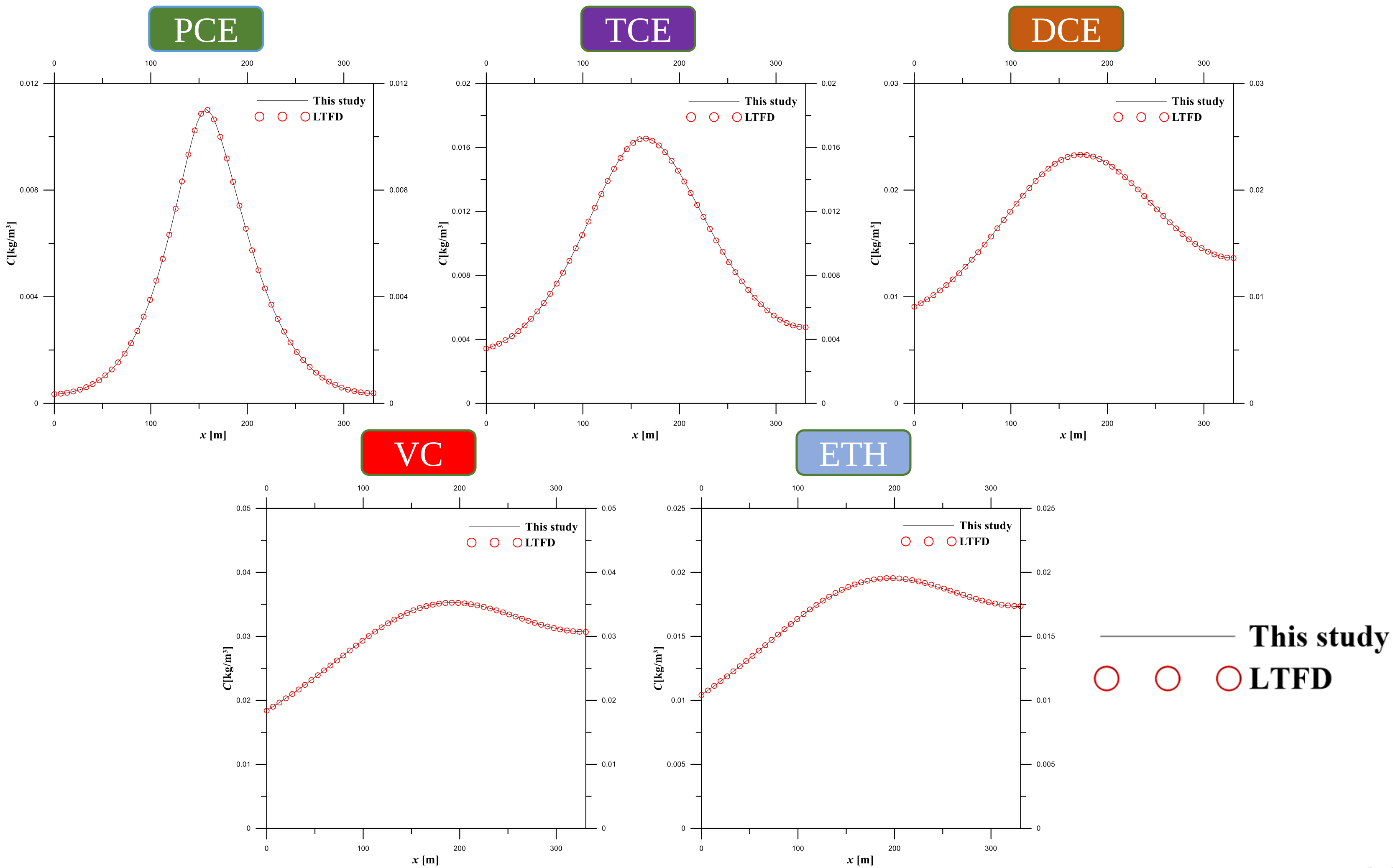
(Chen et al., 2019)

Source parameters	Value	
Mass release [kg]	10	
Release duration [year]	0~1	
Simulation time [year]	10	
Source 1 domain [m]	x: 150~160	y: 100~110
Source 2 domain [m]	x: 50~60	y: 30~40
Source 3 domain [m]	x: 250~260	y: 10~20
Source 4 domain [m]	x: 100~110	y: 180~190
Source 5 domain [m]	x: 300~310	y: 100~110

