Numerical simulation of vadose zone migration and attenuation of organic compounds in produced water from unconventional natural gas extraction

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Produced waters from unconventional natural gas extraction often contain traces of hydraulic fracturing chemicals and naturally occurring organic compounds that may end up in the vadose zone as a result of unintentional release. Naturally occurring organic chemicals considered in this study include phenolic compounds (phenol and 2-methylphenol) and polycyclic aromatic compounds (naphthalene). Chemical additives of hydraulic fracturing fluids included a biocide (bronopol), a surfactant (2-butoxyethanol) and a solvent (limonene). Calculation of natural soil attenuation of the organic compounds involved implementation of biodegradation pathways, i.e. a sequence of organics consecutively undergoing biodegradation and transformation, coupled with sorption onto soil organic carbon. These coupled processes of advection-dispersion equilibrium partitioning – first-order biodegradation in variably-saturated soil were numerically simulated using the HYDRUS-1D simulator. Organic carbon is one of the most important soil properties influencing sorption and transformation of organic compounds. To account for soil organic carbon depth-dependency and its effect on sorption and biodegradation, a new module was developed in HYDRUS-1D which distributes measurements of organic carbon with depth and updates the sorption and degradation parameters accordingly (i.e. depth-dependent). Simulation results showed that for all chemicals considered in the assessment, the combined effect of generally strong sorption and fast biodegradation resulted in nearly complete removal of all chemicals in the top 5 to 10 cm of the soil profile. These results are true for a broad range of sorption and degradation parameter values derived from a literature survey. This indicates that the risk of bioaccumulation in soil and leaching to groundwater is very small for the conditions of this study, i.e. a small infiltration flux approximately equal to the long-term recharge rate of several tens of mm per year.