Analytical modeling and performance evaluation for multi-permeable reactive barrier susceptible to coexistence of original contaminant and its degradation-related byproducts

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Outline

PART 01.
Introduction

PART 02.
Methodology

PART 03.
Preliminary results

PART 04.
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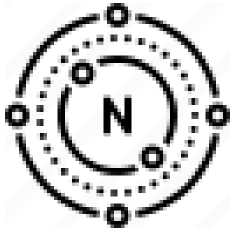
PART 01. Introduction

Why PRB is developed?

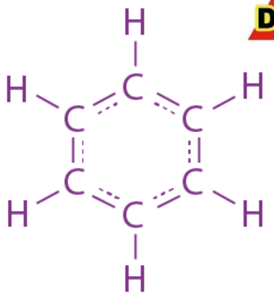
PART 01

- Various geogenic and anthropogenic sources have caused the emergence of numerous toxic contaminants in the groundwater.
- The increasing concentration of contamination has caused adverse effect on humans, animals, and environment.

chlorinated compounds



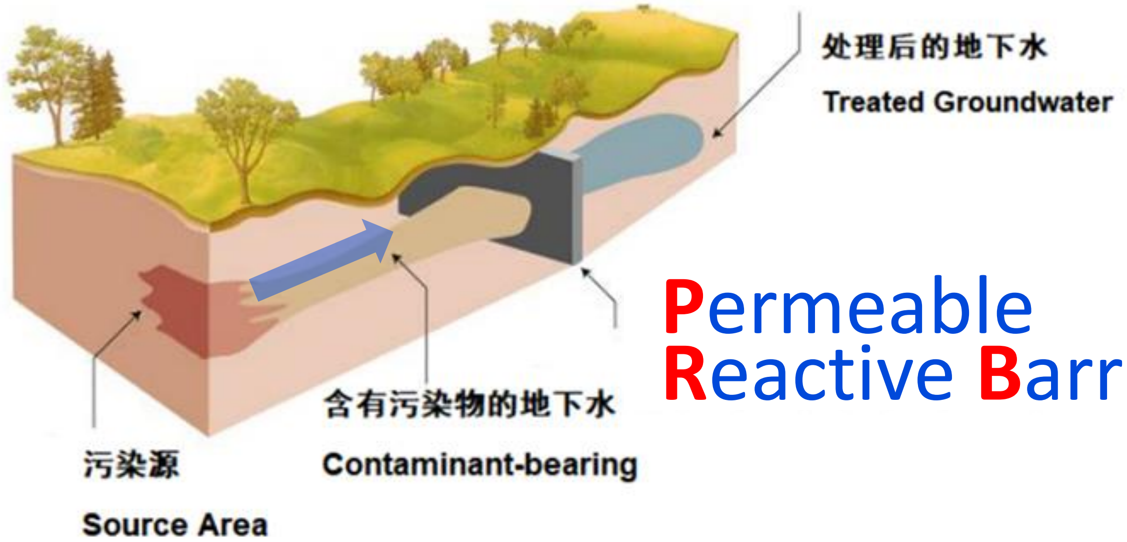
nitrogen



hydrocarbons

radionuclides

Demand for efficient groundwater remediation technique



Permeable Reactive Barrier

- ✓ Physical, chemical, and/or biological processes to remove **contaminants of concern** (COCs)
- ✓ **Cost-effective!**
  No requirement of energy and input resources

