Colloid-facilitated contaminant transport in discretely fractured porous media

1. Numerical formulation and sensitivity analysis

Ibaraki, M., Sudicky, E.A., 1995. Colloid-facilitated contaminant transport in discretely fractured porous media 1. Numerical formulation and sensitivity analysis. *WATER RESOURCES RESEARCH*, **31(12)**, 2945-2960.

Student : Chang-Fu Huang

Advisor : Prof. Jui-Sheng Chen

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Outline

1.Introduction

2.Mathematical model

3.Results and discussion

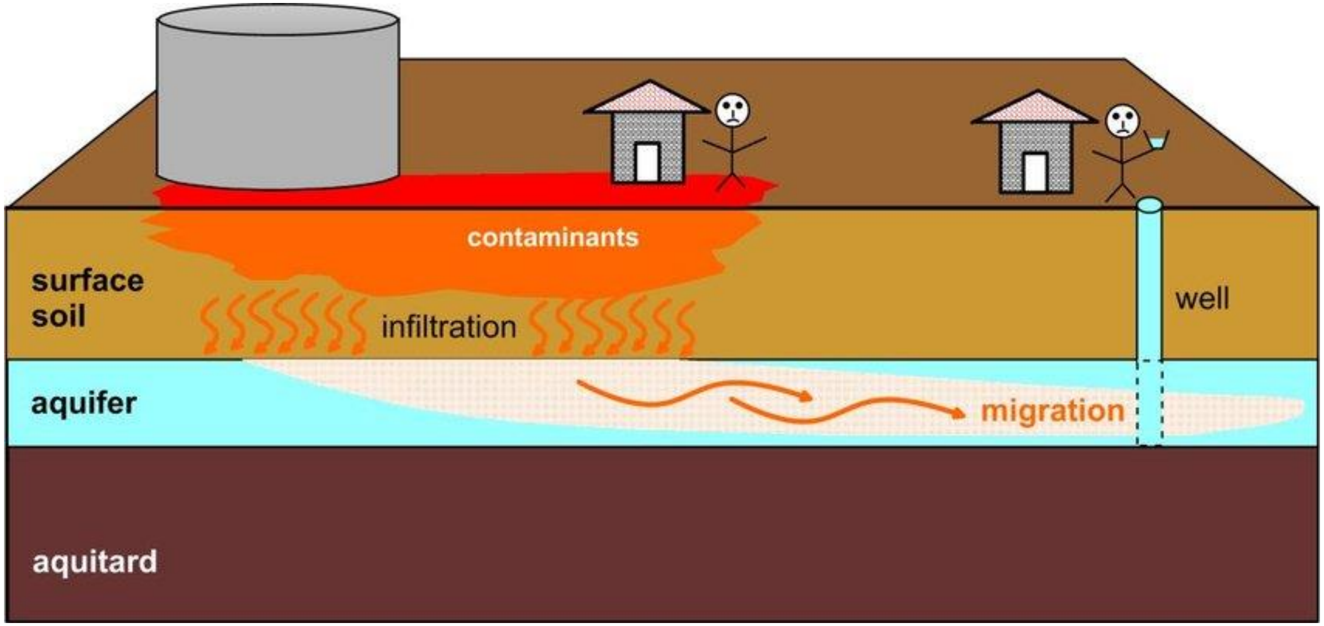
4.Conclusions

1

Introduction

Introduction / Groundwater contamination

- **In recent years, groundwater contaminants such as chlorinated solvents, pesticides and radionuclides can cause human cancer, poisoning, developmental retardation, etc.**

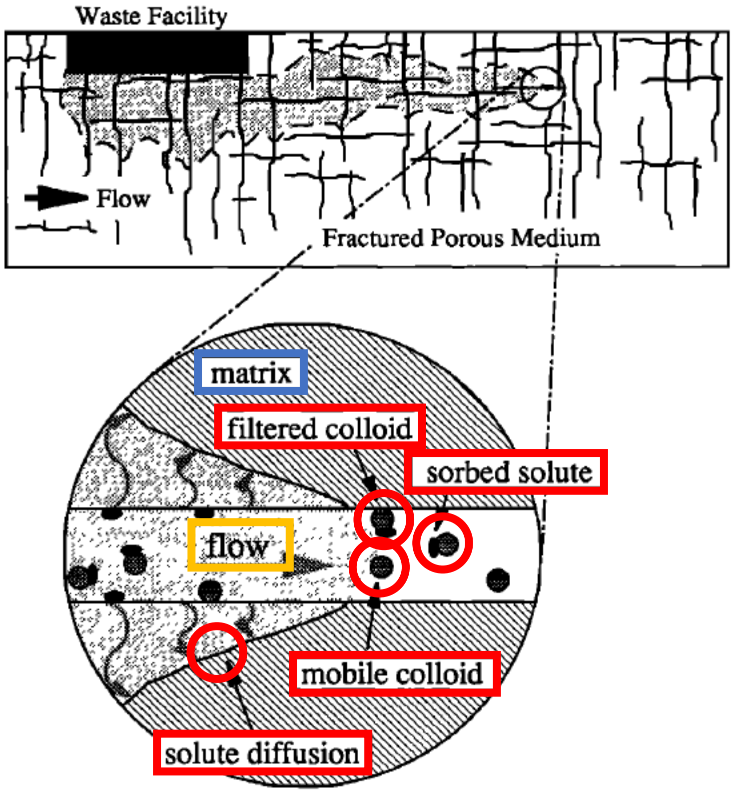


From George Kouretzis, https://www.researchgate.net/figure/Outline-of-the-soil-and-groundwater-contamination-problem_fig24_323256947

