An Improved Simulation Method Using the Dual-Domain Formulation: Mass Transfer vs. Mass Transfer Rate

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Background/Objectives. Numerous site investigations and research studies have shown that the pace of remediation at groundwater sites can be significantly impacted by the presence of low permeability zones where mass transport is generally limited by matrix diffusion and slow advection. During plume development (and plume spreading), dissolved-phase constituents are driven into these low-permeability zones via diffusion (concentration gradients) and slow advection (hydraulic gradients). This can be thought of as a 'mass loading' phase. Once the plume has reached maturity and natural attenuation and/or active remediation has begun, these low permeability zones primarily behave as storage zones. Mass flux from these low permeability zones can significantly contribute to the active groundwater flow and transport system (i.e., the more permeable portions of the aquifer), where constituent movement between the active and less active/inactive domains is typically dominated by the rate of diffusion as well as slow advection.

The dual-domain model is used to represent these effects of aquifer soil structure on plume movement, causing the fast movement of contaminants through sand and gravel horizons as well as the delayed flushing of contaminants observed during remediation. The basis for this approach was developed in the 1950's (Aris, 1956; Aris and Amundson, 1957; McHenry and Wilhelm, 1957), with the generalized solution presented by Dean (1963) and Coats and Smith (1964). The dual-domain model matches breakthrough data observed in the field significantly better than the simple advection-dispersion equation (single domain), allowing quantification of dead-end pores in soils and the effects of velocity on mass transfer through the aquifer. There is extensive literature on the dual-domain model of solute transport (Gillham et al. 1984; Molz et al. 2006; Flach et al. 2004; Harvey and Gorelick 2000; Feehley et al. 2000; Julian et al. 2001; Zheng and Bennet 2002), and it is generally considered the most accurate approach for simulating solute transport in the subsurface.

Approach/Activities. The mass transfer coefficient (MTC) is a superficial parameter incorporated in the dual-domain model intended to account for the complexities of soil structure (physical basis) and the scale-of-observation (curve-fitting parameter). This work is intended to introduce a standard method for evaluating the MTC at contaminated sites and provide guidance for assigning values. Numerous groundwater flow and solute transport model simulations were developed to quantify and evaluate MTC based on a new concept of the 'dual-domain-effect' which represents the influence of Darcian flux on plume migration and attenuation. Simulation results, including breakthrough times and flushing times, were normalized to compare and understand the relationship of the MTC with the mass transfer rate coefficient (MTRC).

Results/Lessons Learned. Modeling results clearly indicate that the MTC is proportional to the Darcian flux. Because of this relationship, a normalized or base MTRC parameter can be supplied to the solute transport model (e.g., MT3DMS) for direct computation of an appropriate MTC on a cell-by-cell basis. The approach allows for the effects of transient flow effects on MTC values. Overall, this new approach allows for better representation of the contaminant mass transfer processes occurring in heterogeneous systems.