Verification of Travel Time Probabilities for Sorbing Solutes in Groundwater

Aditi Bhaskar
REU Summer 2006
Under Dr. Neupauer

Outline

- Introduction
  - Sorbing Solutes
  - Travel Times
  - Probabilities
  - Objective
- Methods
  - Standard Groundwater Codes
  - Random Walk
- Results
- Conclusions

Introduction

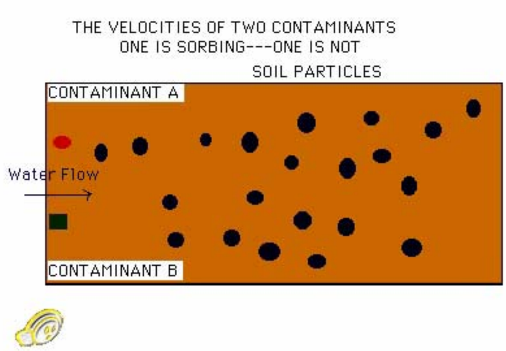
- Sorbing Solutes
  - Non-Equilibrium $\frac{\partial C_s}{\partial t} = \alpha_s (K_d C - C_s)$
  - Equilibrium $C_s = K_d C$

α_s: rate constant
K_d: partition coefficient
C_s: sorbed phase concentration
C: solute concentration

- Advective-Dispersive Eq with Non-Eq Sorption

$$\frac{\partial C}{\partial t} = -v_x \frac{\partial C}{\partial x} + D \frac{\partial^2 C}{\partial x^2} - \frac{\rho_b}{\theta} \frac{\partial C_s}{\partial t}$$

C: solute concentration
ρ_b: bulk density
C_s: sorbed phase concentration
θ: porosity
D: dispersion coefficient
v_x: groundwater velocity in the x direction
t: time
x: spatial dimension



Movie with permission from Daniel Gallagher, Virginia Tech

Introduction

- Sorbing Solutes
  - Non-Equilibrium $\frac{\partial C_s}{\partial t} = \alpha_s (K_d C - C_s)$
  - Equilibrium $C_s = K_d C$

α_s: rate constant
K_d: partition coefficient
C_s: sorbed phase concentration
C: solute concentration

- Advective-Dispersive Eq with Non-Eq Sorption

$$\frac{\partial C}{\partial t} = - v_x \frac{\partial C}{\partial x} + D \frac{\partial^2 C}{\partial x^2} - \frac{\rho_b}{\theta} \frac{\partial C_s}{\partial t}$$

C: solute concentration
ρ_b: bulk density
C_s: sorbed phase concentration
θ: porosity

D: dispersion coefficient
v_x: groundwater velocity in the x direction
t: time
x: spatial dimension

Introduction

- Travel Times
- How this could be useful
- Probability Density Functions (PDFs)
- Aqueous Travel Time PDF

$$f_{T;A}(t; x, x_o) = \frac{vA\theta}{M} C^f(x, t)$$

θ: porosity
C^f: flux concentration
M: source mass
A: cross sectional area

v: average linear groundwater velocity
t: time
x: spatial dimension
x0: location of the initial contamination

Introduction

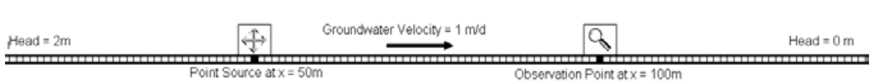
- Sorbed Travel Time Probability $\frac{\text{Mass in Sorbed Phase}}{\text{Total Mass}}$
  - Non-Equilibrium $P(t; x, x_o) = \frac{v\, A\, \rho_b}{\alpha_s M\, R} C_s(x,t)$
  - Equilibrium $f_{T;S}(t; x, x_o) = \frac{v\, A\, \rho_b}{M\, R} C_s(x,t)$

ρ_b: bulk density
M: source mass
v: velocity
A: cross sectional area
α_s: rate constant

C_s: sorbed phase concentration
t: time
x: spatial dimension
x_0: location of the initial contamination

Methods

- Analytical and Semi-Analytical
- Standard Groundwater Codes
  - MODFLOW (Modular Flow)
  - MT3DMS (Mass Transport in 3-D for multiple species)
  - Both are Finite Difference Codes



Methods

- Random Walk Simulation
  - Advection and Dispersion

$$x \text{ location } (t + dt) = x \text{ location } (t) + v\,dt + Z\sqrt{2\,D\,dt}$$

Z: a standard normal random number, D: x dispersion coefficient, v: groundwater velocity, dt: time-step

