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Modeling denitrification's "memory" of oxygen history, from soil aggregates to landscapes

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Oxygen availability regulates many soil biogeochemical processes, including heterotrophic denitrification. While denitrification is canonically expected in hypoxic to anoxic conditions, transient oxygen exposure can promote later denitrification in some systems. This observed phenomenon is hypothesized to result from oxygen stimulating the breakdown of recalcitrant organic carbon in organic-rich soil aggregates or soil lenses, releasing labile organic carbon to heterotrophic denitrifiers and thereby promoting denitrification when hypoxic to anoxic conditions return. The central aim of this numerical modeling study is to understand how nonlinear, history-dependent feedbacks link transient oxygen exposure to present aggregate-scale carbon pool dynamics and future landscape-scale denitrification rates. To model denitrification's dependence on oxygen history, we develop a multiscale, coupled reactive transport model that parameterizes the reaction term in a landscape-scale advection-dispersion-reaction model through two-way coupling with a PFLOTRAN-based model of aerobic respiration, denitrification, carbon release, and diffusion in individual soil aggregates. This numerical model generates mechanistic insights into the relative effects of each of the interdependent processes hypothesized to drive denitrification hysteresis. For example, a Morris method sensitivity analysis indicates that aggregate-scale nitrate fluxes are more sensitive to transport parameters than reaction terms. Nonetheless, the relative magnitudes of the different reaction rates also affect how aggregate-scale nitrate fluxes respond to bulk oxygen concentrations, which translates to a nonlinear response of batch reactor-scale and landscape-scale denitrification rates to bulk oxygen concentrations. Further differences in nitrate fluxes emerge as the aggregates are transferred among different bulk oxygen conditions over time, or as spatially distributed aggregates at the landscape-scale experience diverse oxygen histories. These modeling results suggest a plausible mechanism for denitrification's dependence on oxygen history, which could motivate a non-Markovian, data-driven approach to landscape-scale predictions of denitrification hysteresis. By linking aggregate-scale dynamics to denitrification rates across length scales, our modeling study (1) proposes a conceptual mechanism to explain how and why the system's memory of transient oxygen exposure could promote later denitrification, (2) evaluates the sensitivity of denitrification rates to underlying processes, and (3) lays the theoretical foundation for embedding the emergent history effects into landscape-scale predictions.