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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Date: 113/05/03

Outline

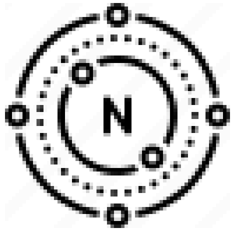
PART 01. Introduction

Why PRB is developed?

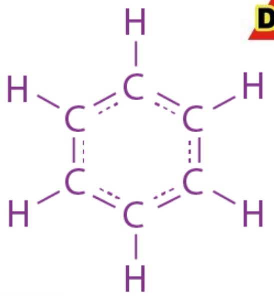
PART 01

- 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



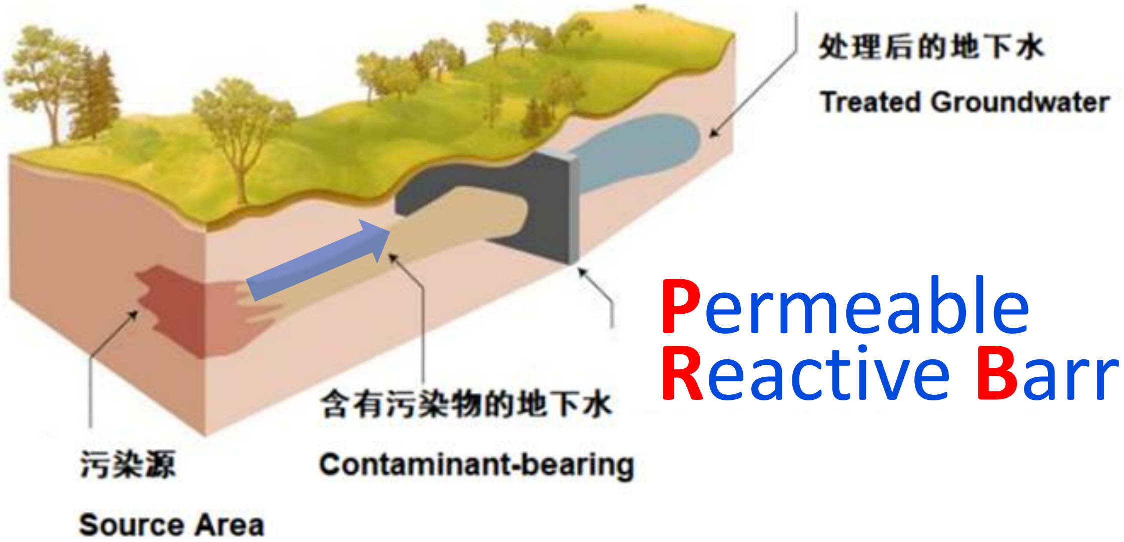
nitrogen



hydrocarbons

radionuclides

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

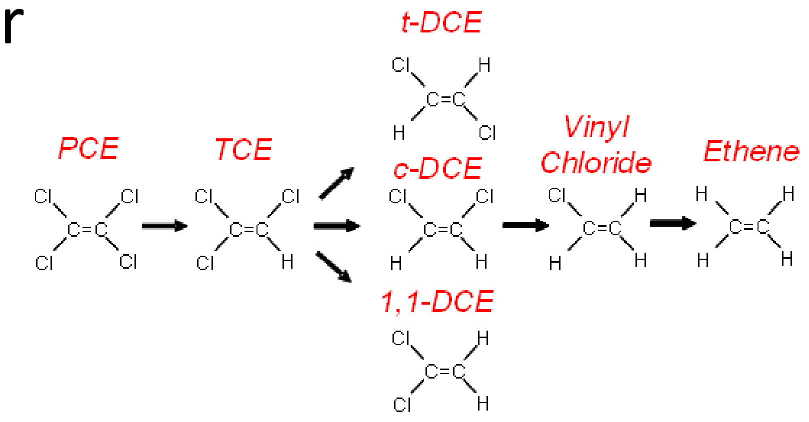
Multi-PRB remediation system

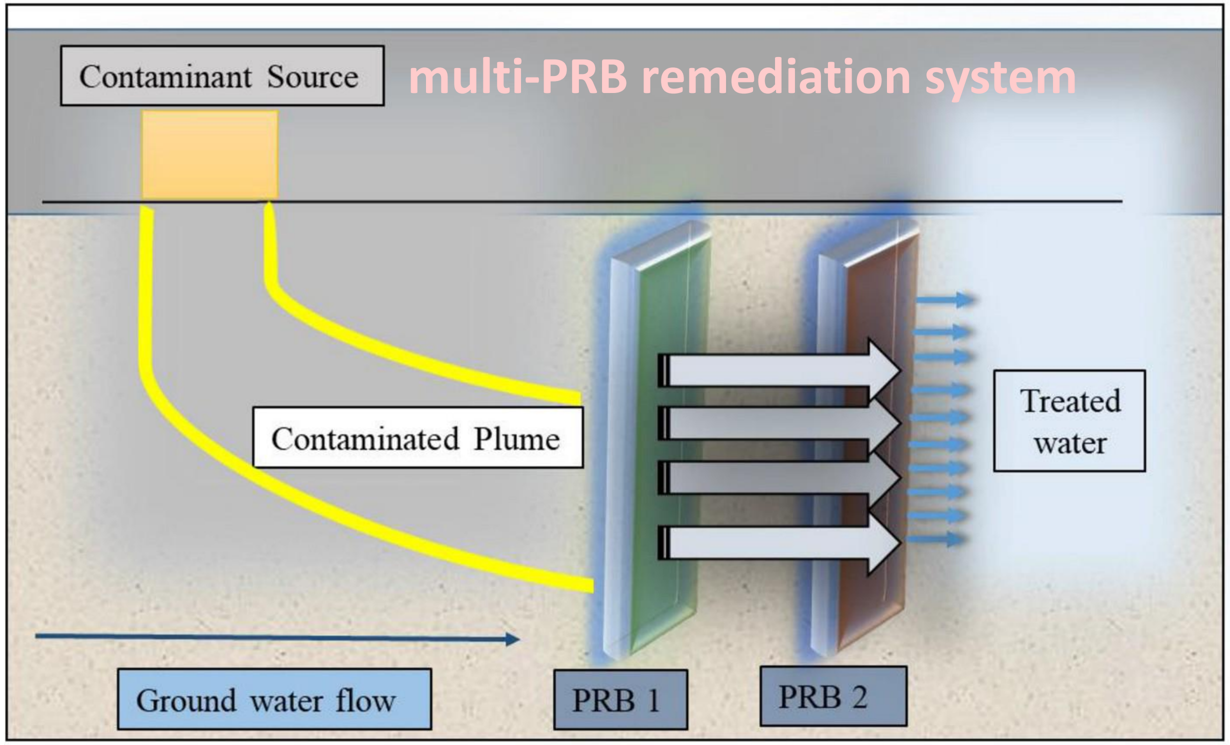
PART 01

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

→ Coexistence of multiple contaminant species