Source: http://www.kaitiangroup.com/business/1803.htm

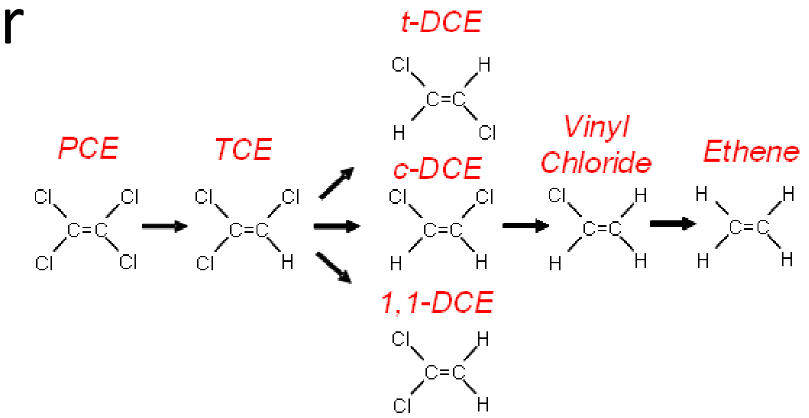
Multi-PRB remediation system

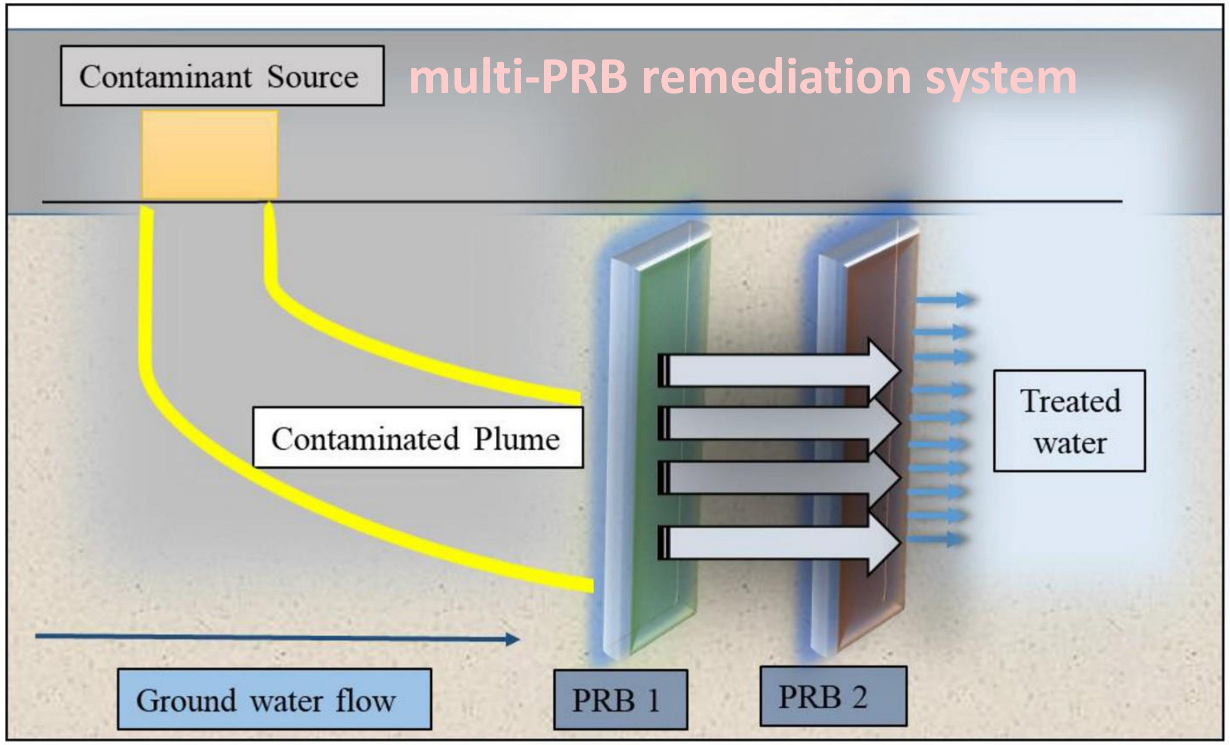
PART 01

- Many **reactive contaminants** would degrade or decay to produce daughter products.

→ Coexistence of multiple contaminant species

→ Existence of daughter species in downstream





Rahul Singh et al. (2020)

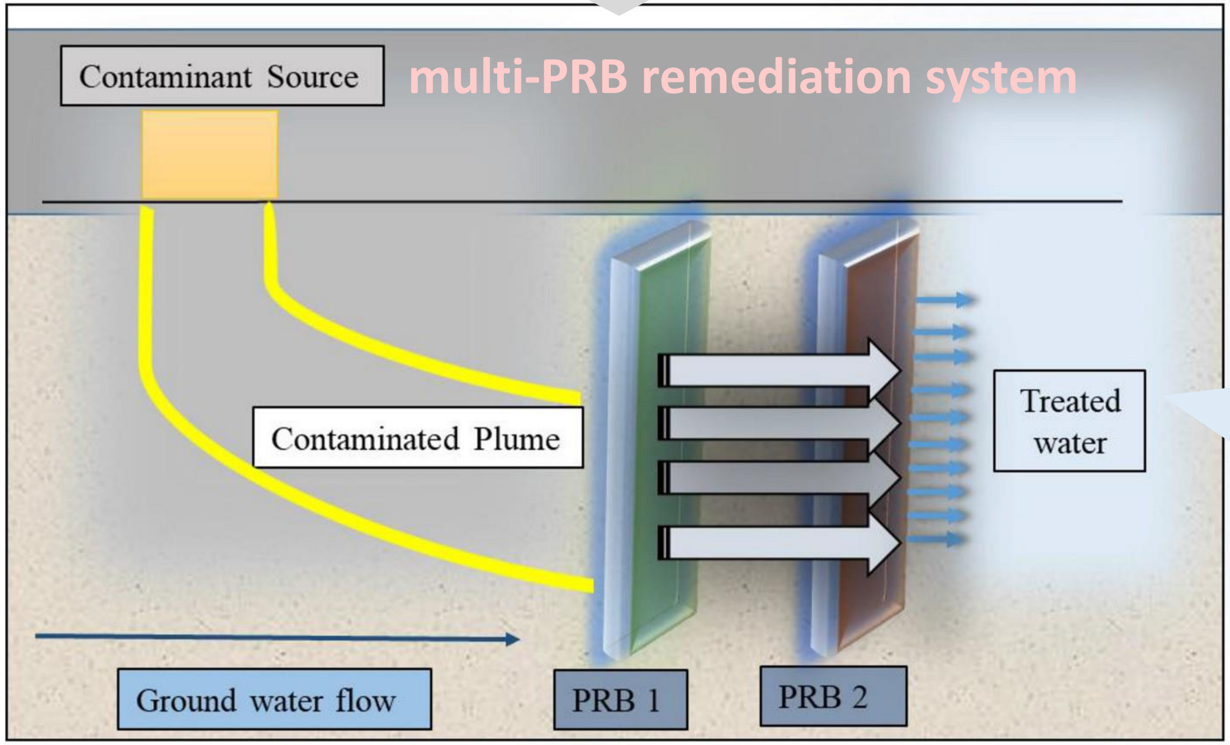
Multi-PRB system has higher removal efficiency for multi contaminants.

- Lee et al. (2010): 2 reactive barriers
- Xu et al. (2012): MODFLOW/MT3DMS
- Singh et al. (2020): MODFLOW

Modelling for Multi-PRB system

PART 01

Modelling of PRB design would aid in analyzing performance of the PRB system for longer time periods and simulate behavior under various plausible scenarios.