Geological parameters	Value
Domain length [m]	330.7
Domain width [m]	213.4
Velocity [m $year^{-1}$]	10
Longitudinal dispersion coefficient [m^2 $year^{-1}$]	2000
Transverse dispersion coefficient [m^2 $year^{-1}$]	1000
Bulk dry density of the solid grain [kg m^{-3}]	1.6
Effective porosity [-]	0.2

Results and Discussion

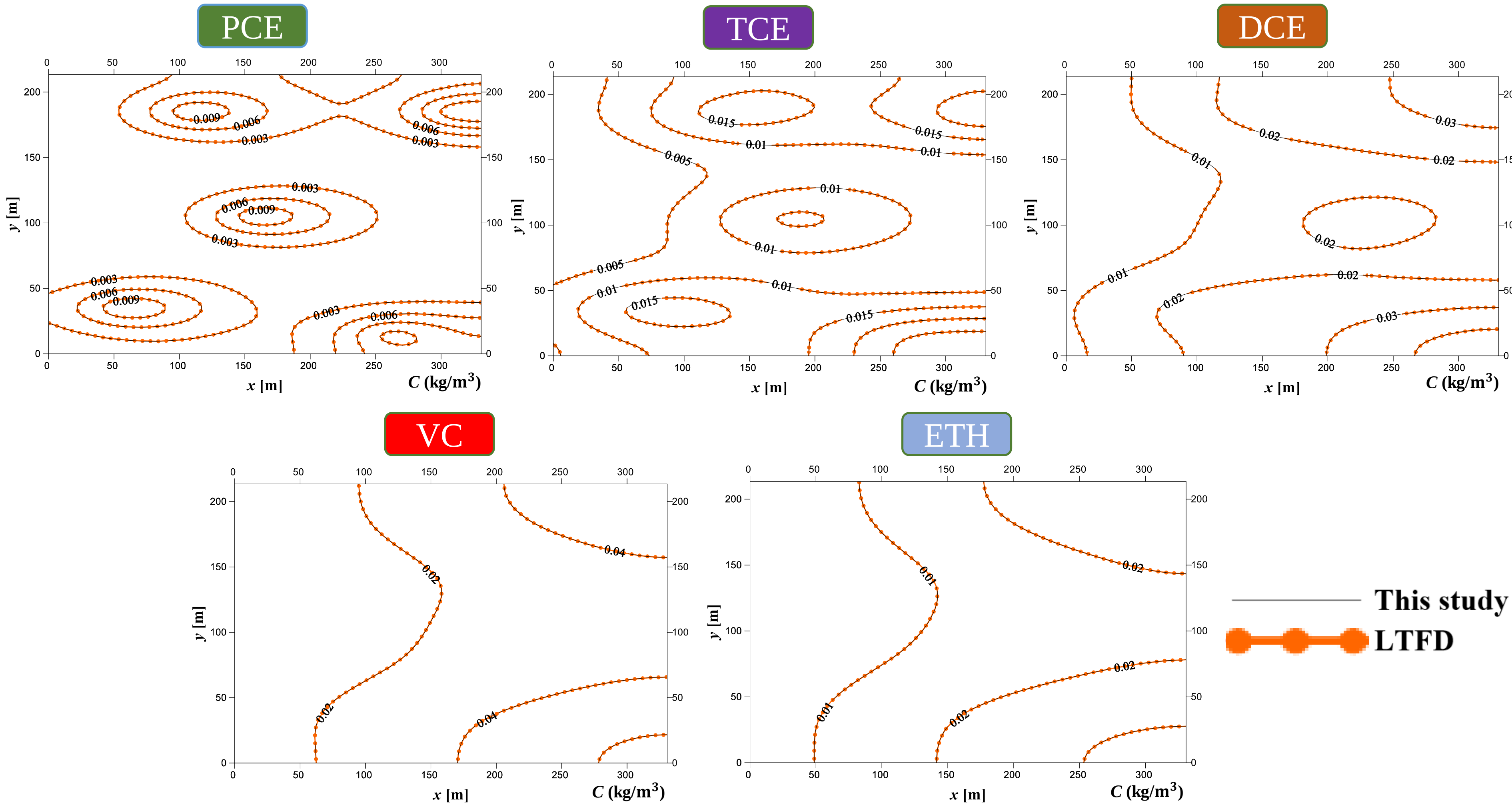
Verification



LTFD: Laplace Transform Finite Difference method (Moridis and Reddell, 1991)