→ Existence of daughter species in downstream





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

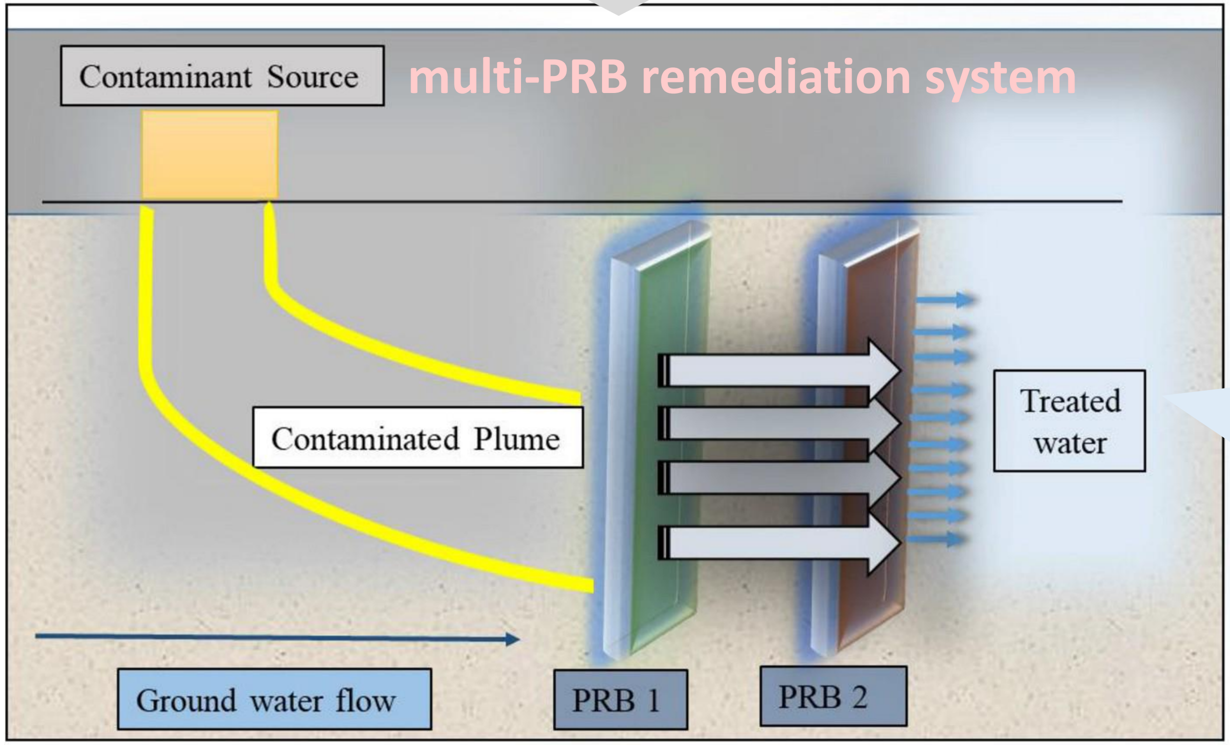
- Lee et al. (2010): 2 reactive barriers
- Xu et al. (2012): MODFLOW/MT3DMS
- Singh et al. (2020): MODFLOW

Rahul Singh et al. (2020)

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 :

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

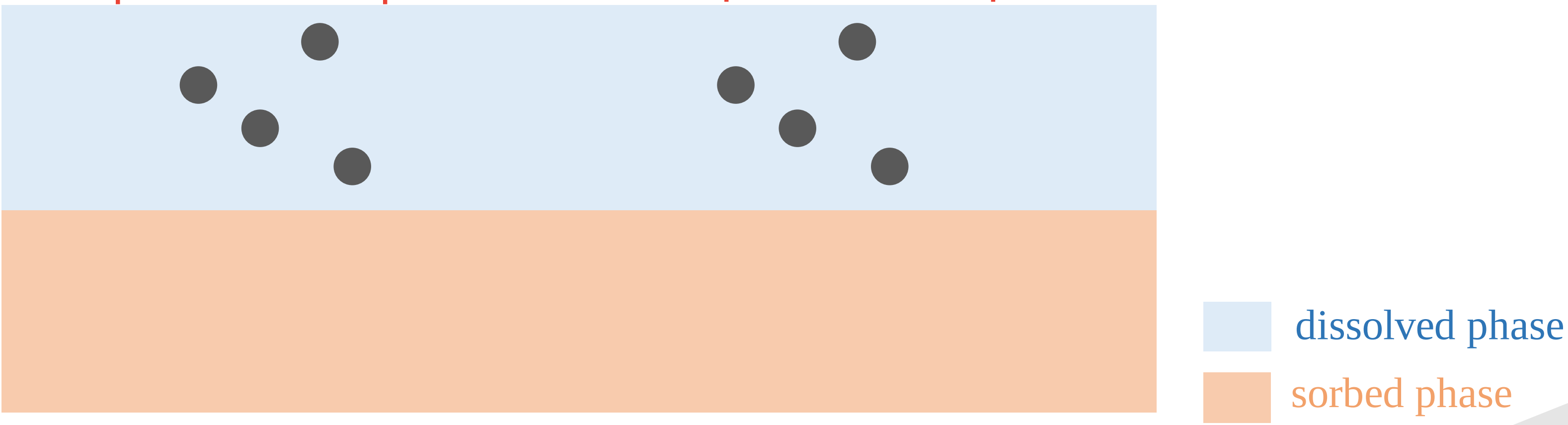
$$D\frac{\partial^2 C_i(x,t)}{\partial x^2} - V\frac{\partial C_i(x,t)}{\partial x} - \mu_i R_i C_i(x,t) + \mu_{i-1} R_{i-1} C_{i-1}(x,t)$$
$$= R_i\frac{\partial C_i(x,t)}{\partial t}. \quad i = 2\ldots N.$$

Chen et al. (2020)