Introduction / Colloids

- **Colloids are substances with sizes ranging from 1 nm to 10 μm. (Russeel t al., 1989)**

- **Many substances can exist in colloidal form, including fine clay particles, humic substances, bacteria, radionuclides, etc.**



A three-phase system

- **Contaminants are effectively prevented from diffusing into the matrix as long as it sorbed onto the colloids, and the attenuation effect of matrix diffusion is lost. Therefore, the distance that the contaminants move will increase.**

Introduction / Sorption processes

- **Sorption processes are classified into two primary categories with respect to the process time of a reaction.**

- **Laboratory studies, have indicated that the sorption process consists of both rapid and slow reactions. (van Genuchten et al., 1974; Sparks, 1989)**

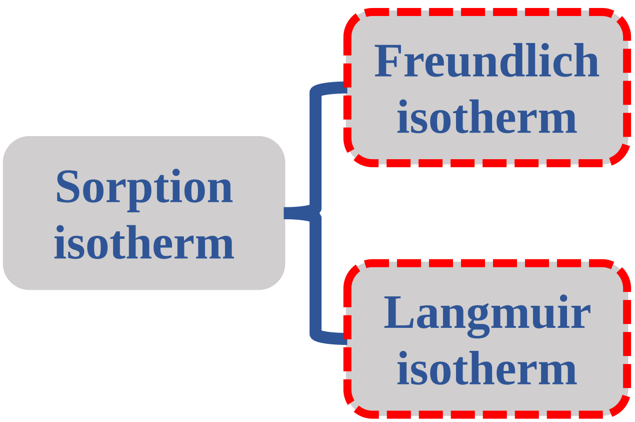
Sorption processes

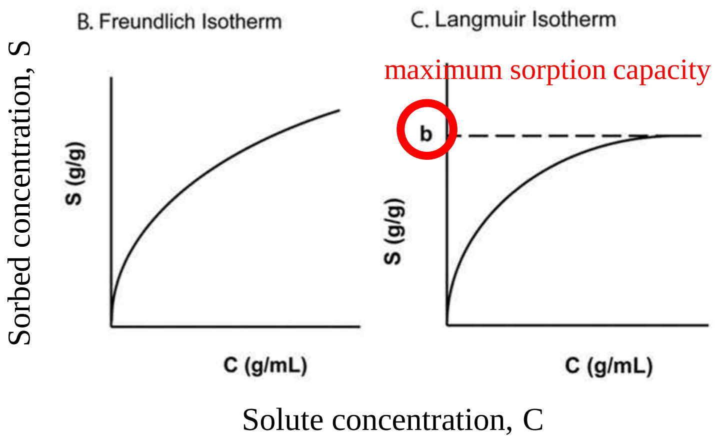
- **Instantaneous reactions (equilibrium sorption, K_m):**
  The desorption and sorption rates are equivalent
- **Time dependent reactions (kinetic sorption, β_m):**
  The desorption and sorption rates are not equivalent

Introduction / Sorption isotherm

➢ **It is a mathematical relation, expressing the mass number between sorbate and sorbent in sorption.**

➢ **Allowing contaminants for either equilibrium or kinetic sorption reactions onto the fracture walls, the matrix solids, and the mobile and filtered colloids according to either a Langmuir or a Freundlich isotherm.**





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Introduction / Literature review

- **Traditional two-phase approaches only contains an immobile solid phase and a mobile aqueous phase, which don’t take into account the role of colloids, therefore have a tendency to underestimate the migration of contaminants.**

- **Field-scale and laboratory-scale observations have shown that colloids in groundwater can act as a third phase which can sorb contaminants, similar to the immobile solid phase. (McCarthy and Zachara, 1989)**

- **At a liquid waste disposal site at Los Alamos, New Mexico, found that both plutonium and americium migrated over 30 m in depth beneath the disposal site. (Nyhan et al., 1985)**

Objective

- **The primary objective of this work is to shed light on processes affecting colloid-facilitated contaminant transport in discretely fractured porous media and to assess the relative importance of various coefficients.**

