HLWYM HEmails

From: Hakan Basagaoglu
Sent: Friday, December 22, 2006 4:11 PM
To: Paul Bertetti; Jude Mcmurry; Scott Painter; David Pickett; Ronald Janetzke; Olufemi Osidele; 'Carol Scherer'
Subject: Colloid Model
Attachments: Colloid_tp.doc

Follow Up Flag: Follow up
Flag Status: Flagged

All,

I have attached a write-up that shows all the steps to obtain Reff for mobile and immobile phases. Apparently, I had a problem with the
(1+Ko) term in the denominator. This was because:

- I had simply (accidentally) forgot to apply the equilibrium isotherm eq in the colloid transport operator (the second term on RHS of Eq. 1)
- I had failed to scale both sides of Eq. (13) by (1/(1+Ko)) in transition from Eq. (13) to Eq. (14).

Thanks Scott for pointing them out.

Now, I feel more comfortable with the model and equations we use.

Hakan

Hearing Identifier: HLW_YuccaMountain_Hold_EX
Email Number: 718

Mail Envelope Properties (000001c7260d$a9ff0000$e6c8a281)

Subject: Colloid Model
Sent Date: 12/22/2006 4:10:53 PM
Received Date: 12/22/2006 4:10:53 PM
From: Hakan Basagaoglu

Created By: hbasagaoglu@cnwra.swri.edu

Recipients:
"Paul Bertetti" <pbertetti@cnwra.swri.edu>
Tracking Status: None
"Jude Mcmurry" <jmcmurry@cnwra.swri.edu>
Tracking Status: None
"Scott Painter" <spainter@cnwra.swri.edu>
Tracking Status: None
"David Pickett" <dpickett@cnwra.swri.edu>
Tracking Status: None
"Ronald Janetzke" <rjanetzke@cnwra.swri.edu>
Tracking Status: None
"Olufemi Osidele" <oosidele@cnwra.swri.edu>
Tracking Status: None
"'Carol Scherer'" <cscherer@cnwra.swri.edu>
Tracking Status: None

Post Office: cnwra.swri.edu

Files	**Size**	**Date & Time**
MESSAGE	565	12/22/2006 4:10:53 PM
Colloid_tp.doc	100928	

Options
Priority: Standard
Return Notification: No
Reply Requested: No
Sensitivity: Normal
Expiration Date:
Recipients Received: Follow up

Mass-balance equation for reversible solved dissolved radionuclides in the mobile (fractures) (Eq. 1) and immobile (matrix) (Eq. 2) phases:

$$\phi_m S_w \frac{\partial C_m}{\partial t} + \rho_b \frac{\partial S_m}{\partial t} + \phi_m S_w \frac{\partial(\sigma_{Cm} C_C)}{\partial t} + \rho'_b \frac{\partial(\sigma_{Cm} C_C)}{\partial t} + \phi_{im} S_{im} \frac{\partial C_{im}}{\partial t} + \rho_b \frac{\partial S_{im}}{\partial t} = -\nabla \cdot J(C_m) - \nabla \cdot J(\sigma_{Cm} C_C) \quad (1)$$

$$\phi_{im} S_{im} \frac{\partial C_{im}}{\partial t} + \rho_b \frac{\partial S_{im}}{\partial t} = \beta(C_m - C_{im}) \quad (2)$$

in which σ_{Cm} is the mass fraction of radionuclides adhered to mobile colloid surfaces per unit mass of mobile colloids, C_C is the mass of mobile colloids per aqueous volume, C_m is the aqueous mass concentration of radionuclides in mobile region (mass of radionuclides per aqueous volume), S_w is the water saturation (aqueous volume per pore volume), ϕ_m is the ratio of pore volume to the bulk volume (porosity) in the mobile flow region, S_m is the sorbed mass of radionuclides per unit mass of available stationary solid surfaces), ρ_b is the ratio bulk density (mass of solid surfaces per unit bulk volume); v is the average linear velocity, and $J(C_m)$ is the transport operator for the radionuclides, $J(\sigma_{Cm} C_C)$ is the transport operator for mobile colloids, β is the mass-transfer coefficient (1/time).

When we assume equilibrium sorption of radionuclides onto mobile colloidal surfaces and stationary matrix, i.e.,

$$\sigma_{vm} = \frac{A_{mat}}{A_{Col}} K_d C_m = A K_d C_m \quad (3)$$

$$S_m = K_d C_m \quad (4)$$

$$S_{im} = K'_d C_{im} \quad (5)$$

in which A_{mat} is the specific surface area of the matrix and A_{Col} is the specific surface area of the colloid; K_d is the distribution coefficient for the mobile flow zone, K'_d is the distribution coefficient for the immobile flow zone.