Influencing factors include:

- Configuration
- Location
- Thickness (residence time)
- Orientation of barrier
- Contaminant properties
- Material filled in

Rahul Singh et al. (2020)

Mechanisms of contaminant transport

PART 01

Example :

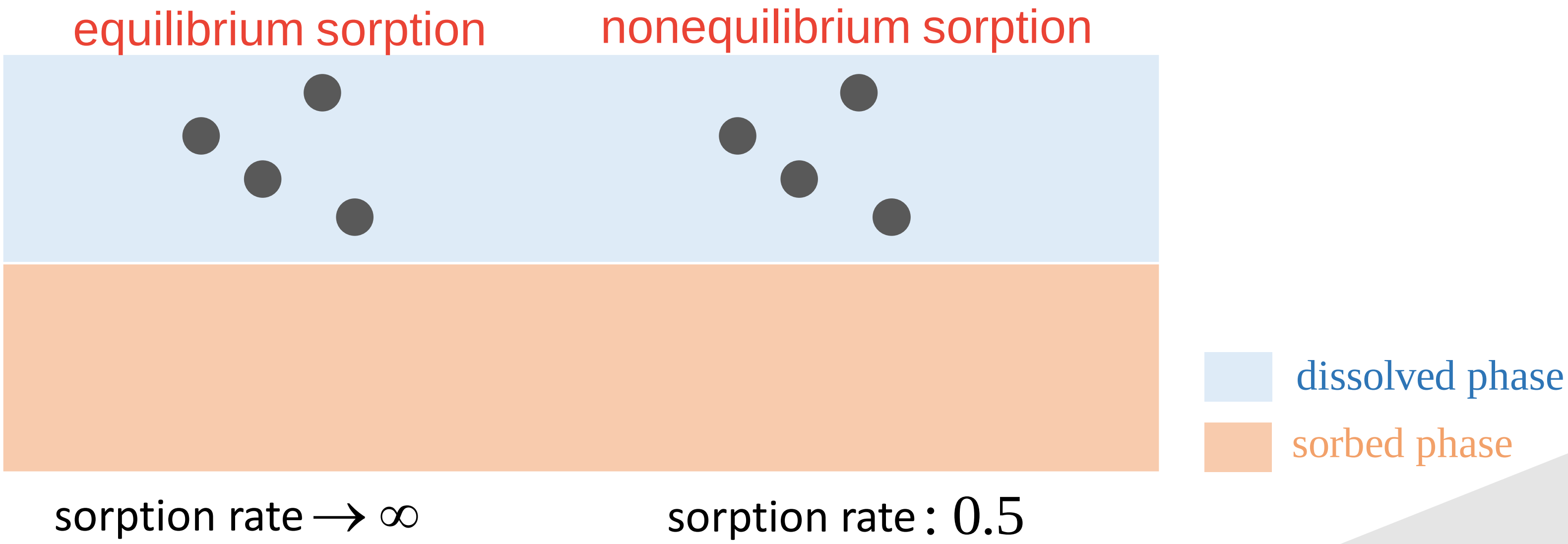
$$D\frac{\partial^2 C_1(x,t)}{\partial x^2} - V\frac{\partial C_1(x,t)}{\partial x} - \mu_1 R_1 C_1(x,t) = R_1\frac{\partial C_1(x,t)}{\partial t}$$

$$D\frac{\partial^2 C_i(x,t)}{\partial x^2} - V\frac{\partial C_i(x,t)}{\partial x} - \mu_i R_i C_i(x,t) + \mu_{i-1} R_{i-1} C_{i-1}(x,t) = R_i\frac{\partial C_i(x,t)}{\partial t}. \quad i = 2\ldots N.$$

Chen et al. (2020)

D : dispersion
V : velocity
μ : decay rate constant
R : retardation coefficient
i : number of species (multispecies)

ratio of speed of plume migration to average groundwater velocity caused by sorption



Literature review of PRB modelling

PART 01

a. transport parameters in PRB and aquifer

b. effective tool for performance evaluation

c. decay reaction in degradation pathway

d. mass transfer between dissolved and sorbed phases

Literature	a. Multiple domain	b. Analytical	c. Multispecies	d. nonequilibrium sorption
Leij et al. (1991)	✓	✓	X	X
Pérez Guerrero et al. (2013)	✓	✓	X	X
Cho (1971)	X	✓	✓	X
Gureghian and Jansen (1985)	✓	✓	✓	X
Singh et al. (2020)	✓	X	X	✓
Guo et al. (2000)	X	✓	X	✓

Objective

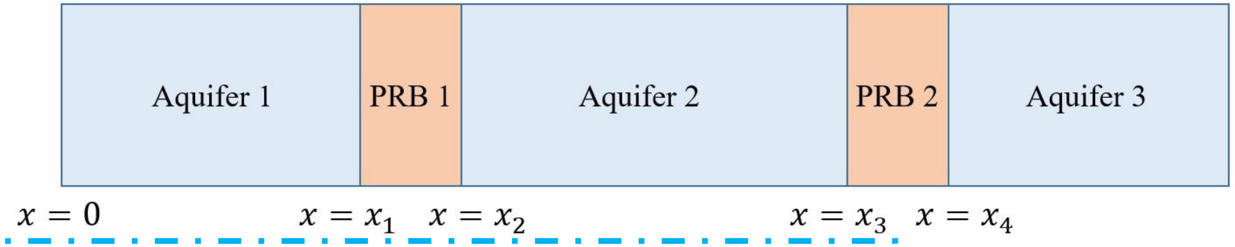
PART 01

- Analytical modeling and performance evaluation for multi-permeable reactive barrier system for groundwater remediation
  - decay reaction and coexistence of multispecies
  - nonequilibrium sorption