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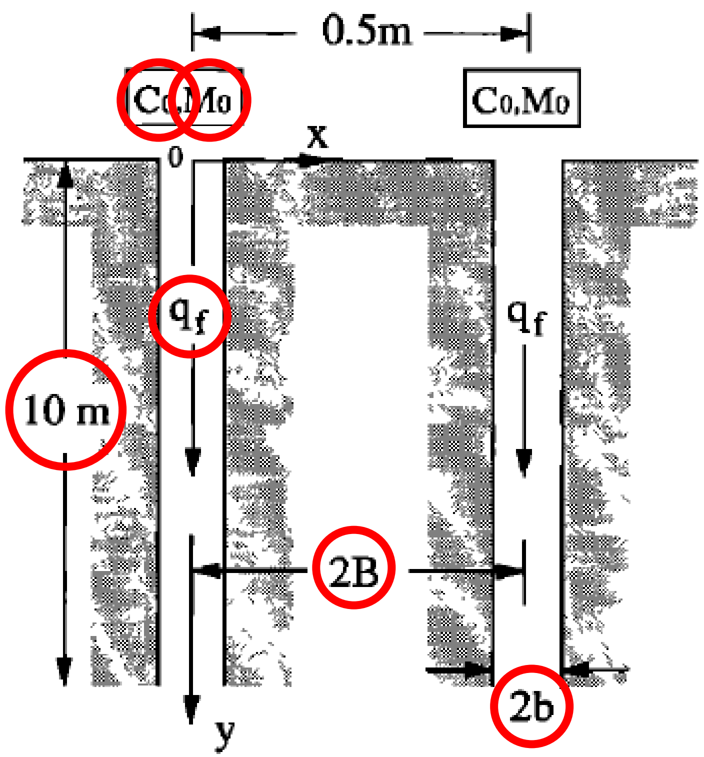
Mathematical model

Mathematical model / Physical system



2B :	**Fracture spacing (L)**
C_0 **:**	**The concentration of the solute (ML^{-3})**
M_0 **:**	**The mobile colloid concentration (ML^{-3})**
q_f **:**	**The fluid flux along the fracture (LT^{-1})**
$2b$ **:**	**Fracture aperture (L)**

- **Solute transport**

$$\theta R\frac{\partial C}{\partial t} + q_l\frac{\partial C}{\partial x_l} - \frac{\partial}{\partial x_l}\theta D_{ij}\frac{\partial C}{\partial x_j} + \theta R\lambda_d C = 0$$

Retardation Advection Dispersion First-order decay

θ	:	The matrix porosity (-)
R	:	The retardation factor (-)
C	:	The concentration of the solute (ML^{-3})
t	:	Time (T)
q_l	:	The velocity (LT^{-1})
$D_{i,j}$	:	The dispersion coefficient ($L^2\ T^{-1}$)
λ_d	:	First-order decay constant (T^{-1})

- **Colloid transport along fractures**

$$\frac{\partial}{\partial t}\left(M + \frac{\sigma}{b}\right) + q_m\frac{\partial M}{\partial l} - \frac{\partial}{\partial l}D_m\frac{\partial M}{\partial l} = 0$$

Advection Dispersion

M	:	The mobile colloid concentration (ML^{-3})
σ	:	The filtered colloid concentration (ML^{-2})
b	:	The half aperture of the fracture (L)
q_m	:	The colloid velocity in the fracture (LT^{-1})
D_m	:	The dispersion coefficient ($L^2\ T^{-1}$)
l	:	The distance along the fracture (L)

Mathematical model / Governing equations

- **For equilibrium-Freundlich reaction (Castellan, 1964)**

$$\rightarrow S_m^* = K_m C_f$$

- **For kinetic-Freundlich reaction (Lapidus and Amundson, 1952)**

$$\rightarrow \frac{\partial S_m^*}{\partial t} = \beta_m (K_m C_f - S_m^*)$$

- **For equilibrium-Langmuir reaction**

$$\rightarrow S_m^* = S_m^{max}\left[K_m C_f / (1 + K_m C_f)\right]$$

S_m^*	:	The mass of contaminant adsorbed onto the mobile colloid (MM^{-1})
K_m	:	The distribution coefficient for the mobile colloid (L^3M^{-1})
C_f	:	The concentration of the solute in the fracture (ML^{-3})
β_m	:	The kinetic rate constants for the mobile colloid (T^{-1})
S_m^{max}	:	The maximum sorption capacity on the mobile colloid (MM^{-1})

- **The change in the concentration of the filtered colloids over time in a fracture (Herzig et al., 1970; Dieulin, 1982)**

$$\rightarrow \frac{\partial \sigma}{\partial t} = \lambda q_m M b$$

σ :	**The filtered colloid concentration (ML^{-2})**
λ :	**The filter coefficient (L^{-1})**
q_m :	**The colloid velocity in the fracture (LT^{-1})**
M :	**The mobile colloid concentration (ML^{-3})**
b :	**The half aperture of the fracture (L)**