Results and Discussion

Verification

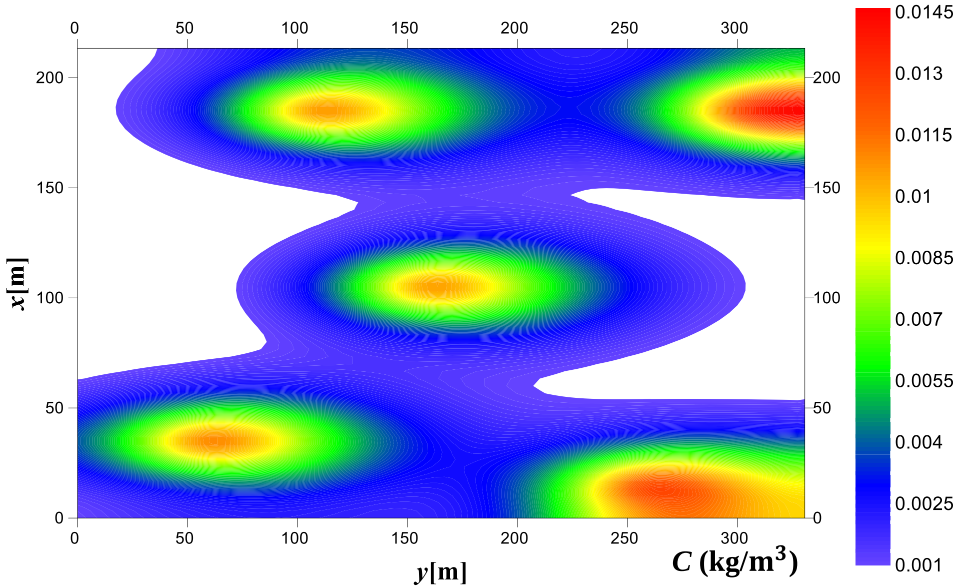


LTFD: Laplace Transform Finite Difference method (Moridis and Reddell, 1991)

Results and Discussion

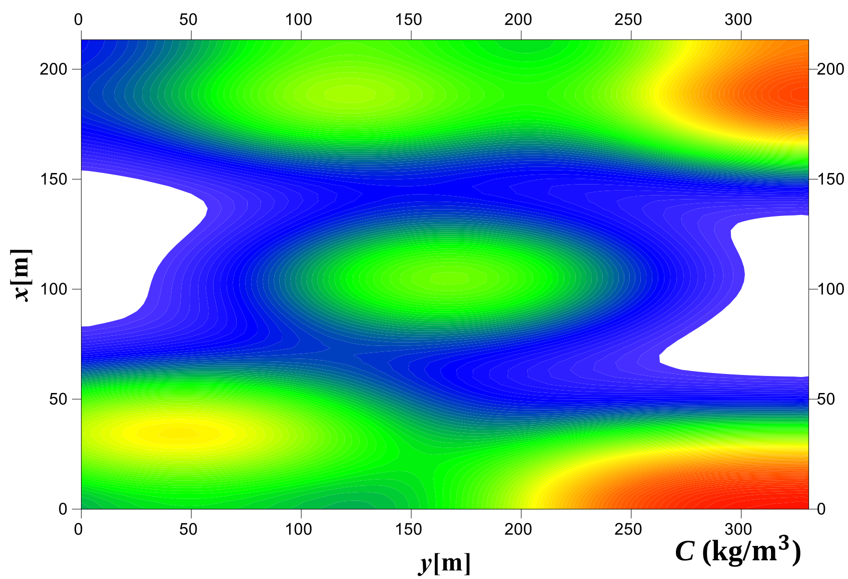
Comparison between equilibrium-controlled and rate-limited sorption