D : dispersion
V : advection
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

equilibrium sorption | nonequilibrium sorption



sorption rate $\rightarrow \infty$ | sorption rate : 0.5

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

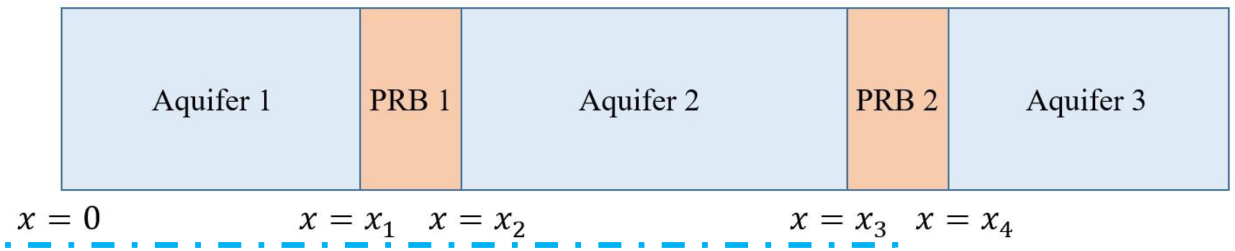
PART 01

- 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

dissolved phase

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

$$\lambda_{a1}^0 = 0 \quad i=1,\dots,N \quad 0 \le x \le x_1,\ t \ge 0$$

sorbed phase

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

$$\gamma_{a1}^0 = 0 \quad i=1,\dots,N \quad 0 \le x \le x_1,\ t \ge 0$$

PRB 1

$$D_{p1}\frac{\partial^2 C_i(x,t)}{\partial x^2} - v_{p1}\frac{\partial C_i(x,t)}{\partial x} - \lambda_{p1}^i C_i(x,t) + y_i\lambda_{p1}^{i-1}C_{i-1}(x,t) + \frac{\beta_{p1}^i}{\theta_{p1}}\left(C_i(x,t)-\frac{S_i(x,t)}{K_{p1}^i}\right) = \frac{\partial C_i(x,t)}{\partial t}$$

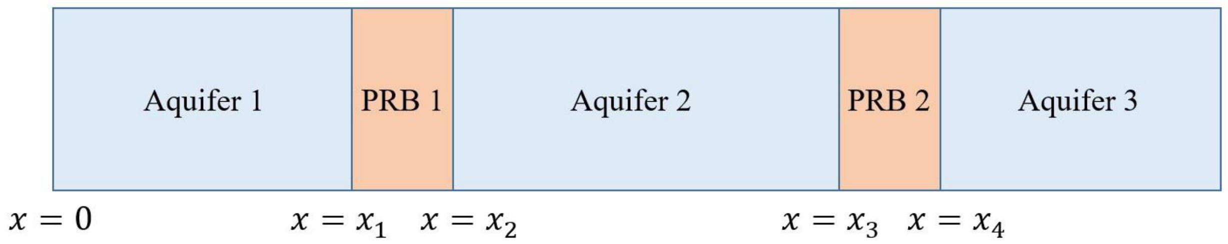
$$\lambda_{p1}^0 = 0 \quad i=1,\dots,N \quad x_1 \le x \le x_2,\ t \ge 0$$

$$\rho_{p1}\frac{\partial S_i(x,t)}{\partial t} = \beta_{p1}^i\left(C_i(x,t)-\frac{S_i(x,t)}{K_{p1}^i}\right) - \gamma_{p1}^i\rho_{p1}S_i(x,t) + y_i\gamma_{p1}^{i-1}\rho_{p1}S_{i-1}(x,t)$$

$$\gamma_{p1}^0 = 0 \quad i=1,\dots,N \quad x_1 \le x \le x_2,\ t \ge 0$$

Governing equations

PART 02



Aquifer 2

$$D_{a2}\frac{\partial^2 C_i(x,t)}{\partial x^2} - v_{a2}\frac{\partial C_i(x,t)}{\partial x} - \lambda_{a2}^i C_i(x,t) + y_i\lambda_{a2}^{i-1}C_{i-1}(x,t) + \frac{\beta_{a2}^i}{\theta_{a2}}\left(C_i(x,t)-\frac{S_i(x,t)}{K_{a2}^i}\right) = \frac{\partial C_i(x,t)}{\partial t}$$

$$\lambda_{a2}^0 = 0 \qquad i=1,\ldots,N \quad x_2 \le x \le x_3, \quad t \ge 0$$

$$\rho_{a2}\frac{\partial S_i(x,t)}{\partial t} = \beta_{a2}^i\left(C_i(x,t)-\frac{S_i(x,t)}{K_{a2}^i}\right) - \gamma_{a2}^i\rho_{a2}S_i(x,t) + y_i\gamma_{a2}^{i-1}\rho_{a2}S_{i-1}(x,t)$$

$$\gamma_{a2}^0 = 0 \qquad i=1,\ldots,N \quad x_2 \le x \le x_3, \quad t \ge 0$$

PRB 2

$$D_{p2}\frac{\partial^2 C_i(x,t)}{\partial x^2} - v_{p2}\frac{\partial C_i(x,t)}{\partial x} - \lambda_{p2}^i C_i(x,t) + y_i\lambda_{p2}^{i-1}C_{i-1}(x,t) + \frac{\beta_{p2}^i}{\theta_{p2}}\left(C_i(x,t)-\frac{S_i(x,t)}{K_{p2}^i}\right) = \frac{\partial C_i(x,t)}{\partial t}$$

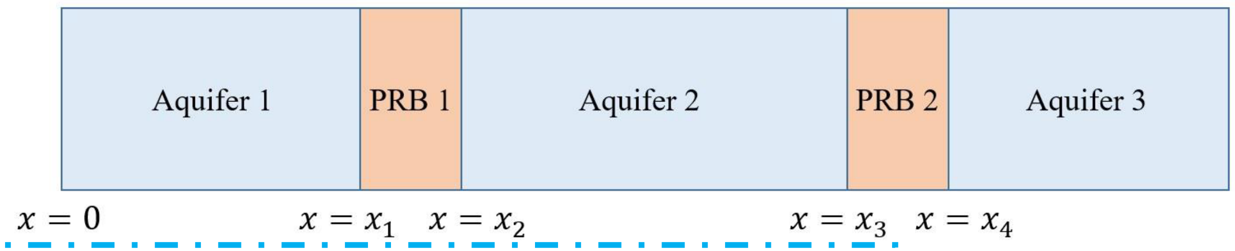
$$\lambda_{p2}^0 = 0 \qquad i=1,\ldots,N \quad x_3 \le x \le x_4, \quad t \ge 0$$