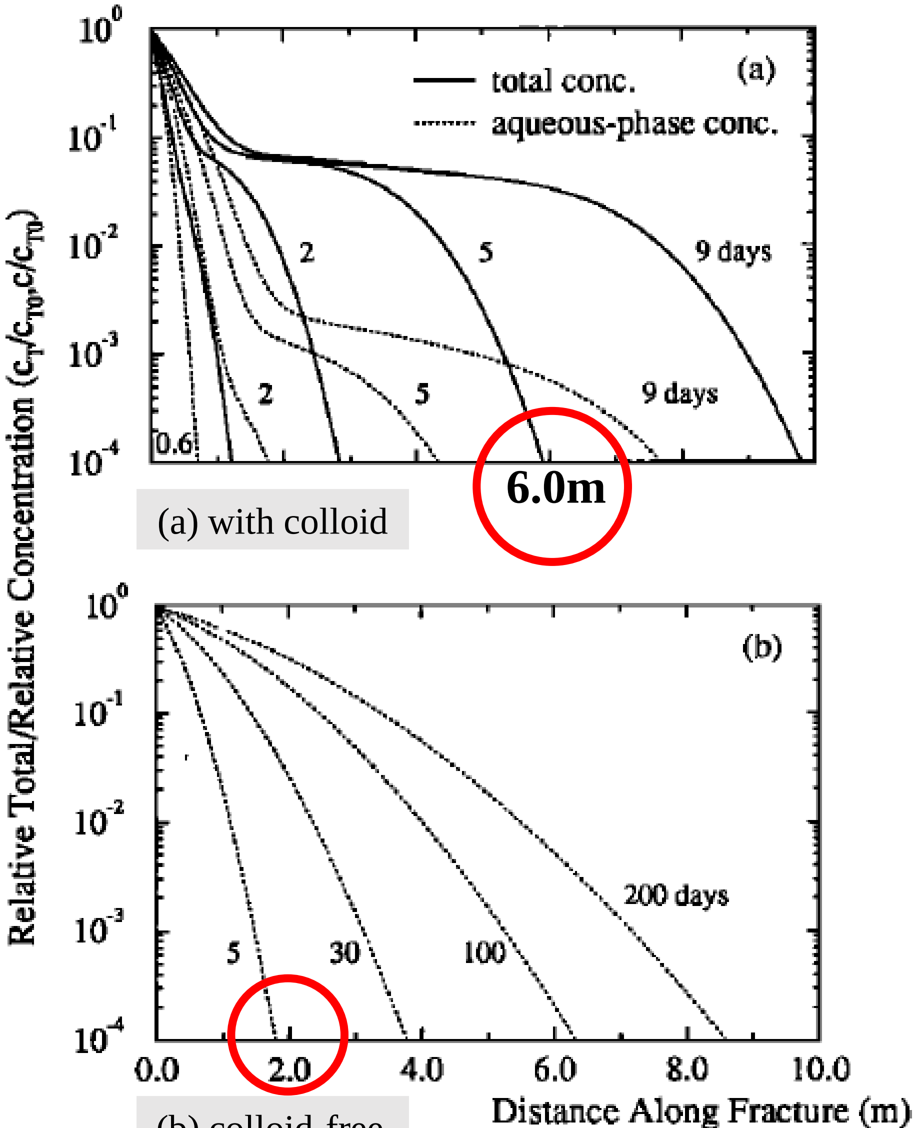
3

Results and discussion

Results and discussion / Parameters for sensitivity analysis

Parameter	Symbol	Value
Matrix porosity	θ	5%
Hydraulic conductivity of the matrix	K	1.0×10^{-10} m s^{-1}
Longitudinal dispersivity for the matrix	α_l	0.0 m
Transverse dispersivity for the matrix	α_t	0.0 m
Matrix retardation factor	R	1.4
Effective diffusion coefficient	τD_d	9.0×10^{-10} m^2 s^{-1}
Fracture aperture	$2b$	100 μm
Fracture spacing	$2B$	0.5 m
Groundwater velocity in the fractures	q_f	1.0 m d^{-1}
Colloid velocity in the fractures	q_m	1.0 m d^{-1}
Longitudinal dispersivity for the fracture	α_l^*	0.1 m
Fracture surface retardation factor	R_f	1.0
Free solution diffusion coefficient	D_d	1.5×10^{-9} m^2 s^{-1}
Decay constant	λ_d	0.0 yr^{-1}
Longitudinal dispersivity for colloids in the fractures	α_{lc}	0.1 m
Free solution diffusion coefficient for colloids	D_{dm}	1.0×10^{-11} m^2 s^{-1}
Filter coefficient	λ	0.0 m^{-1}
Distribution coefficient for mobile colloids	K_m	8.50×10^{-4} L/mg
Kinetic rate constant for mobile colloids	β_m	0.13 d^{-1}