PCE



$\beta_i = 0.5\text{year}^{-1}$

Rate-limited sorption



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

Approaching to equilibrium-controlled sorption

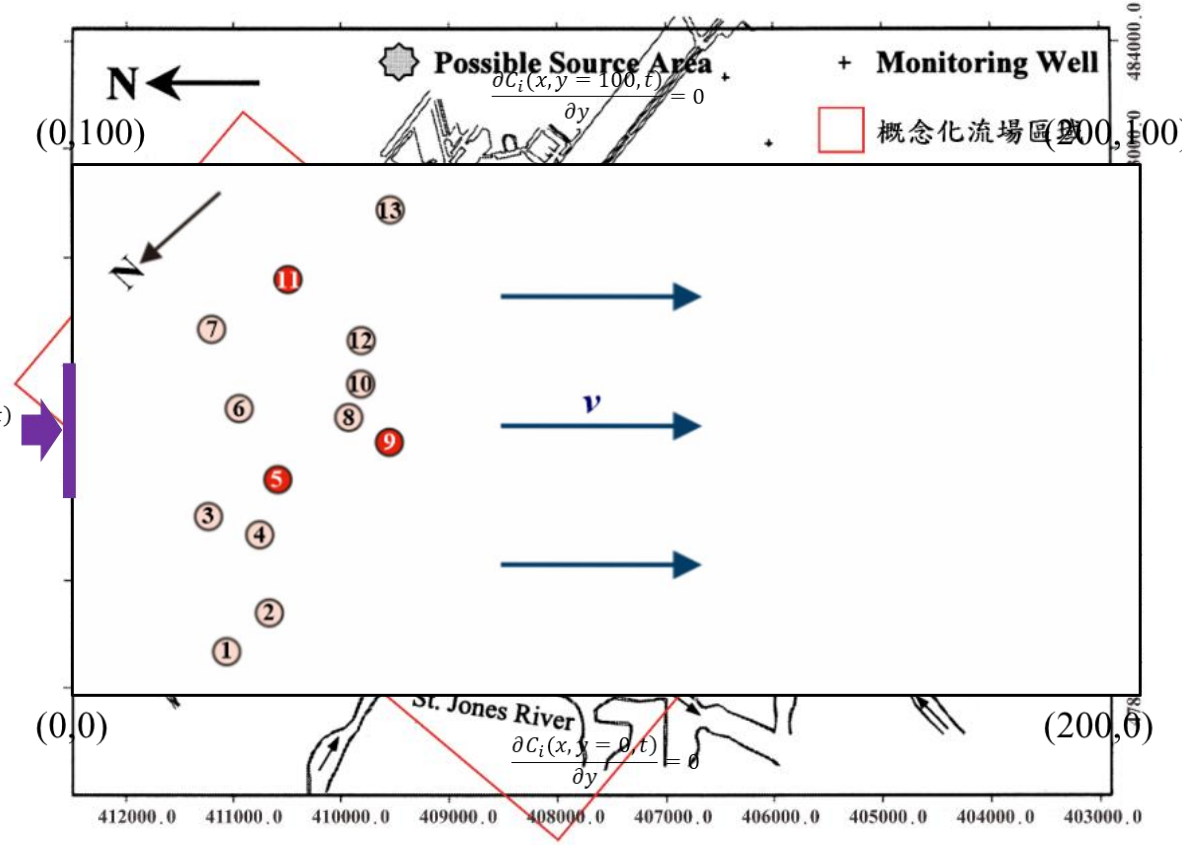
Set the minimum concentration as 0.001 kg/m^3

Results and Discussion

In situ problems - Dover Air Force Base

$$-D_L \frac{\partial C_i(x=0,y,t)}{\partial x} + vC_i(x=0,y,t) = vC_{i,0}[H(y-y_1) - H(y-y_2)]$$

Set $C_{i,0} = 0$



$$\frac{\partial C_i(x=200,y,t)}{\partial x} = 0$$

(Clement, 2000)

Results and Discussion

In situ problems - Dover Air Force Base

Contaminant parameters	PCE	TCE	DCE	VC	ETH
Distribution coefficient [kg m^{-3}]	0.062	0.041	-	-	-
Sorption reaction rate constant [$year^{-1}$]	0.5	0.5	-	-	-
Decay constant [$year^{-1}$]	0.1314	0.1261	-	-	-

(Clement, 2000)

Geological parameters	Value
Domain length [m]	200
Domain width [m]	100
Velocity [m $year^{-1}$]	1.117
Longitudinal dispersion coefficient [m^2 $year^{-1}$]	44.68
Transverse dispersion coefficient [m^2 $year^{-1}$]	4.468
Bulk dry density of the solid grain [kg m^{-3}]	1.7
Effective porosity [-]	0.35

(J.R. Barbaro, 2002)

Source parameters	Value
Mass release [kg]	Shown in table
Release duration [year]	Shown in table
Simulation time [year]	10 / 20 / 30 / 40
Source domain [m]	Shown in figure