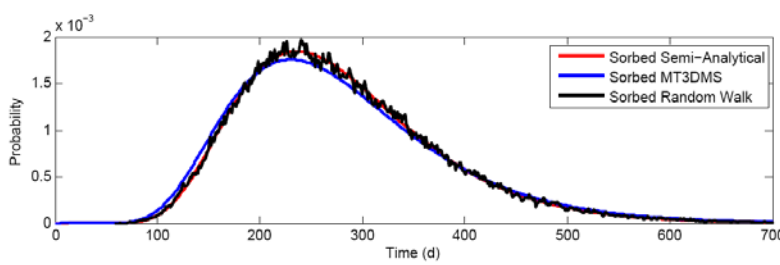
  - Sorption and Desorption

$$t_{A \to S} = -\frac{\log(\varepsilon)}{k_f} = \frac{-\log(\varepsilon)}{(R-1)\,\alpha_s} \qquad t_{S \to A} = -\frac{\log(\varepsilon)}{k_b} = -\frac{\log(\varepsilon)}{\alpha_s}$$

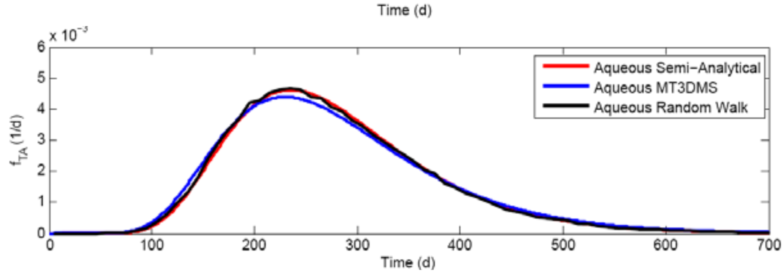
$t_{S \to A}$: time until the phase change from sorbed to aqueous
$t_{A \to S}$: is the time until the phase change from aqueous to sorbed
ε is a random number picked from a uniform distribution,
k_b: backwards reaction rate = α_s the rate constant
k_f: forward reaction rate = (R-1) α_s where R is the retardation coefficient