Results and discussion / The base case



(a) with colloid

(b) colloid-free

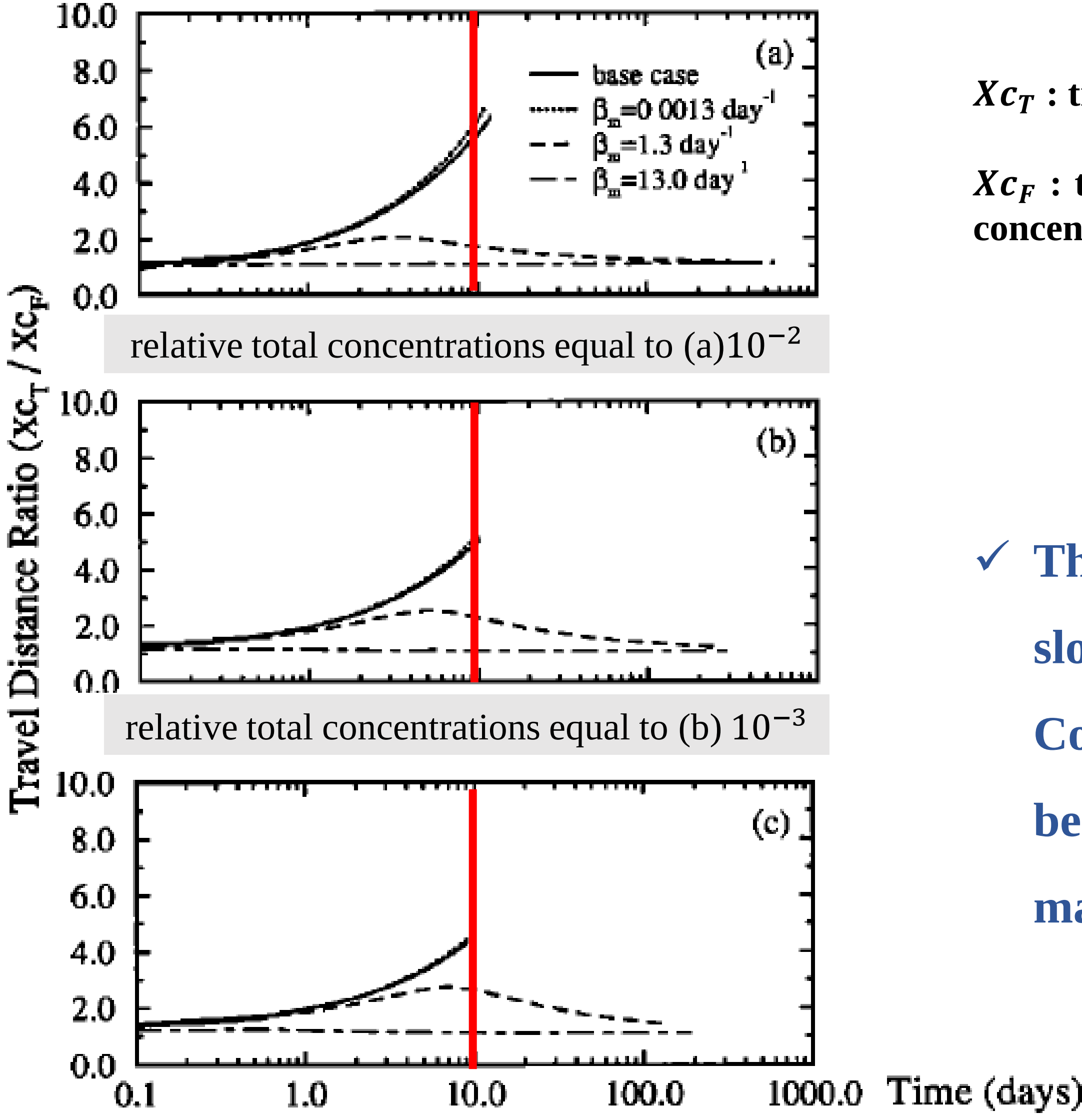
C_T : total concentration

C_{T0} : initial total concentration

C : concentration in aqueous phase (not include concentration in colloid)

✓ **Colloids facilitate the migration of contaminants.**

Results and discussion / Effect of Kinetic rate constant (β_m)



relative total concentrations equal to (a)10^{-2}

relative total concentrations equal to (b) 10^{-3}

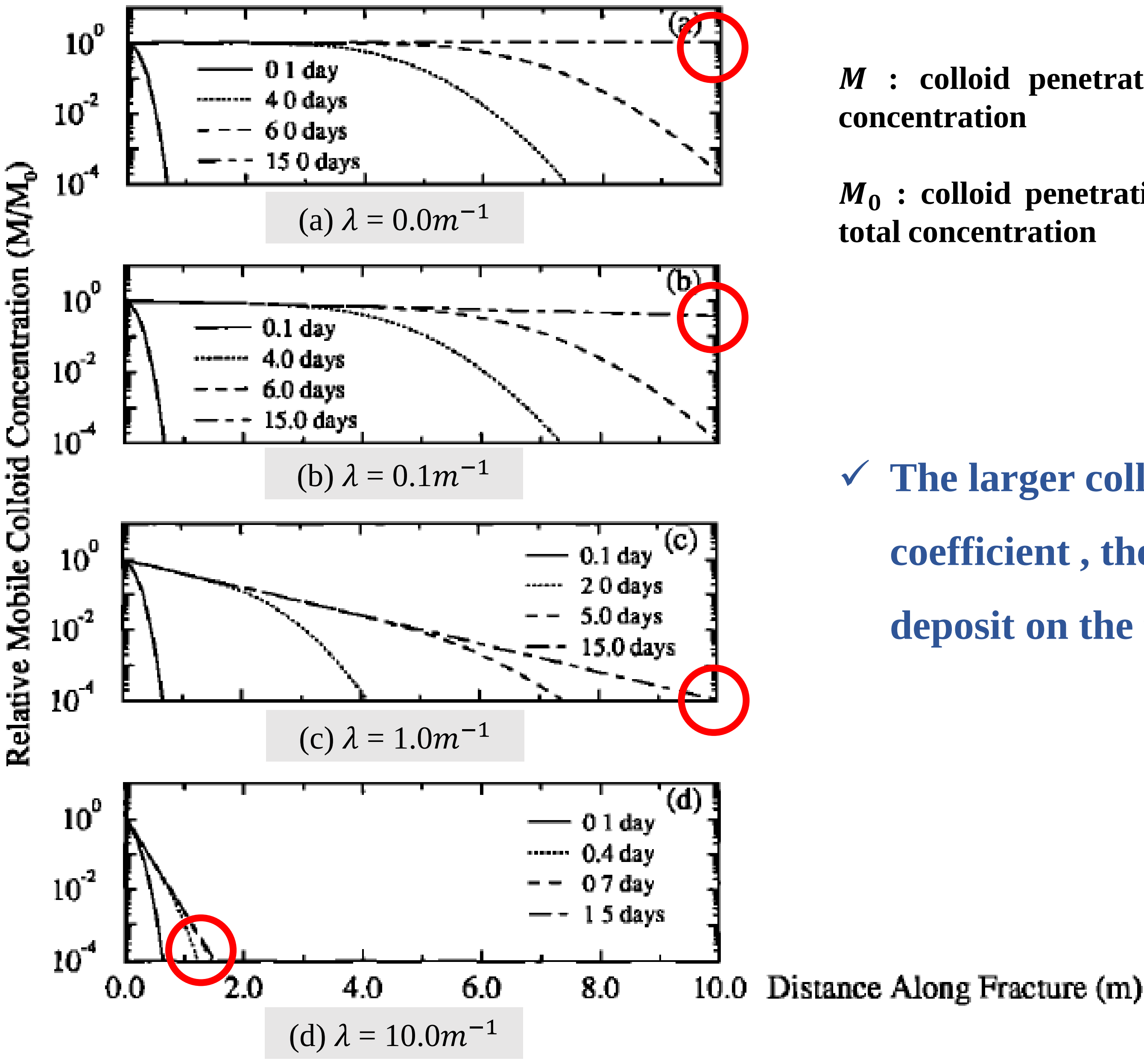
relative total concentrations equal to (c) 10^{-4}