$$(\phi_m S_w + K_d \rho_b)\frac{\partial C_m}{\partial t} + (\phi_m S_w + 1) A K_d \frac{\partial(C_m C_C)}{\partial t} + (\phi_{im} S_{im} + K'_d \rho_b)\frac{\partial C_{im}}{\partial t} = -\nabla \cdot J(C_m) - (A K_d)\nabla \cdot (C_m C_C) \quad (6)$$

$$(\phi_{im} S_{im} + K'_d \rho_b)\frac{\partial C_{im}}{\partial t} = \beta(C_m - C_{im}) \quad (7)$$

For a constant C_C, Eq. 6 becomes,

$$\left(\phi_m S_w + K_d \rho_b\right)\frac{\partial C_m}{\partial t} + \left(\phi_m S_w + 1\right) A K_d C_C \frac{\partial C_m}{\partial t} + \left(\phi_{im} S_{im} + K'_d \rho_b\right)\frac{\partial C_{im}}{\partial t} \tag{8}$$
$$= -\left(1 + A K_d C_C\right)\left[\nabla \cdot J\left(C_m\right) + \nabla \cdot \left(C_m\right)\right]$$

Let $K_0 = A K_d C_C$, then Eq. (8) and (9) becomes,

$$\phi_m S_w \left(1 + \frac{K_d \rho_b}{\phi_m S_w}\right)\frac{\partial C_m}{\partial t} + \phi_m S_w \left(1 + \frac{1}{\phi_m S_w}\right) K_0 \frac{\partial C_m}{\partial t} + \phi_{im} S_{im}\left(1 + \frac{K'_d \rho_b}{\phi_{im} S_{im}}\right)\frac{\partial C_{im}}{\partial t} \tag{9}$$
$$= -\left(1 + K_0\right)\left[\nabla \cdot J\left(C_m\right) + \nabla \cdot \left(C_m\right)\right]$$

$$\phi_{im} S_{im}\left(1 + \frac{K'_d \rho_b}{\phi_{im} S_{im}}\right)\frac{\partial C_{im}}{\partial t} = \beta\left(C_m - C_{im}\right) \tag{10}$$

Let $R = 1 + \frac{K_d \rho_b}{\phi_m S_w}$, $R_C = 1 + \frac{1}{\phi_m S_w}$, and $R_{im} = 1 + \frac{K'_d \rho_b}{\phi_{im} S_{im}}$, Eq. (9),

$$\phi_m S_w R \frac{\partial C_m}{\partial t} + \phi_m S_w R_C K_0 \frac{\partial C_m}{\partial t} + \phi_{im} S_{im} R_{im} \frac{\partial C_{im}}{\partial t} = -\left(1 + K_0\right)\left[\nabla \cdot J\left(C_m\right) + \nabla \cdot \left(C_m\right)\right] \tag{11}$$

or

$$\phi_m S_w \left(\frac{R + R_C K_0}{1 + K_0}\right)\frac{\partial C_m}{\partial t} + \phi_{im} S_{im}\left(\frac{R_{im}}{1 + K_0}\right)\frac{\partial C_{im}}{\partial t} = -\left[\nabla \cdot J\left(C_m\right) + \nabla \cdot \left(C_m\right)\right] \tag{12}$$

and Eq. (10) becomes

$$R_{im} \frac{\partial C_{im}}{\partial t} = \beta\left(C_m - C_{im}\right) \tag{13}$$

By comparing Eqs (10) and (11), (and dividing both sides of Eq. 13 by $1 + K_0$)

$$\frac{R_{im}}{1 + K_0}\frac{\partial C_{im}}{\partial t} = \frac{\beta}{1 + K_0}\left(C_m - C_{im}\right) \tag{14}$$

So, we have the following system of equation:

$$\phi_m S_w \left(\frac{R + R_C K_0}{1 + K_0}\right)\frac{\partial C_m}{\partial t} + \phi_{im} S_{im}\left(\frac{R_{im}}{1 + K_0}\right)\frac{\partial C_{im}}{\partial t} = -\left[\nabla \cdot J\left(C_m\right) + \nabla \cdot \left(C_m\right)\right] \tag{15}$$

$$\frac{R_{im}}{1 + K_0}\frac{\partial C_{im}}{\partial t} = \frac{\beta}{1 + K_0}\left(C_m - C_{im}\right) \tag{16}$$

By defining

$R_{eff} = \frac{R + R_C K_0}{1 + K_0}$ and $R'_{eff} = \frac{\beta}{1 + K_0}$, Eqs. 15 and 16 become

$$\phi_m S_w R_{eff} \frac{\partial C_m}{\partial t} + \phi_{im} S_{im} R'_{eff} \left(C_m - C_{im}\right) = -\left[\nabla \cdot J\left(C_m\right) + \nabla \cdot \left(C_m\right)\right] \tag{17}$$

$$R'_{eff} \left(C_m - C_{im}\right) = \frac{R_{im}}{1 + K_0} \frac{\partial C_{im}}{\partial t} \tag{18}$$