1-D Non-Equilibrium Homogenous Aquifer

K_d = 0.3, α_s = 2, ρ_b = 4, θ = 0.3, R= 5



Sorbed Phase



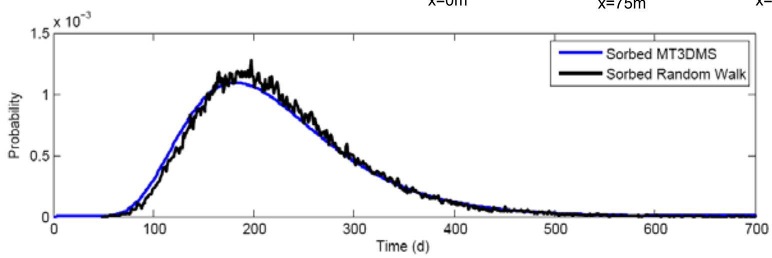
Aqueous Phase

1-D Non-Equilibrium Variable Sorption Properties

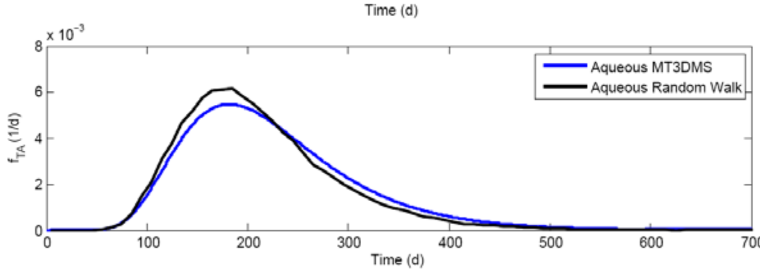
K_d, α_s = 2, ρ_b = 4, θ = 0.3, R= 5

K_d = 0.3 cm³/g	K_d = 0.15 cm³/g

x=0m x=75m x=150m



Sorbed Phase



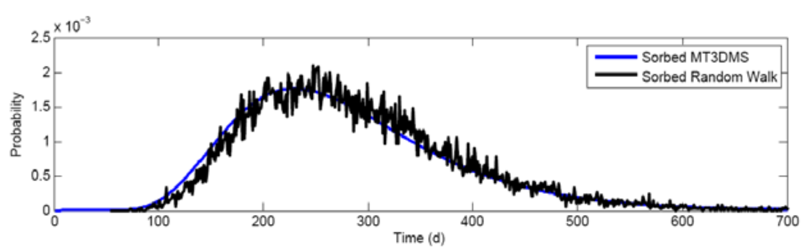
Aqueous Phase

1-D Non-Equilibrium Variable Rate Constant

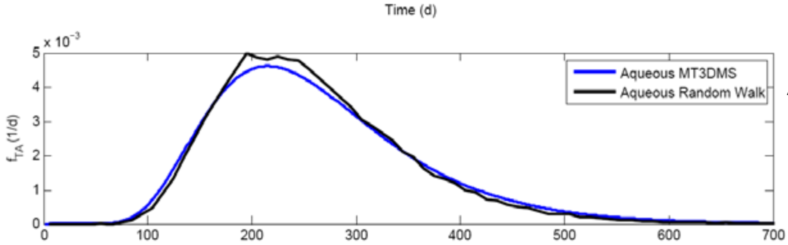
K_d = 0.3, **α_s**, ρ_b = 4, θ = 0.3, R= 5

α_s = 2 d^{-1}	α_s = 4 d^{-1}

x=0m x=75m x=150m



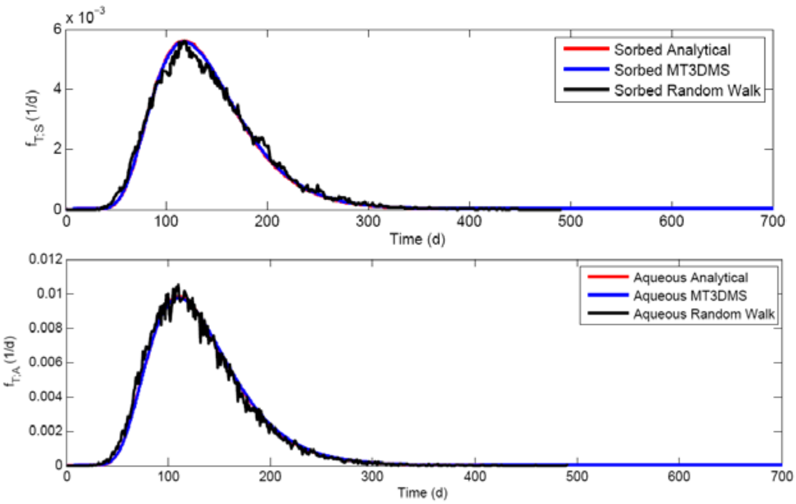
Sorbed Phase



Aqueous Phase

1-D Equilibrium Homogeneous Aquifer

$K_d = 0.3$, $\rho_b = 1.5$, $\theta = 0.3$, R= 2.5



Sorbed Phase

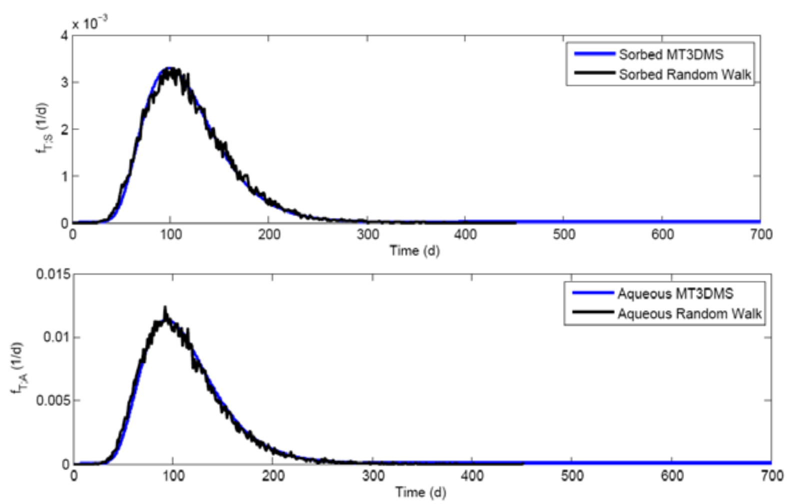
Aqueous Phase

1-D Equilibrium Variable Sorption Properties

$\mathbf{K_d}$, $\rho_b = 1.5$, $\theta = 0.3$, R= 2.5

$K_d = 0.3$ cm³/g	$K_d = 0.6$ cm³/g

x=0m x=75m x=150m



Sorbed Phase

Aqueous Phase

Conclusions

- Verification of travel time probability for sorbing solutes:
  - Equilibrium
    - Homogenous aquifers
    - Variable sorption properties
  - Non-equilibrium
    - Homogenous aquifers
    - Variable sorption properties
    - Variable rate constant
- Future Work

Acknowledgements

- Thank you to:
  - Dr. Roseanna M. Neupauer
  - Dr. Angela Bielefeldt
  - Guadalupe Gutierrez-Padilla
  - Dr. Scott Summers
  - Heather O’Shea
  - The other REU students
  - The NSF REU Program at the University of Colorado-Boulder