Xc_T : travel distances for total concentration

Xc_F : travel distances for the aqueous phase concentration in the colloid-free case

- ✓ The smaller the value of β_m, the slower the desorption speed. Contaminants can move fast because they don't diffuse into matrix.

Results and discussion / Effect of colloidal filtration (λ)

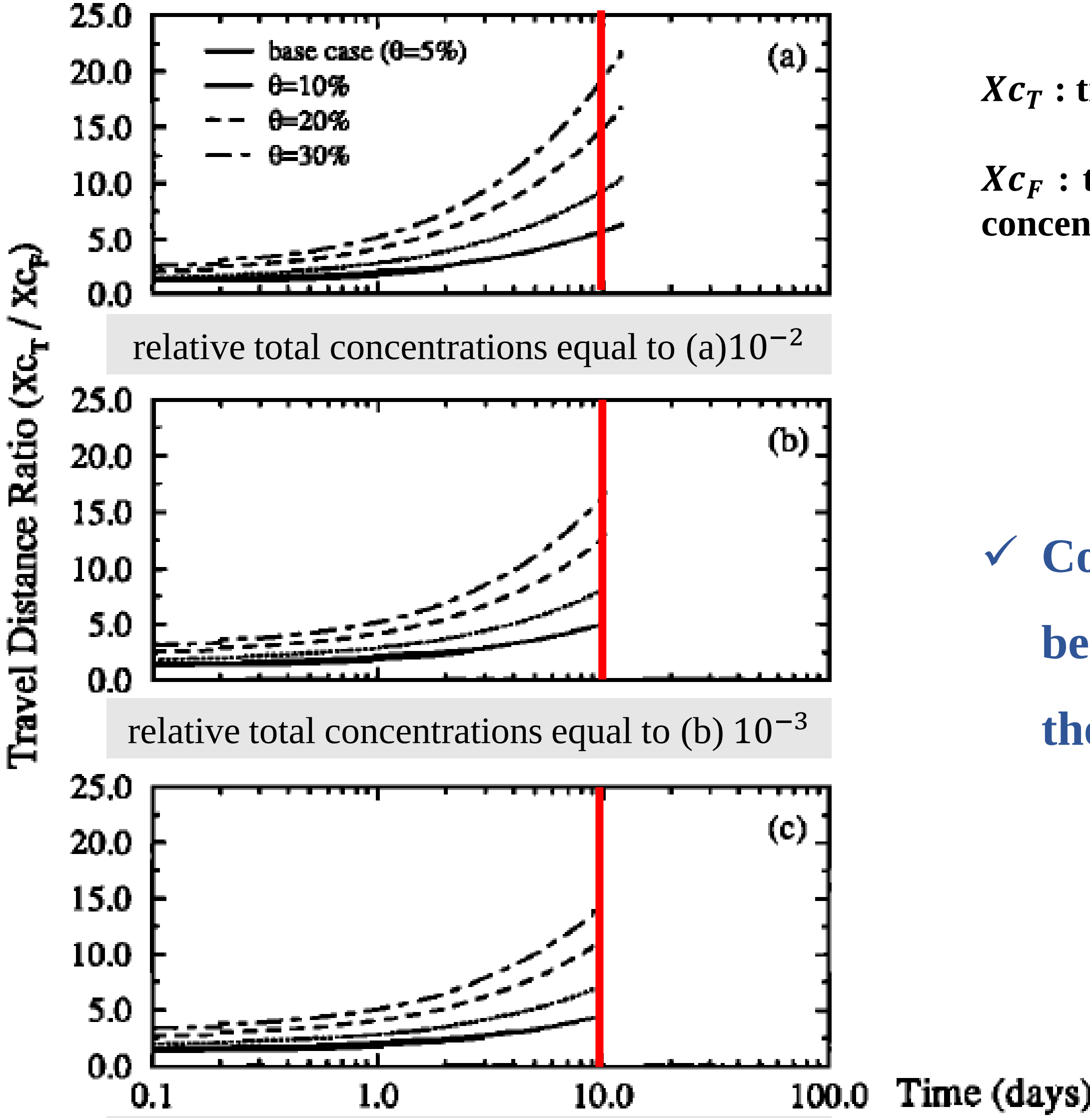


M **: colloid penetration distance for total concentration**

$\boldsymbol{M_0}$ **: colloid penetration distance for initial total concentration**

