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From: David Pickett
Sent: Tuesday, January 21, 2003 6:52 PM
To: Ronald Janetzke
Cc: David Turner; Paul Bertetti
Subject: reversible colloids
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Ron,

Attached is a document outlining my abstraction for incorporating reversible colloidal attachment in TPA. It's a little more complicated than simply providing you a list of KD's and RD's. Rather, it shows how they should be calculated. I hope it's reasonably clear, but I'm sure you'll have questions...and so will I.

What's involved:

1. Adjustment of matrix KD's for UZ tuff.
2. Adjustment of "immobile" RD's for SZ tuff.
3. Adjustment of matrix RD's for alluvium.

David

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Proposed Equations and Parameters for Irreversible Colloid Attachment in TPA Transport Abstractions

David Pickett
January 21, 2003

The TPA approach to modeling reversible attachment involves an (optional) adjustment to transport parameters that account for the increased mobility due to reversible attachment. Values for K_D and R_D are re-calculated. Retardation in fractures is not modeled, consistent with the non-colloid case. **Note: none of these adjustments should be made to the new irreversible colloid species.**

1. Unsaturated Zone

The affected parameters in the UZ are the matrix K_D's for the various tuff units (because there is no retardation in the fractures). The adjustment will be made to all radioelements that have a non-zero K_D, but it should be noted that the effect is smaller the smaller the starting K_D. The affected elements are Am, Pu, U, Np, Th, Ra, Pb, Cs, Ni, and Se. Curium should be included in this list if it is given a non-zero K_D; the current zero value is highly conservative.

Alternatively, the adjustment could be made to all radioelements, because those that are assigned a zero value will remain zero. This would simplify later efforts if any elements are no longer assumed to have no sorption. In any case, the adjustment should be made after the K_D is sampled. The adjustment should be made to every unit, e.g., MatrixKD_TSw_Am, MatrixKD_ChnvAm, etc.

The adjustment is as follows:

$$K_{D,eff} = \frac{K_D}{1 + C_U F_T K_D}$$

(Contardi et al., 2001, after Vilks et al., 1998) where K_D is the given matrix K_D (m^3/kg) sampled in TPA, C_U is the colloid concentration in unsaturated zone water (kg/m^3), and F_T is a unitless factor accounting for surface area differences between tuff matrix and colloids (Contardi et al., 2001). C_U and F_T should be easily adjustable by the user; default values are:

> $C_U = 0.001$ kg/m^3 (bounds 78% of the concentration data compiled by Contardi et al., 2001)
> $F_T = 590$ (typical value for tuff in Contardi et al., 2001).

FractureRD_... values for the UZ can remain unaltered, as long as they continue to be unity.

2. Saturated Zone

A. SZ Tuff

For transport in the SZ tuff, relevant parameters are the "immobile" phase retardation factors and the diffusion rate. (Fracture_RD_... values can remain unaltered as long as they continue to be unity.) These two parameters affect how solute is transferred from the mobile fracture phase to the "immobile" matrix. They are affected by reversible colloid attachment according to these equations (note: these are not the equations that will be used in TPA):

$$R_{D,eff} = 1 + \frac{(1-\phi)\rho K_D}{\phi(1 + C_T F_T K_D)}$$

(Contardi et al., 2001, after Vilks et al., 1998) and

$$D_{eff} = \frac{D}{(1 + C_T F_T K_D)^2}$$

(modified from CRWMS M&O, 2000, after CRWMS M&O, 1997). φ is the tuff matrix porosity, equivalent to the input parameter ImmobilePorosity_STFF (currently a constant value of 0.2). ρ is the grain density of the tuff matrix; a value of 2650 kg/m^3 is appropriate (Contardi et al., 2001). D is the diffusion coefficient, K_D is the matrix K_D (m^3/kg), C_T is the colloid concentration in water in saturated tuff matrix (kg/m^3), and F_T is a unitless factor accounting for surface area differences between matrix and colloids (Contardi et al., 2001). C_T and F_T should be easily adjustable by the user; default values are:

> C_T = 0.001 kg/m^3 (bounds 78% of the concentration data compiled by Contardi et al., 2001)
> F_T = 590 (typical value for tuff in Contardi et al., 2001).