$$\rho_{p2}\frac{\partial S_i(x,t)}{\partial t} = \beta_{p2}^i\left(C_i(x,t)-\frac{S_i(x,t)}{K_{p2}^i}\right) - \gamma_{p2}^i\rho_{p2}S_i(x,t) + y_i\gamma_{p2}^{i-1}\rho_{p2}S_{i-1}(x,t)$$

$$\gamma_{p2}^0 = 0 \qquad i=1,\ldots,N \quad x_3 \le x \le x_4, \quad t \ge 0$$

Governing equations

PART 02



Aquifer 3

$$D_{a3}\frac{\partial^2 C_i(x,t)}{\partial x^2} - v_{a3}\frac{\partial C_i(x,t)}{\partial x} - \lambda_{a3}^i C_i(x,t) + y_i\lambda_{a3}^{i-1}C_{i-1}(x,t) + \frac{\beta_{a3}^i}{\theta_{a3}}\left(C_i(x,t) - \frac{S_i(x,t)}{K_{a3}^i}\right) = \frac{\partial C_i(x,t)}{\partial t} \quad \lambda_{a3}^0 = 0 \quad i = 1,\ldots,N \quad x_4 \le x \le L,\ t \ge 0$$

dissolved phase

$$\rho_{a3}\frac{\partial S_i(x,t)}{\partial t} = \beta_{a3}^i\left(C_i(x,t) - \frac{S_i(x,t)}{K_{a3}^i}\right) - \gamma_{a3}^i\rho_{a3}S_i(x,t) + y_i\gamma_{a3}^{i-1}\rho_{a3}S_{i-1}(x,t) \quad \gamma_{a3}^0 = 0 \quad i = 1,\ldots,N \quad x_4 \le x \le L,\ t \ge 0$$

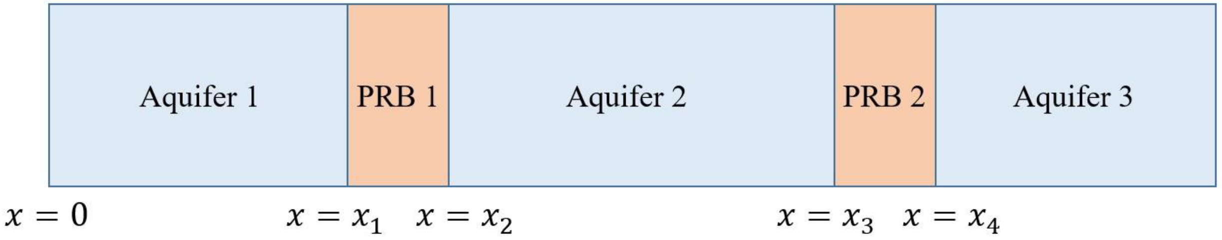
sorbed phase

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 sorbed 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

Initial conditions

PART 02



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

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

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

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

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

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

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

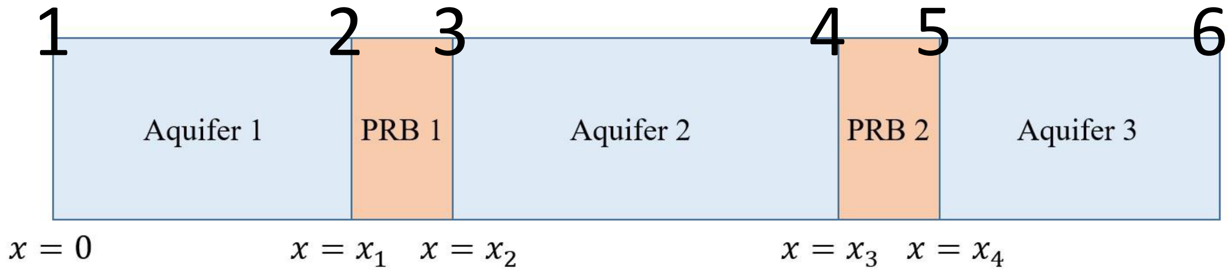
$$S_i(x, t=0) = 0 \qquad x_2 \le x \le x_3 \quad i = 1, \dots, N$$

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

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

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

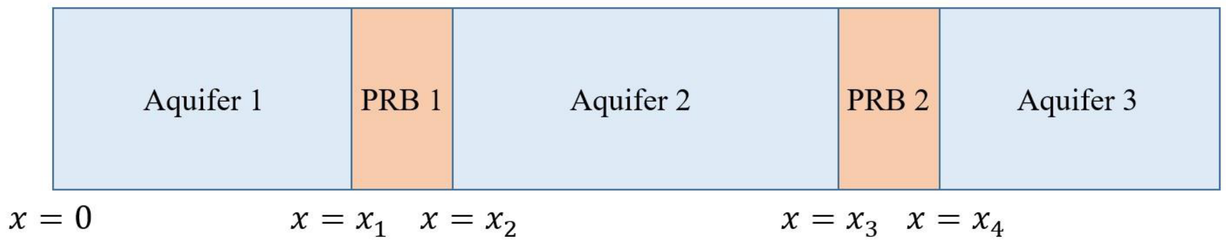
KEY

Satisfy the continuities of species concentrations and mass flux at interfaces

PART 03. Preliminary results

Solution of Species 1

PART 03



❖ Aquifer1

$$C_{1,L}(x,s)=A_1 e^{\alpha_1 x}+B_1 e^{\beta_1 x} \qquad 0\le x\le x_1$$

$$\alpha_1=\frac{v_{a1}+\sqrt{(v_{a1})^2+4D_{a1}\theta_1^{a1}(s)}}{2D_{a1}}$$

$$\beta_1=\frac{v_{a1}-\sqrt{(v_{a1})^2+4D_{a1}\theta_1^{a1}(s)}}{2D_{a1}}$$

❖ PRB1

$$C_{1,L}(x,s)=X_1 e^{\chi_1 x}+\Delta_1 e^{\delta_1 x} \qquad x_1\le x\le x_2$$

$$\chi_1=\frac{v_{p1}+\sqrt{(v_{p1})^2+4D_{p1}\theta_1^{p1}(s)}}{2D_{p1}}$$

$$\delta_1=\frac{v_{p1}-\sqrt{(v_{p1})^2+4D_{p1}\theta_1^{p1}(s)}}{2D_{p1}}$$

❖ Aquifer2

$$C_{1,L}(x,s)=E_1 e^{\varepsilon_1 x}+\Phi_1 e^{\phi_1 x} \qquad x_2\le x\le x_3$$

