2006 Fall Meeting

Donado, L.D, X. Sanchez-Vila and M. Dentz (2006), **Multi-Component Reactive Transport in Physically Heterogeneous Media**, ***Eos Trans. AGU, 87***(52), Fall Meet. Suppl., Abstract H13F-06

Multi-Component Reactive Transport in Physically Heterogeneous Media

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Reactive transport in the subsurface is governed by mixing of waters with different geochemical signature. Mixing yields to chemical disequilibrium in the resulting mixed water, leading to homogeneous (same phase) or heterogeneous (different phase) reactions. In parallel, solute transport of non-conservative species is highly influenced by heterogeneity of physical and chemical properties of the media. A challenging problem resides in the combination of both problems, which is the study of multi-component transport in physically heterogeneous media under equilibrium conditions. This work aims at obtaining an analytical expression for the reaction rates of the different species involved in a given water mixing problem. The methodology presented accounts both for acid-base and/or precipitation/dissolution reactions. The approach consists in defining a number of components, which are conservative quantities obtained by stoichiometric combinations of the aqueous chemical species, which allows partial decoupling of the full reactive transport problem. Here, physical heterogeneity is modeled by means of an effective dynamic equation, which considers the transfer of mass between the mobile zone and a suite of immobile zones which occurs at some pre-specified rates. The resulting expression for the reaction rates is expressed as the sum of two terms, one corresponding to the equivalent homogeneous media, plus the additional term that is expressed in terms of the memory function characterizing the multi-rate mass transfer model. The implications and relative significance of the latter term are explored.

1012 Reactions and phase equilibria (3612, 8412)
1829 Groundwater hydrology
1832 Groundwater transport
1869 Stochastic hydrology

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