✓ **The larger colloid filter coefficient , the easier colloids deposit on the fracture surface.**

Results and discussion / Effect of matrix porosity (θ)



relative total concentrations equal to (a)10^{-2}

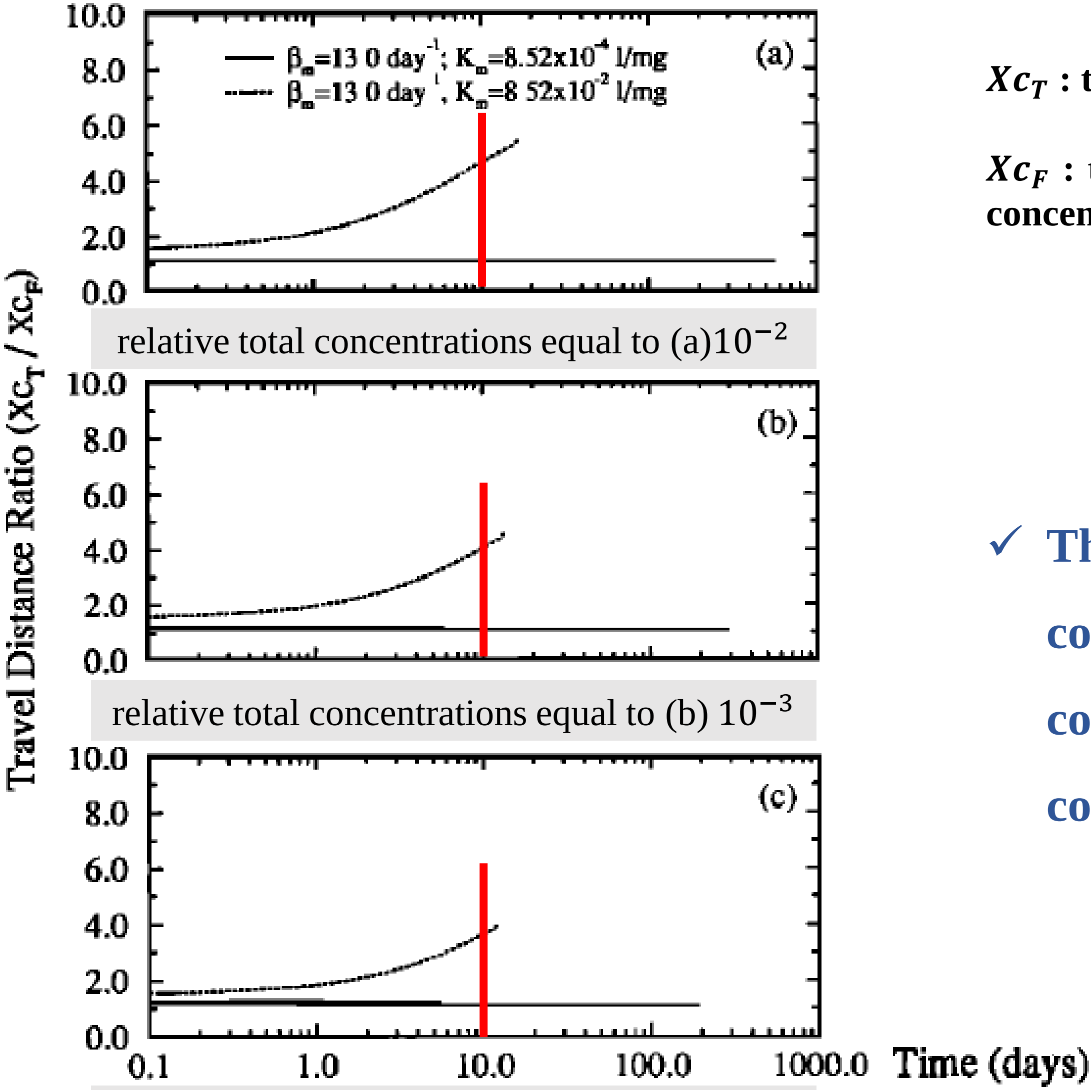
relative total concentrations equal to (b) 10^{-3}

relative total concentrations equal to (c) 10^{-4}

Xc_T : travel distances for total concentration

Xc_F : travel distances for the aqueous phase concentration in the colloid-free case