Results and Discussion

In situ problems - Dover Air Force Base

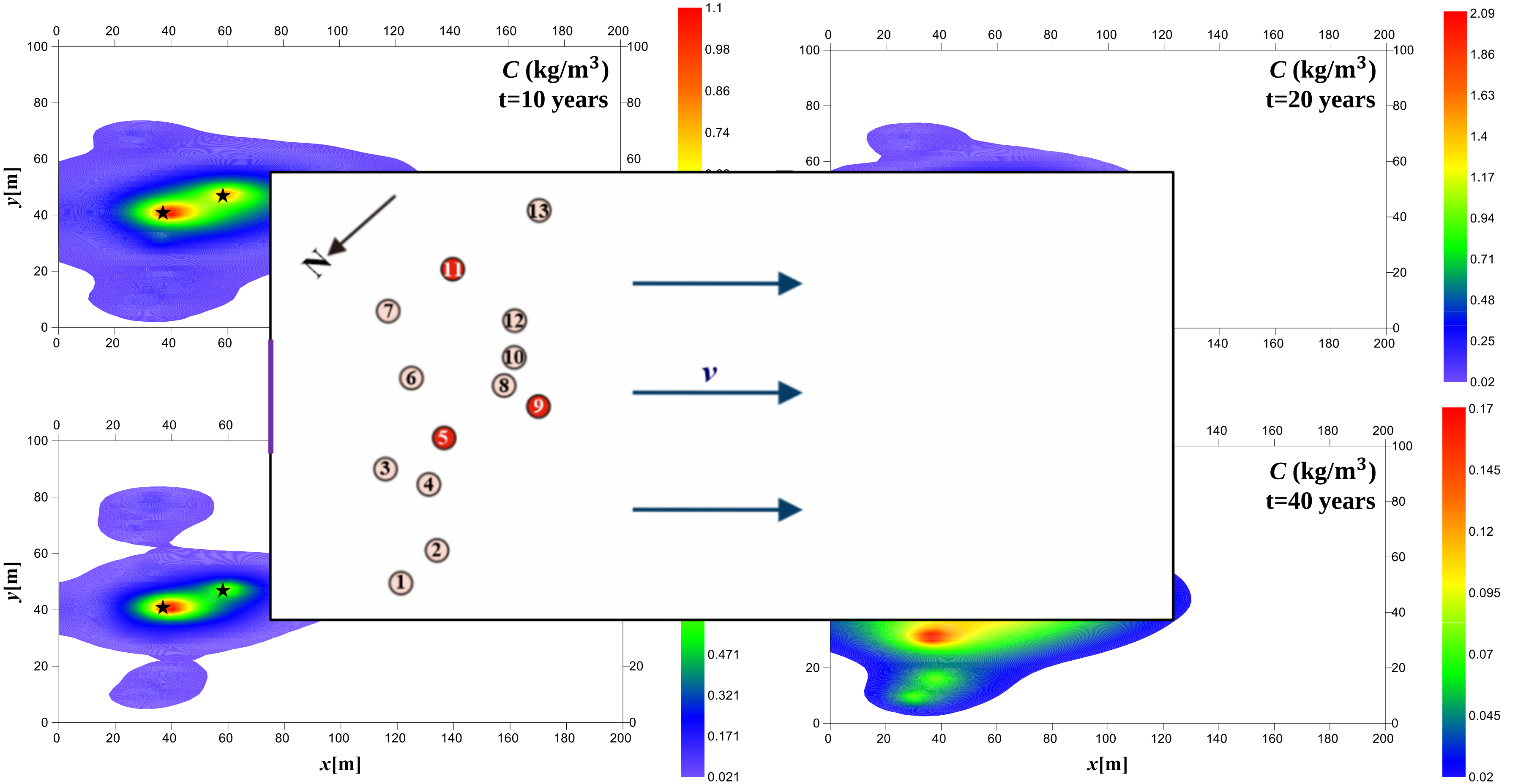
Source	Stress period#1		Stress period#2		Stress period#3		Stress period#4	
number	PCE	TCE	PCE	TCE	PCE	TCE	PCE	TCE
1	1	10	2	10	1	8	1	1
2	1	2	1	2	1	1	1	0
3	1	52	1	1	0	1	0	1
4	1	19	2	19	2	8	2	2
5	25	413	25	165	17	74	0	17
6	1	9	0	1	0	1	0	1
7	1	1	1	1	1	1	0	0
8	0	5	0	5	0	5	0	5
9	10	1	31	517	10	1	1	1
10	0	41	0	41	0	4	0	2
11	2	0	0	413	0	0	0	0
12	0	21	0	21	0	17	0	2
13	0	0	0	0	0	0	0	0

(Clement, 2000)

Results and Discussion

In situ problems - Dover Air Force Base

PCE



Outline

Conclusions

- Since most of contaminated remediation problems involved the internal pollution sources in the contaminated sites, this model can serve as the basis for preliminary assessment of remediation strategy.

- Most of current models considered equilibrium-controlled sorption, which may underestimate the concentration in the groundwater, the model in this study could considered rate-limited sorption to avoid the problems.

Thank you for your attention