$$\varepsilon_1=\frac{v_{a2}+\sqrt{(v_{a2})^2+4D_{a2}\theta_1^{a2}(s)}}{2D_{a2}}$$

$$\phi_1=\frac{v_{a2}-\sqrt{(v_{a2})^2+4D_{a2}\theta_1^{a2}(s)}}{2D_{a2}}$$

❖ PRB2

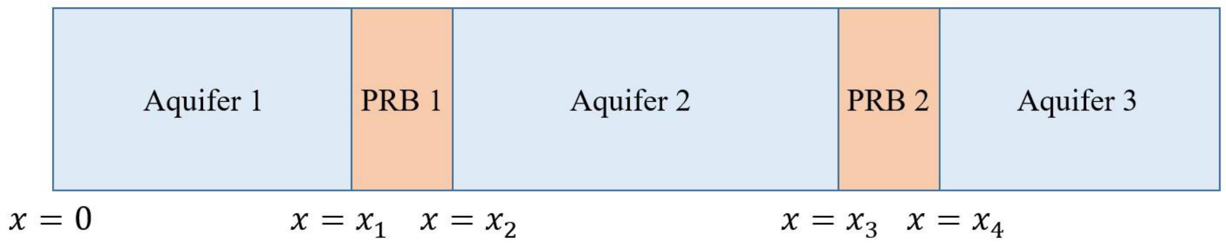
$$C_{1,L}(x,s)=\Gamma_1 e^{\varphi_1 x}+H_1 e^{\gamma_1 x} \qquad x_3\le x\le x_4$$

$$\varphi_1=\frac{v_{p2}+\sqrt{(v_{p2})^2+4D_{p2}\theta_1^{p2}(s)}}{2D_{p1}}$$

$$\gamma_1=\frac{v_{p2}-\sqrt{(v_{p2})^2+4D_{p2}\theta_1^{p2}(s)}}{2D_{p2}}$$

Solution of Species 1

PART 03



❖ Aquifer3

$$C_{1,L}(x,s) = \mathrm{I}_1 e^{\eta_1 x} + \mathrm{K}_1 e^{\iota_1 x} \qquad x_4 \le x \le \infty$$

$$\eta_1 = \frac{v_{a3} + \sqrt{(v_{a3})^2 + 4D_{a3}\theta_1^{a3}(s)}}{2D_{a3}}$$

$$\iota_1 = \frac{v_{a3} - \sqrt{(v_{a3})^2 + 4D_{a3}\theta_1^{a3}(s)}}{2D_{a3}}$$

where

$$\mathrm{K}_1 = \frac{-\dfrac{e^{\varphi_1 x} i1}{e^{\gamma_1 x} g1 - e^{\varphi_1 x} h1} + \dfrac{pi1}{g1q - ph1}}{\dfrac{g1r}{g1q - ph1} - \dfrac{e^{\iota_1 x} g1}{e^{\gamma_1 x} g1 - e^{\varphi_1 x} h1}}$$

$$\mathrm{H}_1 = \frac{g1r}{g1q - ph1}\mathrm{K}_1 - \frac{pi1}{g1q - ph1}$$

$$\Gamma_1 = \frac{i1 - h1\mathrm{H}_1}{g1}$$

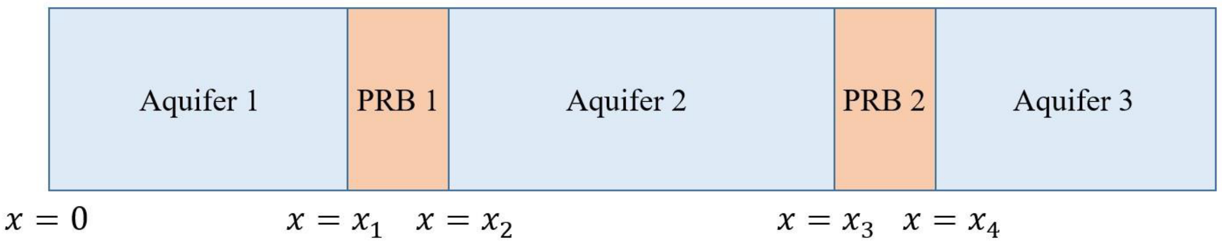
$$\Phi_1 = \frac{d1n}{d1m - le1}\Gamma_1 + \frac{d1o}{d1m - le1}\mathrm{H}_1 - \frac{lf1}{d1m - le1}$$

$$\mathrm{E}_1 = \frac{f1 - e1\Phi_1}{d1}$$

$$\Delta_1 = \frac{a1j}{a1i - hb1}\mathrm{E}_1 + \frac{a1k}{a1i - hb1}\Phi_1 - \frac{hc1}{a1i - hb1}$$

Solution of Species 1

PART 03



$$X_1 = \frac{c1 - b1\Delta_1}{a1}$$

$$B_1 = \frac{af}{ae-bd} X_1 + \frac{ag}{ae-bd}\Delta_1 - \frac{cd}{ae-bd}$$

$$A_1 = \frac{c\text{-}bB_1}{a}$$

where

$$a = v_{a1}e^{\alpha_1 x} - D_{a1}\alpha_1 e^{\alpha_1 x}$$

$$b = v_{a1}e^{\beta_1 x} - D_{a1}\beta_1 e^{\beta_1 x}$$

$$c = \frac{v_{a1}c_{1,0}}{s}$$

$$d = \theta_{a1}D_{a1}\alpha_1 e^{\alpha_1 x}$$

$$e = \theta_{a1}D_{a1}\beta_1 e^{\beta_1 x}$$

$$f = \theta_{p1}D_{p1}\chi_1 e^{\chi_1 x}$$

$$g = \theta_{p1}D_{p1}\delta_1 e^{\delta_1 x}$$

$$h = \theta_{p1}D_{p1}\chi_1 e^{\chi_1 x}$$

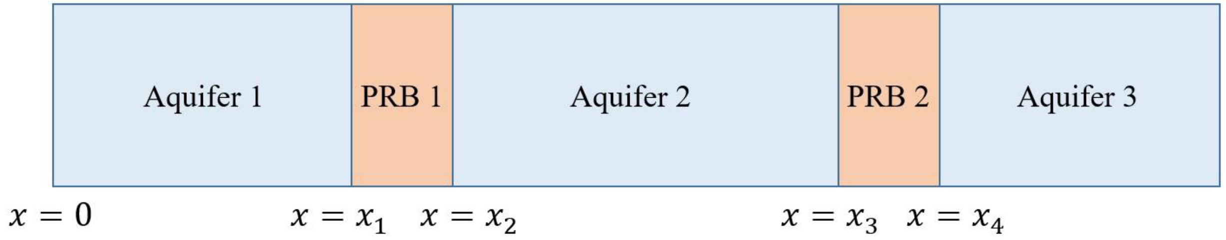
$$i = \theta_{p1}D_{p1}\delta_1 e^{\delta_1 x}$$