PART 02. Methodology

Governing equations

PART 02



Aquifer 1

$$D_{a1}\frac{\partial^2 C_i(x,t)}{\partial x^2} - v_{a1}\frac{\partial C_i(x,t)}{\partial x} - \lambda_{a1}^{i} C_i(x,t) + y_i \lambda_{a1}^{i-1} C_{i-1}(x,t) + \frac{\beta_{a1}^{i}}{\theta_{a1}}\left(C_i(x,t) - \frac{S_i(x,t)}{K_{a1}^{i}}\right) = \frac{\partial C_i(x,t)}{\partial t} \quad \lambda_{a1}^{0} = 0 \quad i = 1,\ldots,N \quad 0 \le x \le x_1,\ t \ge 0$$

dissolved phase

$$\rho_{a1}\frac{\partial S_i(x,t)}{\partial t} = \beta_{a1}^{i}\left(C_i(x,t) - \frac{S_i(x,t)}{K_{a1}^{i}}\right) - \gamma_{a1}^{i}\rho_{a1}S_i(x,t) + y_i \gamma_{a1}^{i-1}\rho_{a1}S_{i-1}(x,t) \quad \gamma_{a1}^{0} = 0 \quad i = 1,\ldots,N \quad 0 \le x \le x_1,\ t \ge 0$$

sorbed phase

PRB 1

$$D_{p1}\frac{\partial^2 C_i(x,t)}{\partial x^2} - v_{p1}\frac{\partial C_i(x,t)}{\partial x} - \lambda_{p1}^{i} C_i(x,t) + y_i \lambda_{p1}^{i-1} C_{i-1}(x,t) + \frac{\beta_{p1}^{i}}{\theta_{p1}}\left(C_i(x,t) - \frac{S_i(x,t)}{K_{p1}^{i}}\right) = \frac{\partial C_i(x,t)}{\partial t} \quad \lambda_{p1}^{0} = 0 \quad i = 1,\ldots,N \quad x_1 \le x \le x_2,\ t \ge 0$$

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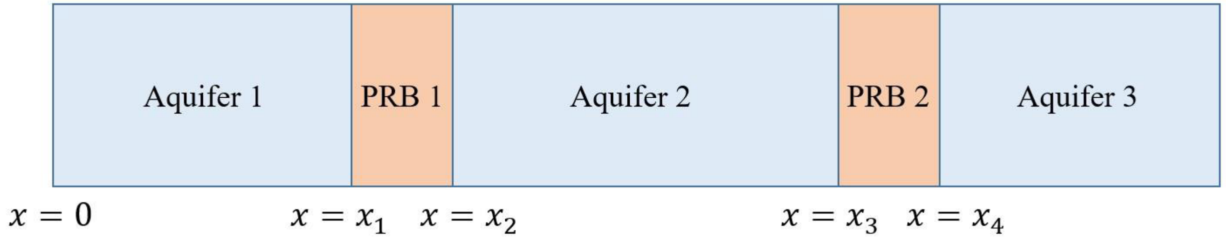
Governing equations

PART 02



Aquifer 2

$$D_{a2}\frac{\partial^2 C_i(x,t)}{\partial x^2} - v_{a2}\frac{\partial C_i(x,t)}{\partial x} - \lambda_{a2}^i C_i(x,t) + y_i\lambda_{a2}^{i-1}C_{i-1}(x,t) + \frac{\beta_{a2}^i}{\theta_{a2}}\left(C_i(x,t)-\frac{S_i(x,t)}{K_{a2}^i}\right) = \frac{\partial C_i(x,t)}{\partial t} \qquad \lambda_{a2}^0 = 0 \qquad i=1,\dots,N \quad x_2 \le x \le x_3,\ \ t\ge 0$$

$$\rho_{a2}\frac{\partial S_i(x,t)}{\partial t} = \beta_{a2}^i\left(C_i(x,t)-\frac{S_i(x,t)}{K_{a2}^i}\right) - \gamma_{a2}^i\rho_{a2}S_i(x,t) + y_i\gamma_{a2}^{i-1}\rho_{a2}S_{i-1}(x,t) \qquad \gamma_{a2}^0 = 0 \qquad i=1,\dots,N \quad x_2 \le x \le x_3,\ \ t\ge 0$$

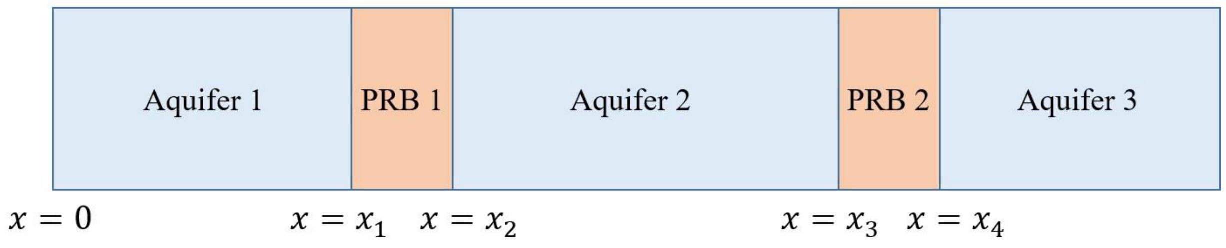
PRB 2

$$D_{p2}\frac{\partial^2 C_i(x,t)}{\partial x^2} - v_{p2}\frac{\partial C_i(x,t)}{\partial x} - \lambda_{p2}^i C_i(x,t) + y_i\lambda_{p2}^{i-1}C_{i-1}(x,t) + \frac{\beta_{p2}^i}{\theta_{p2}}\left(C_i(x,t)-\frac{S_i(x,t)}{K_{p2}^i}\right) = \frac{\partial C_i(x,t)}{\partial t} \qquad \lambda_{p2}^0 = 0 \qquad i=1,\dots,N \quad x_3 \le x \le x_4,\ \ t\ge 0$$

$$\rho_{p2}\frac{\partial S_i(x,t)}{\partial t} = \beta_{p2}^i\left(C_i(x,t)-\frac{S_i(x,t)}{K_{p2}^i}\right) - \gamma_{p2}^i\rho_{p2}S_i(x,t) + y_i\gamma_{p2}^{i-1}\rho_{p2}S_{i-1}(x,t) \qquad \gamma_{p2}^0 = 0 \qquad i=1,\dots,N \quad x_3 \le x \le x_4,\ \ t\ge 0$$