- ✓ **Colloid-facilitated transport becomes more pronounced as the matrix porosity increases.**



relative total concentrations equal to (a) 10^{-2}

relative total concentrations equal to (b) 10^{-3}

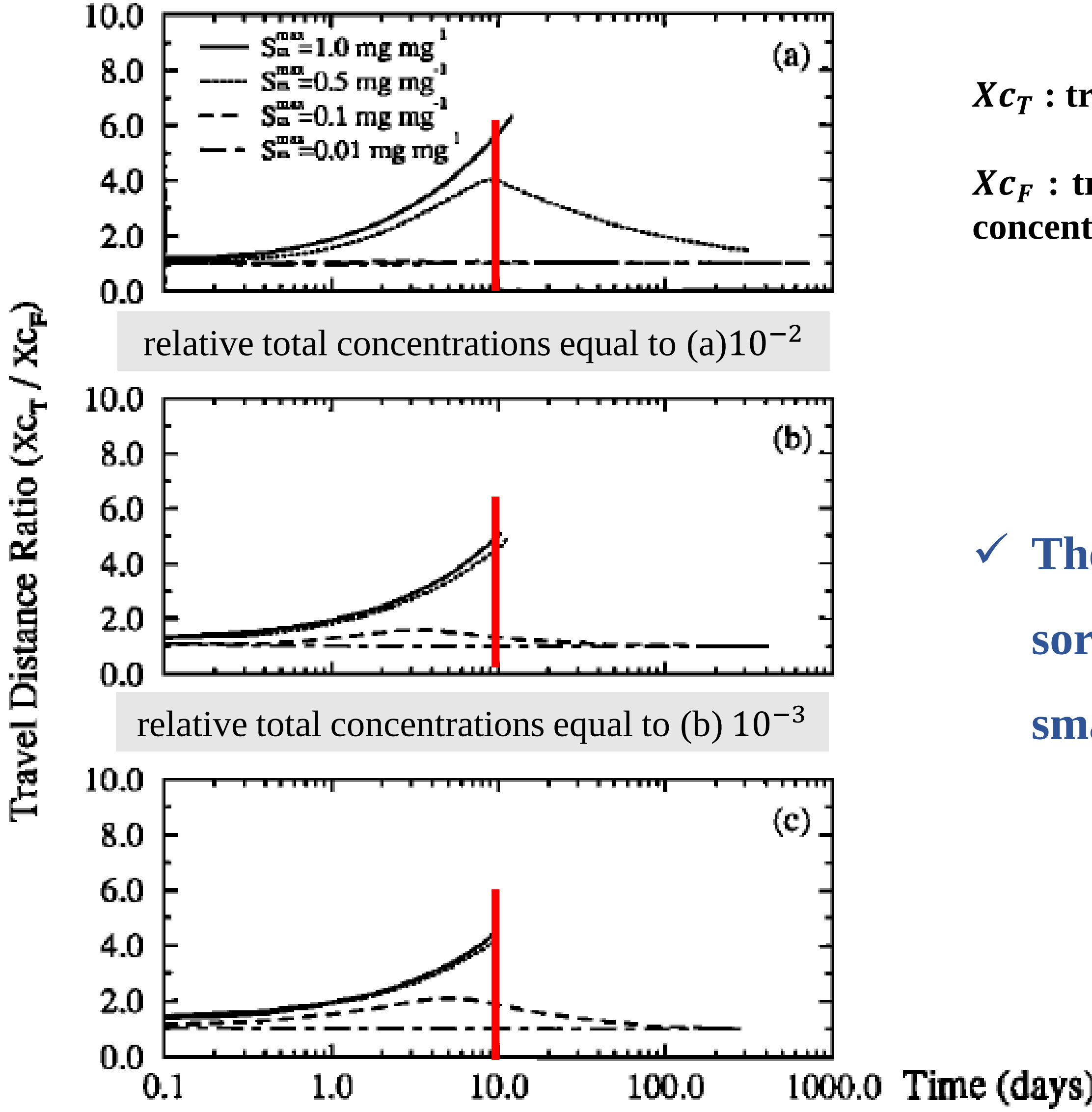
relative total concentrations equal to (c) 10^{-4}

Xc_T : travel distances for total concentration

Xc_F : travel distances for the aqueous phase concentration in the colloid-free case

- ✓ The higher the distribution coefficient , the more contaminants are sorbed on the colloid.

Results and discussion / Effect of Langmuir Isotherm (S_m^{max})



relative total concentrations equal to (a)10^{-2}

relative total concentrations equal to (b) 10^{-3}

relative total concentrations equal to (c) 10^{-4}

Xc_T : travel distances for total concentration

Xc_F : travel distances for the aqueous phase concentration in the colloid-free case

- ✓ **The smaller the maximum sorption capacity value, the smaller the travel distance ratio.**

4

Conclusions

Conclusions

- **Numerical analyses involving colloid-facilitated contaminant transport in discretely fractured porous media were performed to assess the relative importance of various coefficients.**

- **The presence of mobile colloids onto which the contaminant can adsorb can strongly affect contaminant migration rates.**

- **Slow kinetic desorption of the contaminant from the colloids can significantly enhance transport.**

- **When the colloidal particles are filtered onto the fracture surfaces, contaminant migration isn’t enhanced because of the low colloid mobility, even when the sorption capacity of the colloids is large.**

Thank you for your attention