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Numerical modelling of soil/atmosphere exchange of POPs with MIN3P

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Soil/atmosphere exchange processes are of vital role not only for the cycling of water and the transport of nutrients and oxygen, but also for the long-term fate of many persistent organic pollutants (POPs). This study focuses on modelling the vapor phase exchange of a representative POP, i.e. phenanthrene, across the soil/atmosphere interface using the numerical code MIN3P, which was extended to include an atmospheric boundary layer. The numerical code was validated with analytical solutions of the advection-dispersion equation and additionally considering pure diffusion with linear sorption in the porous medium. We ran several scenarios to test the relevant processes influencing soil/atmosphere exchange at various time scales, i.e. diffusion/dispersion, advection, sorption, re-volatilization, biodegradation, and temperature changes. The atmospheric boundary layer near the ground surface was assumed to be well mixed, and overall fluxes of phenanthrene were found to be limited within the soil compartment for downward migration from the atmosphere. Sorption to soil organic carbon causes strong retardation of phenanthrene in seepage water, thus affecting re-volatilization and biodegradation. After phenanthrene deposition, sorption limits the spreading in the short term while biodegradation leads to steady-state concentration profiles in the long term (e.g. centuries). Temperature increases, e.g. from nighttime to daytime, lead to a release of sorbed phenanthrene. While the model shows dynamically fluctuating atmospheric concentration gradients for diurnal temperature changes, eddy diffusion is sufficient to mix concentrations in the atmospheric boundary layer for seasonal and longer-term temperature increases. The model can be further used to estimate levels of other POPs in soils with varying physico-chemical properties and under different environmental loadings and climate scenarios to evaluate their long-term fate in soils.