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Modeling soil gas dynamics in the context of noble gas tracer applications

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Noble gas tracer applications show a particular relevance for the investigation of gas dynamics in the unsaturated zone, but also for a treatment of soil contamination as well as concerning exchange processes between soil and atmosphere. In this context, reliable conclusions require a profound understanding of underlying biogeochemical processes. With regard to noble gas tracer applications, the dynamics of reactive and inert gases in the unsaturated zone is investigated. Based on long-term trends and varying climatic conditions, this is the first study providing general insights concerning the role of unsaturated zone processes. Modeling approaches are applied, in combination with an extensive set of measured soil air composition data from appropriate sampling sites. On the one hand, a simple modeling approach allows to identify processes which predominantly determine inert gas mixing ratios in soil air. On the other hand, the well-proven and sophisticated modeling routine Min3P is applied to describe the measured data by accounting for the complex nature of subsurface gas dynamics. Both measured data and model outcomes indicate a significant deviation of noble gas mixing ratios in soil air from the respective atmospheric values, occurring on seasonal scale. Observed enhancements of noble gas mixing ratios are mainly caused by an advective balancing of depleted sum values of O_2+CO_2, resulting from microbial oxygen depletion in combination with a preferential dissolution of CO_2. A contrary effect, meaning an enhanced sum value of O_2+CO_2, is shown to be induced at very dry conditions due to the different diffusivities of O_2 and CO_2. Soil air composition data show a yearlong mass-dependent fractionation, occurring as a relative enhancement of heavier gas species with respect to lighter ones. The diffusive balancing of concentration gradients between soil air and atmosphere is faster for lighter gas species compared to heavier ones. The rather uniform fractionation is a consequence of the time scale of diffusive transport which is decoupled from the typically stronger fluctuating advective impact.