$$j = \theta_{a2}D_{a2}\varepsilon_1 e^{\varepsilon_1 x}$$

$$k = \theta_{a2}D_{a2}\phi e^{\phi_1 x}$$

Solution of Species 1

PART 03



$$l = \theta_{a2} D_{a2} \varepsilon_1 e^{\varepsilon_1 x}$$

$$m = \theta_{a2} D_{a2} \phi e^{\phi_1 x}$$

$$n = \theta_{p2} D_{p2} \varphi_1 e^{\varphi_1 x}$$

$$o = \theta_{p2} D_{p2} \gamma e^{\gamma_1 x}$$

$$p = \theta_{p2} D_{p2} \varphi_1 e^{\varphi_1 x}$$

$$q = \theta_{p2} D_{p2} \gamma_1 e^{\gamma_1 x}$$

$$r = \theta_{a3} D_{a3} \iota_1 e^{\iota_1 x}$$

$$a1 = \frac{ae^{\chi_1 x}}{ae^{\beta_1 x} - be^{\alpha_1 x}} - \frac{af}{ae - bd}$$

$$b1 = \frac{ae^{\delta_1 x}}{ae^{\beta_1 x} - be^{\alpha_1 x}} - \frac{ag}{ae - bd}$$

$$c1 = \frac{ce^{\alpha_1 x}}{ae^{\beta_1 x} - be^{\alpha_1 x}} - \frac{cd}{ae - bd}$$

$$d1 = \frac{a1j}{a1i - hb1} - \frac{a1e^{\varepsilon_1 x}}{a1e^{\delta_1 x} - e^{\chi_1 x} b1}$$

$$e1 = \frac{a1k}{a1i - hb1} - \frac{a1e^{\phi_1 x}}{a1e^{\delta_1 x} - e^{\chi_1 x} b1}$$

$$f1 = \frac{hc1}{a1i - hb1} - \frac{e^{\chi_1 x} c1}{a1e^{\delta_1 x} - e^{\chi_1 x} b1}$$

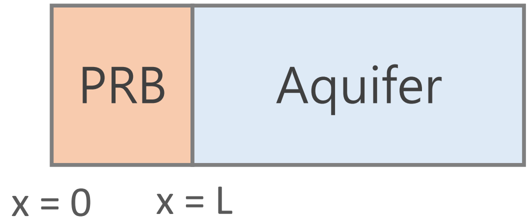
$$g1 = \frac{d1n}{d1m - le1} - \frac{d1e^{\varphi_1 x}}{d1e^{\phi_1 x} - e^{\varepsilon_1 x} e1}$$

$$h1 = \frac{d1o}{d1m - le1} - \frac{d1e^{\gamma_1 x}}{d1e^{\phi_1 x} - e^{\varepsilon_1 x} e1}$$

$$i1 = \frac{lf1}{d1m - le1} - \frac{e^{\varepsilon_1 x} f1}{d1e^{\phi_1 x} - e^{\varepsilon_1 x} e1}$$