Governing equations

PART 02



Aquifer 3

$$D_{a3}\frac{\partial^2 C_i(x,t)}{\partial x^2} - v_{a3}\frac{\partial C_i(x,t)}{\partial x} - \lambda_{a3}^i C_i(x,t) + y_i\lambda_{a3}^{i-1}C_{i-1}(x,t) + \frac{\beta_{a3}^i}{\theta_{a3}}\left(C_i(x,t) - \frac{S_i(x,t)}{K_{a3}^i}\right) = \frac{\partial C_i(x,t)}{\partial t}$$

$$\lambda_{a3}^0 = 0 \quad i = 1,\dots,N \quad x_4 \le x \le L, \quad t \ge 0$$

$$\rho_{a3}\frac{\partial S_i(x,t)}{\partial t} = \beta_{a3}^i\left(C_i(x,t) - \frac{S_i(x,t)}{K_{a3}^i}\right) - \gamma_{a3}^i\rho_{a3}S_i(x,t) + y_i\gamma_{a3}^{i-1}\rho_{a3}S_{i-1}(x,t)$$

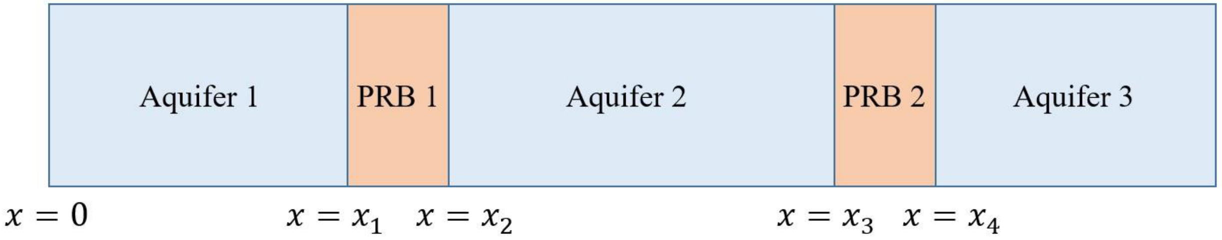
$$\gamma_{a3}^0 = 0 \quad i = 1,\dots,N \quad x_4 \le x \le L, \quad t \ge 0$$

N : total number of species coexisting in the chemical mixture
$C_i(x,t)$: concentration of species i in the dissolved phase
$S_i(x,t)$: concentration of species i in the sorbed phase
v_* : average steady-state pore water velocity
x : spatial coordinate
D_* : dispersion coefficient

λ_*^i : first-order degradation rate constant of specie i in the dissolved phase
γ_*^i : first-order degradation rate constant of specie i in the dissolved phase
β_*^i : retardation factor
y^i : stoichiometric yield factor from species i-1 to species i
$a1$, $p1$, $a2$, $p2$ and $a3$: aquifer 1, PRB1, aquifer 2, PRB2 and aquifer 3

Initial conditions

PART 02



$$C_i(x, t=0) = 0 \qquad 0 \le x \le x_1 \quad i = 1, \ldots, N$$

$$C_i(x, t=0) = 0 \qquad x_1 \le x \le x_2 \quad i = 1, \ldots, N$$

$$C_i(x, t=0) = 0 \qquad x_2 \le x \le x_3 \quad i = 1, \ldots, N$$

$$C_i(x, t=0) = 0 \qquad x_3 \le x \le x_4 \quad i = 1, \ldots, N$$

$$C_i(x, t=0) = 0 \qquad x_4 \le x \le \infty \quad i = 1, \ldots, N$$

$$S_i(x, t=0) = 0 \qquad 0 \le x \le x_1 \quad i = 1, \ldots, N$$

$$S_i(x, t=0) = 0 \qquad x_1 \le x \le x_2 \quad i = 1, \ldots, N$$

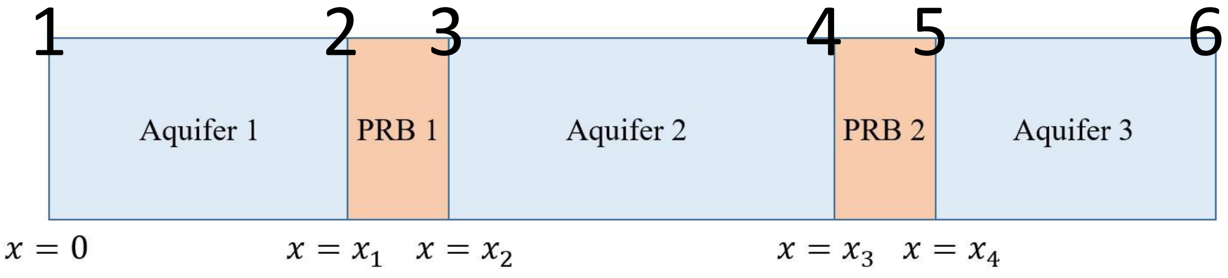
$$S_i(x, t=0) = 0 \qquad x_2 \le x \le x_3 \quad i = 1, \ldots, N$$

$$S_i(x, t=0) = 0 \qquad x_3 \le x \le x_4 \quad i = 1, \ldots, N$$

$$S_i(x, t=0) = 0 \qquad x_4 \le x \le \infty \quad i = 1, \ldots, N$$

Boundary conditions

PART 02



1
$$v_{a1}C_i(x=0,t)-D_{a1}\frac{\partial C(x=0,t)}{\partial x}=v_{a1}c_{i,0} \qquad i=1,\ldots,N$$

