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The Mechanism of Field-Scale Solute Transport: An insight from Numerical Simulations

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Field-scale transport of conservative (chloride) and reactive (nitrate) solutes was analyzed by means of two different model processes for the local description of the transport. The first is the classical, one-region advection dispersion equation (ADE) model, while the second is the two-region, mobile-immobile (MIM) model. The analyses were performed by means of detailed three-dimensional (3-D), numerical simulations of the flow and the transport considering realistic features of the soil-water-plant-atmosphere system, pertinent to a turf field located in the Glil Yam site, Israel, irrigated with treated waste water (TWW). Simulated water content and concentration profiles were compared with available measurements of their counterparts. Results of the analyses suggest that the behavior of both the conservative and the reactive solutes in the Glil Yam site is quantified better when the transport on the local scale is modeled as a two-region, MIM model, than when a single-region, ADE model is used. Reconstruction of the shape of the measured solute concentration profiles using the MIM transport model, required relatively large immobile water content fraction and relatively small mass transfer coefficient. These results suggest that in the case of initially non-zero solute concentration profile (e.g., chloride and nitrate), the 3-D ADE transport model may significantly overestimate the groundwater contamination hazard posed by the solutes moving through the vadose zone, as compared with the 3-D MIM transport model, while the opposite is true in the case of initially zero solute concentration profile (e.g., carbamazepine). These findings stem from the combination of relatively large immobile water content fraction and relatively small mass transfer coefficient taken into account in the MIM transport model. In the first case, this combination forces a considerable portion of the solute mass to remain in the immobile region of the water-filled pores, while the opposite is true in the second case.