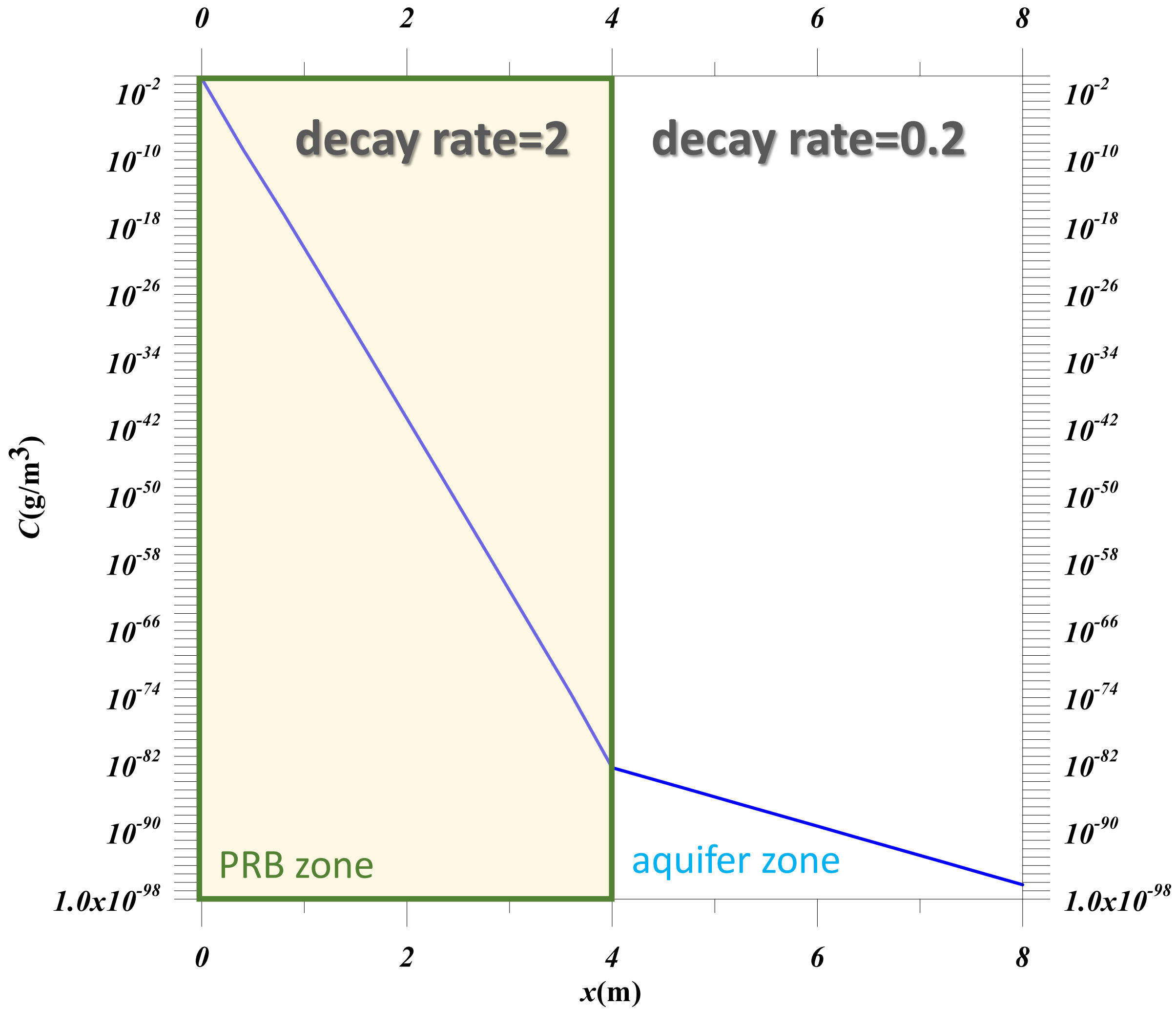
2-layer PRB system

PART 03

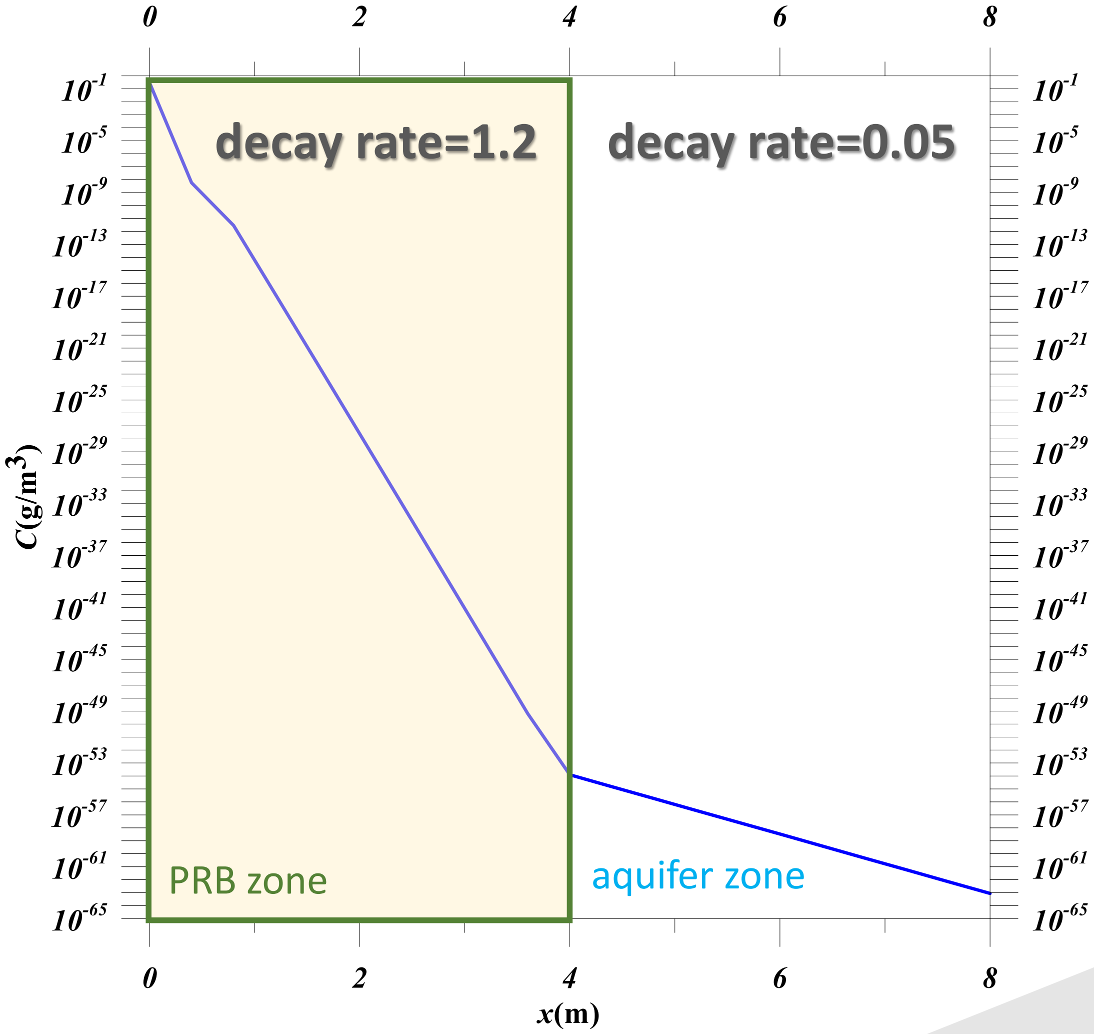


PRB thickness= 4 m

❖ Species 1

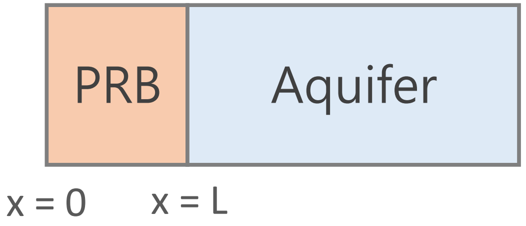


❖ Species 2



Parameters considered

PART 03

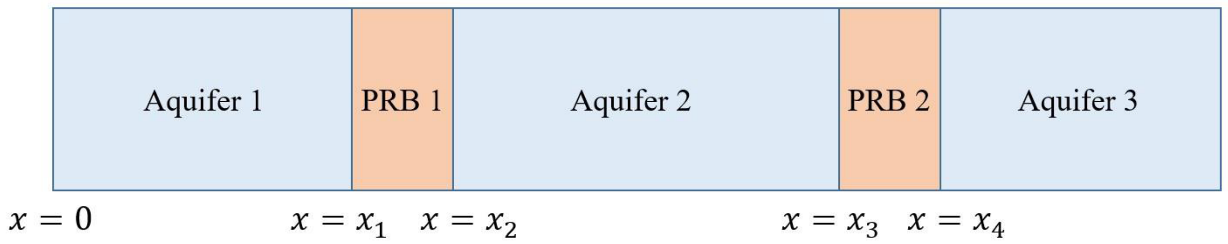


Parameters	Values
Domain length, L [m]	4
velocity in PRB, v_p [m day^{-1}]	0.2
velocity in aquifer, v_a [m day^{-1}]	0.33
Dispersion coefficient in PRB, D_p [m^2 day^{-1}]	0.01
Dispersion coefficient in PRB, D_a [m^2 day^{-1}]	0.67
Bulk density, ρ_b [kg L^{-1}]	1.3
Sorption reaction rate constant, β_i [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. Multi-PRB system design scenarios

Thanks for your attention!

