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Modelling multicomponent soil-gas exchange as a tool for process identification near water saturation

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One-compound Fick diffusion facilitates the assessment of gas exchange within the soil provided that influx and outflux are balanced and the soil is well aerated. The more diffusion in the air-filled pore space is restricted, the more the simplifications of this approach become erroneous and the complexity of multicomponent diffusion processes becomes obvious, e.g. through enrichment of inert compounds or diffusion along inverse concentration gradients. We developed a structural model consisting of an air-filled pore space that has on one side, known gas sources or sinks, and on the other side is connected via a bundle of capillaries to the atmosphere. The capillaries are filled either with air or water. Gas concentrations are iteratively modelled by a combination of a Maxwell-Stefan equation for multicomponent diffusion through the air-filled pore space and one-compound diffusion through the water filled pores. The model yields an equilibrium atmosphere of N_2, O_2, Ar, CO_2, N_2O. Parameters included are porosity, water-filled pore space, respiration rate, respiratory quotient, and production terms of N_2 and N_2O. The modelled atmospheres reveal a high sensitivity to water saturation at high levels of water-filled pore space. Independent from a source/sink term N_2 can be heavily enriched or depleted. With regard to the Ar/N_2 ratio as an indicator of N_2 production the model allows the definition of practical measuring limits. The CO_2 / N_2O ratio reflects the ratio of the source terms. Field data of gas concentrations from soils with different water regimes revealed the same types of ratios that we derived from our model. Although the soil system is extremely simplified in our model, it facilitates the derivation of qualitative indicators of soil exchange processes in subsoils near water saturation. In real soils we expect a mi-

croscopic distribution of pores with unique tortuosity and gas sources as well as a highly variable diffusive distance to the free atmosphere. Using the model to quantify the gas fluxes would require an almost impossible 3-dimensional parametrization of these microscopic structures. However, the modelled concentration ratios could allow the quantification of N_2O sources and sinks or denitrification in relation to probably more easy to quantify fluxes such as soil respiration.