2
$$C_i(x=x_1^-,t)=C_i(x=x_1^+,t) \quad i=1,\ldots,N$$
$$\theta_{a1}D_{a1}\frac{\partial C_i(x=x_1^-,t)}{\partial x}=\theta_{p1}D_{p1}\frac{\partial C_i(x=x_1^+,t)}{\partial x} \qquad i=1,\ldots,N$$

3
$$C_i(x=x_2^-,t)=C_i(x=x_2^+,t) \quad i=1,\ldots,N$$
$$\theta_{p1}D_{p1}\frac{\partial C_i(x=x_2^-,t)}{\partial x}=\theta_{a2}D_{a2}\frac{\partial C_i(x=x_2^+,t)}{\partial x} \qquad i=1,\ldots,N$$

4
$$C_i(x=x_3^-,t)=C_i(x=x_3^+,t) \quad i=1,\ldots,N$$
$$\theta_{a2}D_{a2}\frac{\partial C_i(x=x_3^-,t)}{\partial x}=\theta_{p2}D_{p2}\frac{\partial C_i(x=x_3^+,t)}{\partial x} \qquad i=1,\ldots,N$$

5
$$C_i(x=x_4^-,t)=C_i(x=x_4^+,t) \quad i=1,\ldots,N$$
$$\theta_{p2}D_{p2}\frac{\partial C_i(x=x_4^-,t)}{\partial x}=\theta_{a3}D_{a3}\frac{\partial C_i(x=x_4^+,t)}{\partial x} \qquad i=1,\ldots,N$$