Reactive Materials	Geochemical Process
Activated carbon	Adsorption
Amorphous Ferric Oxyhydroxide	Adsorption
Basic Oxygen Furnace Slag (BOFS)	Sorption
Ion exchange resins	Adsorption
Zero-Valent Iron	Reduction and precipitation
Limestone	Precipitation
Apatite	Precipitation
Sodium Dithionite	Reduction & precipitation
Sulfate Reducing Bacteria	Microbial degradation
Zeolites	Adsorption
Sand/Gravel beds + nutrients + oxygen	Promotes microbial degradation

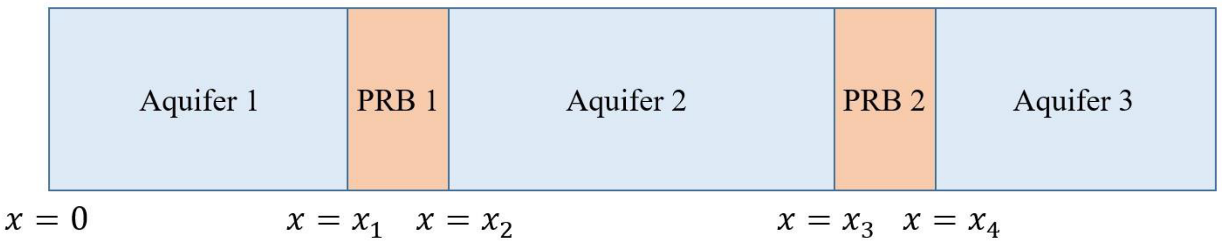
Table 1: Reactive materials used in Permeable Reactive Barriers. (Bronstein, 2005)

$$3Fe^0 \rightarrow 2Fe^{2+} + 4e^-$$
$$3H_2O \rightarrow 3H^+ + 3OH^-$$
$$2H^+ + 2e^- \rightarrow H_2$$
$$\underline{R\text{–}Cl + H^+ + 2e^- \rightarrow R\text{–}H + Cl^-}$$
$$3Fe^0 + 3H_2O + R\text{–}Cl \rightarrow 2Fe^{2+} + 3OH^- + H_2 + R\text{–}H + Cl^-$$

Figure 3b: Abiotic reduction of a chlorinated organic compound (Vogan, 1999)

Solution of Species 1

PART 03



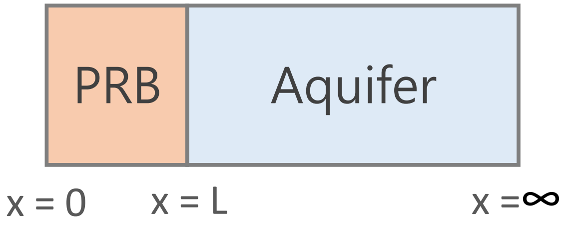
❖ The current problem..

```
!!!!!!!!!!!!!! !!!!!!!!!!!!!! !!!!!!!!!!!!!!
!          LAPLACE inverse
!!!!!!!!!!!!!! !!!!!!!!!!!!!! !!!!!!!!!!!!!!

      ALPHA=0.D0
      RELERR=1.D-7
      KMAX=100000

      call DINLAP (Fun, NT, T, ALPHA, RELERR, KMAX, FINV)
      write(*,*) "RESULT=",x,FINV
```

```
  3.829534862675795E-019  2.443336273005137E-005 -5.731702958084554E-026
 ----------------------------------------------
 !!!!!check!!!!!  2.646977960169689E-023  0.000000000000000E+000
 -2.646977960169689E-023 -5.293955920339377E-023 -2.646977960169689E-023
 -1.455837878093329E-022  0.000000000000000E+000  1.389663429089086E-022
 -1.323488980084844E-022

 *** FATAL    ERROR 1 from DINLAP.  The accuracy requested cannot be achieved
 ***          within KMAX = 10000 function evaluations for some T(I).
Press any key to continue
```

Parameters considered

PART 03



Parameters	Values
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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

```
COMMON /PART6/theta_a1,theta_p1,theta_a2,theta_p2,the

T=1.d0
!!!初始濃度
c10=10.d0

x=0.4d0

va1=0.2d0
vp1=0.33d0
va2=0.33d0
vp2=0.33d0
va3=0.33d0

Da1=0.01d0
Dp1=0.67d0
Da2=0.670
Dp2=0.67d0
Da3=0.67d0

!!!decay
Dlambda_a1=1.2d0
Dlambda_p1=0.2d0
Dlambda_a2=0.2d0
Dlambda_p2=0.2d0
Dlambda_a3=0.2d0
!!!sorption rate
beta_a1=50.d0
beta_p1=50.d0
beta_a2=50.d0
beta_p2=50.d0
beta_a3=50.d0
!!!bulk density
rho_a1=1.3d0
rho_p1=1.3d0
rho_a2=1.3d0
rho_p2=1.3d0
rho_a3=1.3d0
!!!distribution Coefficient
DIS_Ka1=1.89d0
DIS_Kp1=1.89d0
DIS_Ka2=1.89d0
DIS_Kp2=1.89d0
DIS_Ka3=1.89d0
!!!porosity
theta_a1=0.5d0
theta_p1=0.3d0
theta_a2=0.3d0
theta_p2=0.3d0
theta_a3=0.3d0

!!!!!!!!!!!!!! !!!!!!!!!!!!!! !!!!!!!!!!!!!!
!          LAPLACE inverse
!!!!!!!!!!!!!! !!!!!!!!!!!!!! !!!!!!!!!!!!!!

ALPHA=0.D0
RELERR=1.D-7
KMAX=100000

call DINLAP (Fun, NT, T, ALPHA, RELERR, KMAX, FINV)
write(*,*) "RESULT=",x,FINV
```

- 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%2FzY2jQBP6HnRx4bMJnGV7dsbrA6bbFMEtjCwfEAOGw4fHR75VgWkgW46E3yaFTXLc1brwxsbltmA3e%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

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

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 sorbed 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