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A consistent framework to predict mass fluxes and depletion times for DNAPL contaminations in heterogeneous aquifers under uncertainty

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At many hazardous waste sites and accidental spills, dense non-aqueous phase liquids (DNAPLs) such as TCE, PCE, or TCA have been released into the subsurface. Once a DNAPL is released into the subsurface, it serves as persistent source of dissolved-phase contamination. In chronological order, the DNAPL migrates through the porous medium and penetrates the aquifer, it forms a complex pattern of immobile DNAPL saturation, it dissolves into the groundwater and forms a contaminant plume, and it slowly depletes and bio-degrades in the long-term. In industrial countries the number of such contaminated sites is tremendously high to the point that a ranking from most risky to least risky is advisable. Such a ranking helps to decide whether a site needs to be remediated or may be left to natural attenuation. Both the ranking and the designing of proper remediation or monitoring strategies require a good understanding of the relevant physical processes and their inherent uncertainty. To this end, we conceptualize a probabilistic simulation framework that estimates probability density functions of mass discharge, source depletion time, and critical concentration values at crucial target locations. Furthermore, it supports the inference of contaminant source architectures from arbitrary site data.

As an essential novelty, the mutual dependencies of the key parameters and interacting physical processes are taken into account throughout the whole simulation. In an uncertain and heterogeneous subsurface setting, we identify three key parameter fields: the local velocities, the hydraulic permeabilities and the DNAPL phase saturations. Obviously, these parameters depend on each other during DNAPL infiltration, dissolution and depletion.

In order to highlight the importance of these mutual dependencies and interactions, we present results of several model set ups where we vary the physical and stochastic dependencies of the input parameters and simulated processes. Under these changes, the probability density functions demonstrate strong statistical shifts in their expected values and in their uncertainty. Considering the uncertainties of all key parameters but neglecting their interactions overestimates the output uncertainty. However, consistently using all available physical knowledge when assigning input parameters and simulating all relevant interactions of the involved processes reduces the output uncertainty significantly back down to useful and plausible ranges. When using our framework in an inverse setting, omitting a parameter dependency within a crucial physical process would lead to physical meaningless identified parameters. Thus, we conclude that the additional complexity we propose is both necessary and adequate. Overall, our framework provides a tool for reliable and plausible prediction, risk assessment, and model based decision support for DNAPL contaminated sites.