6
$$C_i(x\to\infty,t)=0 \quad i=1,\ldots,N$$

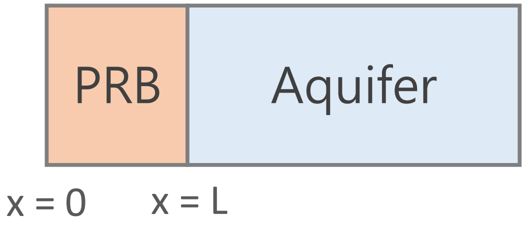
KEY

Satisfy the continuities of species concentrations and mass flux at interfaces

PART 03. Preliminary results

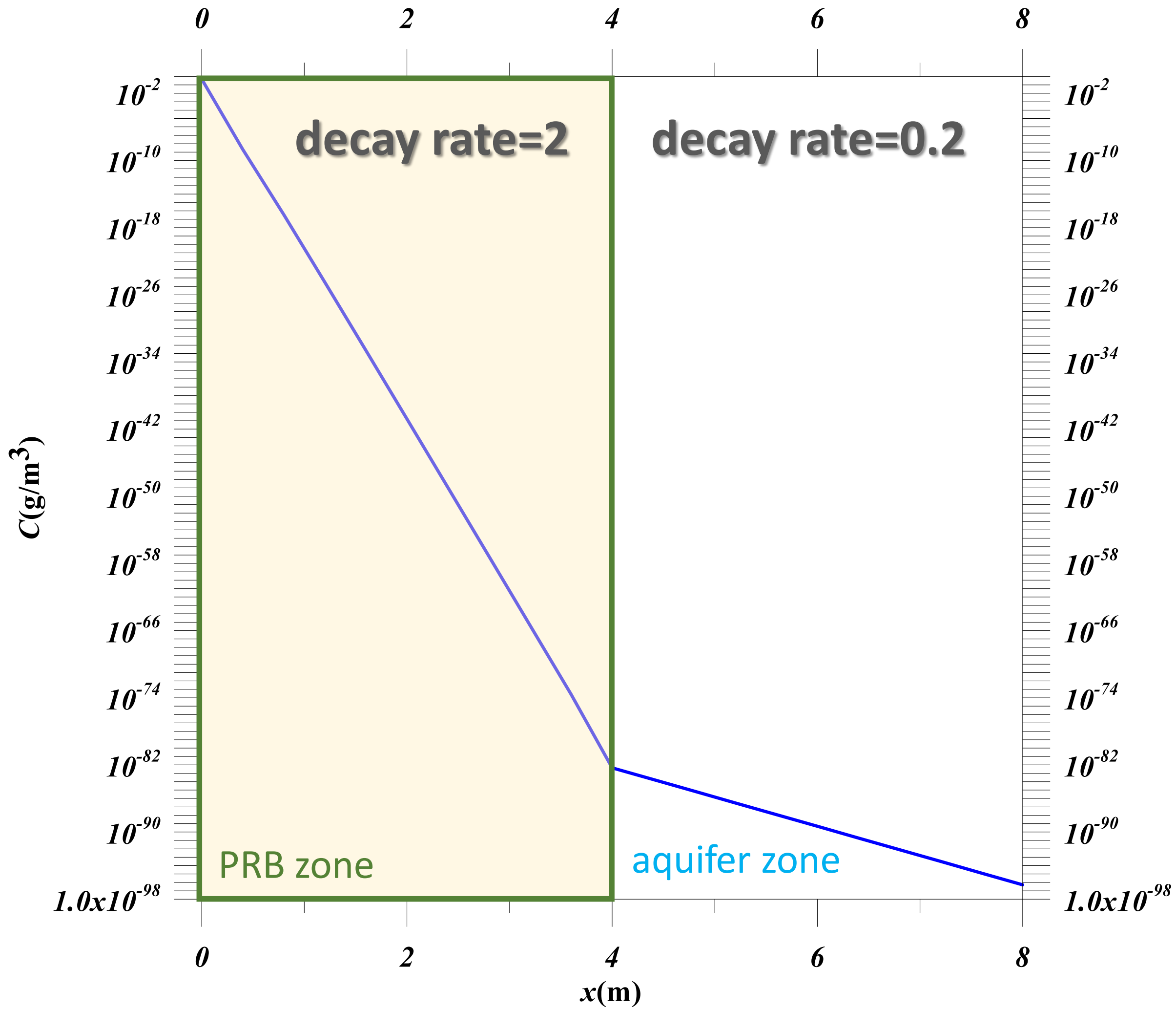
2-layer PRB system

PART 03

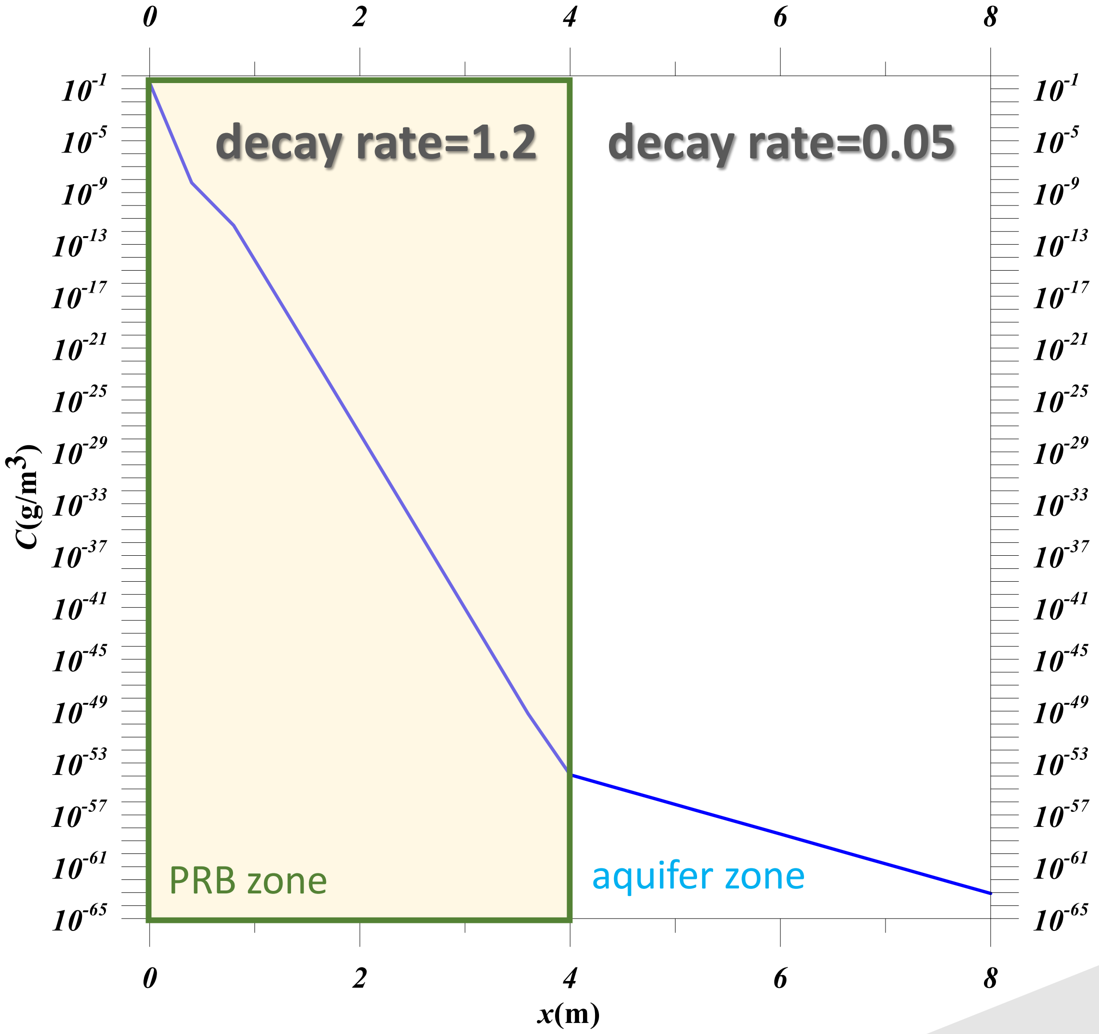


PRB thickness= 4 m

- Species 1

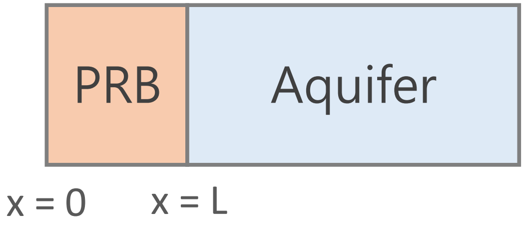


- Species 2



Parameters considered

PART 03

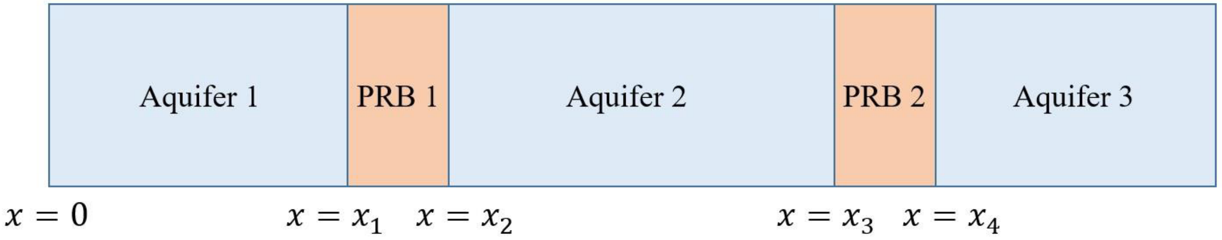


Parameters	Values
Domain length, L [m]	4
velocity in PRB, v_p [m day^{-1}]	0.2
velocity in aquifer, v_a [m day^{-1}]	0.33
Dispersion coefficient in PRB, D_p [m^2 day^{-1}]	0.01
Dispersion coefficient in PRB, D_a [m^2 day^{-1}]	0.67
Bulk density, ρ_b [kg L^{-1}]	1.3
Sorption reaction rate constant, β_i [year^{-1}]	
Species 1	50
Species 2	50
Source concentration, $C_{i,0}$ [g m^{-3}]	
Species 1	0.05
Species 2	0.03
Yield coefficient, $y_{i-1\rightarrow i}$ [-]	
$y_{species1\rightarrow species2}$	0.8

PART 04. Future works

Future works

PART 04



1. Solving equations of multi-PRB system (5 layers) analytically
2. Model verification (numerical model)
3. Sensitivity analysis
4. PRB design scenarios

Thanks for your attention!

