A Two-Independent-Region Model for Gas Diffusivity of Aggregated, Unsaturated Soil

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To obtain reliable numerical simulation of the fate and transport of gaseous phase chemicals, knowledge of the variation of the gas diffusion coefficient (Dp) as function of the soil moisture condition (in terms of soil-air content, e) is needed. Based on recent studies, the magnitude of soil-gas diffusivity (Dp/Do, where Do is the gas diffusion coefficient in free air) and its variation with soil-air content for aggregated soils is strongly dependent on soil structure and bimodal pore size distribution. In this study, a two-region flexible Dp/Do model is presented taking into account the separate contributions from the inter-aggregate and intra-aggregate pore space regions. The form of the inter-aggregate Dp/Do model includes a nonlinear water-induced blockage effect of connected water films on soil-gas diffusion, whereas a simple linear model is sufficient to describe the behavior of Dp/Do in the intra-aggregate pore space region. This Two-Independent Region (TIR) Dp/Do model described well the Dp/Do of pure aggregates and highly structured soils at different compaction levels. By using the average parameter values for the TIR Dp/Do model, a better prediction of Dp/Do was observed within the total range of soil-air content than the widely-used classical Dp/Do models.