The retardation factors (e.g., ImmobileRD_STFF_Am) are element specific, and so could be adjusted for colloids with the above equation. However, a single diffusion coefficient, DiffusionRate_STFF = 0.001 m^2/yr, is applied to all elements in TPA; adjustment of this parameter would be inappropriate because elements are affected to very different degrees by reversible attachment (see K_D term in D_{eff} equation). According to equations 10-1 and 10-2 of CNWRA (2002; TPA 4.0 Module Description and User's Guide), the retardation factor is inversely proportional to the rate of change of concentration in the immobile phase, while the diffusion coefficient is directly proportional. Therefore, the ratio of the diffusion coefficient to the retardation factor, both adjusted for reversible attachment, implements the colloidal effect on matrix diffusion. Because the diffusion coefficient cannot be adjusted (i.e., we cannot calculate D_{eff} for each element), the retardation factor $R_{D,eff}$ can be further adjusted so that the ratio is element specific. That is:

$$\frac{0.001}{R'_{D,eff}} = \frac{D_{eff}}{R_{D,eff}}$$

Using the equations above for D_{eff} and $R_{D,eff}$, knowing that D = 0.001 m^2/yr, and rearranging gives:

$$R'_{D,eff} = (1 + C_T F_T K_D)\left[(1 + C_T F_T K_D) + \left(\frac{1-\phi}{\phi}\right)\rho K_D\right]$$

This calculation should be applied to each "immobile" R_D value in the TPA input (e.g., ImmobileRD_STFF_Am) using an element-specific K_D (see below). The colloid adjustment can either be applied only to those radioelements with a non-unity value (Am, Np, Cm, U, Pu, Th, Ra, Pb, Cs, Ni, Se, and Nb) or to all radioelements (values that are unity will remain at unity, because the K_D calculated below will be zero). This formulation accounts for the competing effects of the two parameters on matrix diffusion.

The K_D value in the equation is not in the TPA input file; it must be extracted from the starting R_D (e.g., ImmobileRD_STFF_Am) in the input file, using this equation:

$$K_D = \frac{\phi}{(1-\phi)\rho}(R_D - 1)$$

(Freeze and Cherry, 1979), with φ and ρ as defined above. $R_{D,eff}$' can now be calculated and used in place of the input file value for the "immobile" R_D for each element.

B. SZ Alluvium

In TPA, transport in the alluvial aquifer is simulated with an element-specific retardation factor, e.g., AlluviumMatrixRD_SAV_Am. The equation for the R_D that accounts for reversible attachment is:

$$R_{D,eff} = 1 + \frac{(1-\phi)\rho K_D}{\phi(1 + C_A F_A K_D)}$$

(Contardi et al., 2001, after Vilks et al., 1998), where K_D is the matrix K_D (m^3/kg), C_A is the colloid concentration in water in saturated alluvium (kg/m^3), and F_A is a unitless factor accounting for surface area differences between alluvium and colloids (Contardi et al., 2001). C_A and F_A should be easily adjustable by the user; default values are:

> C_A = 0.001 kg/m^3 (in middle of range of concentration data compiled by Contardi et al., 2001)

F_A = 630 (calculated for alluvium in Contardi et al., 2001).

φ is the alluvium matrix porosity; a value of 0.125, in the middle of the range for TPA parameter AlluviumMatrixPorosity_SAV, should be used to be consistent with Contardi et al. (2001). ρ is the grain density of the alluvium matrix; a value of 2500 kg/m^3 should be used (Contardi et al., 2001).

The K_D value in the equation is not in the TPA input file; it must be extracted from the starting R_D (e.g., AlluviumMatrixRD_SAV_Am) in the input file, using this equation:

$$K_D = \frac{\phi}{(1-\phi)\rho}(R_D - 1)$$

(Freeze and Cherry, 1979), with φ and ρ as defined in the previous paragraph (note that φ and ρ differ for the tuff and alluvial aquifers). $R_{D,eff}$ can now be calculated. This calculation can either be applied to only those radioelements with non-unity alluvium retardation factors (Am, Np, Cm, U, Pu, Th, Ra, Pb, Cs, Ni, Se, and Nb) or to all radioelements. Those with R_D equal to one will be unaffected by the calculation because calculated K_D will be zero. **Note: this adjustment should be made after the starting R_D has been sampled and/or calculated with D. Turner's method.**