- Hongbin Zhan 2012
- https://pdf.sciencedirectassets.com/271864/1-s2.0-S0169772212X00068/1-s2.0-S0169772212000538/main.pdf?X-Amz-Security-Token=IQoJb3JpZ2luX2VjEBYaCXVzLWVhc3QtMSJIMEYCIQCFOkNLdgIxhPHPQZfXJKhS8ynLqdjl0ljbtBOPoymm1gIhAP9cAFE7IyAjZRuGy4rTGyEh0tvsWS8IsGvr5tSiec2kKrwFCP%2F%2F%2F%2F%2F%2F%2F%2F%2F%2F%2FwEQBRoMMDU5MDAzNTQ2ODY1IgxSHlZ30DUkCzv6yf0qkAUM9acN1Oj5WkCrve%2BS8SMZVQC4E6%2BFEh22JPL%2BREfLYysoKAXriw%2FzY2jQBP6HnRx4bMJnGV7dsbrA6bbFMEtjCwfEAOGw4fHR75VgWkgW46E3yaFTXLc1brwxsbItmA3e%2FRIe1Amjej9ZHzp7Qp4zhm8vQgrKk6YXfsSWJuz882HPXKS3W3HQwJRnFmf9jyqxSSEaS1IWAPQFsyP%2FDfwsMq5yHkztXpjEdgx1l%2Bs7jIYMMWWtbt%2FP%2BvW2lSP1M9B6FMM5cEWAUG4BYq2Ach5FNCzzFOdS%2BxJnDglekPWwiu43hWLxbwxE3yYNQ1Oloz6i%2B4q341832ULY40SdQMUizl3KnjYtiffKDf%2FXX1VD8RYGqyURBOsjsYWy2jcsgWTSgCprC3M%2BEJNygtVtqQ1EmTzjzaXGvpCYnRczgBbJlYkc6au4YpLPMmg9SFybtIExSWDvEUYuRKSaaLIHO%2F5OCVtwzr6HTJF10MwBqDe1q3IIpF3%2BOz17BEA55RG2rQNf3clN14tO5jTokzSf8Fq3nZ80yWOGI6TJv4vNztueth%2FZl4h2S9zqZZoLaKgizOvWrekGV%2BpueNMrH911zD26HRORfZGAtpfQCjzxwtOvMR5iMUQ7R0pNLmkm3Mu7gpNLpydpM4NzMCuhfieVAJa%2BwiHdK%2F9W%2Bn7S6fs78DuRA1tpY6boWD891Pb7SQI%2Biah2HchAdXr5xPVOPmZ8dMK%2Bk6gnz1xW0Kw%2BZ0Sg%2FLQDRuS9ox4ILvQYxo73i2Hac8ioAXg%2F12qoeGf8CUmCTvLx6TmmcN2ESA7VzLn8Vt0jcLjAoN91W3frWYXChpfJ%2BF1CGWY3jEIrzx12HRUR3z2uKdXbzhU2T0HNrTvRWeetKzCh3LSoBjqwAfqRmKOiEu8gMD1aKu3jR5OZtBWkvfub64Jp6lT3slcU7IHIhU0KFG4VOpawCTJRX8NiPPCLljQLYKxy0slV1ioWBnLFIEA8S%2B%2BxAF4swDmtp%2B6QFGrBnHNdNcWGNeT7OGnX9FHAHmCMwzT%2F3JJY8wIjyRCD1NbOhNm8OBxDdEHRJNNnlA5p%2BTQG4achQ3SdV8i0OXRwtKFypZbp5bVSrGEbwrTWS72badehAswOJAFn&X-Amz-Algorithm=AWS4-HMAC-SHA256&X-Amz-Date=20230922T065742Z&X-Amz-SignedHeaders=host&X-Amz-Expires=299&X-Amz-Credential=ASIAQ3PHCVTY745XELDJ%2F20230922%2Fus-east-1%2Fs3%2Faws4_request&X-Amz-Signature=aa6523494221aab67efdcccd06202c1e236c7c8cd0cbbd1c1c3c1318b0138155&hash=40447d2a1b3480be96ea07a5439aeca9c0724ee5064718a6b4fd9a92828291e7&host=68042c943591013ac2b2430a89b270f6af2c76d8dfd086a07176afe7c76c2c61&pii=S0169772212000538&tid=spdf-64a674b1-6d49-4350-a0ac-340782fda802&sid=ce4a27293894b440009bf8d25617aec10bebgxrqa&type=client&tsoh=d3d3LnNjaWVuY2VkaXJlY3QuY29t&ua=0e11585305560659065753&rr=80a8a7c01bd66b69&cc=tw

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γ_*^i : first-order degradation rate constant of specie i in the dissolved phase
y^i : stoichiometric yield factor from species i-1 to species i
$a1$, $p1$, $a2$, $p2$ and $a3$: aquifer 1, PRB1, aquifer 2, PRB2 and aquifer 3

λ_*^i : first-order degradation rate constant of specie i in the dissolved phase
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