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Solute dissipation regimes and rates controlled by soil evaporation and rainfall variability in heterogeneous soils

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Reactive solute leaching from the top soil has received wide attention as it relates to major environmental challenges like groundwater and river water pollution by leached reactive solutes such as agricultural pesticides or biochemical pollutants. Adequate understanding of how fast, when and how such solutes and possible contaminants are leached from the top soil is necessary to enhance agricultural practice, pollution risk assessment and overall water quality management. Many empirical studies have been carried on the subject, with varied their approaches and complexity, and have been carried out under different site and atmospheric conditions. Some of such studies argue that properties of soils and solutes are dominant for the leaching process, while others emphasize atmospheric drivers as a main trigger for preferential flow. Long residence times have also been observed, with solutes lingering in the soils long after initially introduced and after experiencing rainfall events. Modelling and analytical studies have been put forward to better explain these behaviours, but often neglecting some of of the sources of complexity (such as preferential flow and soil heterogeneity) or with simplified modelling strategies.

In this work, we study reactive solute dissipation processes in a soil column with a contaminated top soil layer in response to rainfall events. To cope with a heterogeneous soil structure, within an intermediate-complexity and physically-based framework, we solve Richards equation together with a mobile-immobile soil model together with a non-equilibrium advection-diffusion reaction model in Hydrus1D. We perform an extensive analysis of the sensitivity of solute dissipation rates from the top soil in response to all permutations of a parameter space comprised of soil properties (immobile fraction, mobile-immobile mass transfer coefficient), solute properties (decay coefficient, adsorption coefficient), rainfall parameters (total precipitation, duration, frequency) and the presence or absence of evaporation. Results are assessed in terms of the resulting solute dissipation curves and are fitted to exponential decay curves for comparison purposes.

The results show that different solute dissipation regimes exist in response to the dominant physical process under a particular set of conditions. We identify three dissipation regimes which exhibit characteristic time scales and dissipation curve shapes: an advection dominated regime occurring under particular rainfall conditions, an evaporation dominated regime occurring under low rainfall volume and intensity and a decay-dominated regime exists, in which the bio- or chemical- decay rate of the substance is large and therefore dominant. Our results also provide further evidence and rationale for long residence times (which have been previously noted in the literature) in the top soil under preferential flow conditions, as the complex interactions between different processes may favour at mobilisation or immobilisation of the solute, which can be related to the characteristic shapes of the dissipation curves and in turn the regimes.

The results allow a better understanding of the controlling processes and the related parameters interactions that dominate each regime. The thorough sensitivity analysis shows that, within those regimes, certain properties have higher weight and respectively more attention should be given when investigating them in comprehensive leaching risk assessment.