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Image-based model quantification of pore-scale nitrogen diffusion and potential microbial 'dead zones' induced by fertilization application

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Soil microbial communities contribute many ecosystem services including soil structure maintenance, crop synergy, and carbon sequestration. However, it is not fully understood how the health of microbial communities is effected by fertilization at the pore scale. This study investigates the nature of nitrogen (N) transport and reactions at the soil pore scale in order to better understand the influence of soil structure and moisture content on microbial community health. Using X-ray Computed Tomography (XRCT) scans, we reconstructed a microscale description of a dry soil-pore geometry as a computational mesh. Solving two-phase water/air models produced pore-scale water distributions at 15, 30 and 70% water-filled pore volume. The model considers ammonium (NH_4^+), nitrate (NO_3^-) and dissolved organic N (DON), and includes N immobilization, ammonification and nitrification processes, as well as diffusion in soil-solution. We simulated the dissolution of a fertilizer pellet and a pore scale N cycle at the three different water saturation conditions. To aid interpretation of the model results, microbial activity at a range of N concentrations was quantified experimentally using labelled C to infer microbial activity based on CO_2 respiration measurements in bulk soil. The pore-scale model showed that the diffusion and concentration of N in water films is critically dependent upon soil moisture and N species. We predicted that the maximum NH_4^+ and NO_3^- concentrations in soil solution around the pellet under low water saturation conditions (15%) are in the order of $1\text{x}10^3$ and $1\text{x}10^4$ mol m^{-3} respectively (1-10 M), and under higher water saturation conditions (70%) where on the order of $2\text{x}10^2$ and $1\text{x}10^3$ mol m^{-3}, respectively (0.1-1 M). Supporting experimental evidence regarding microbial respiration suggests that these concentrations at the pore-scale would be sufficient to reduce microbial activity in the zone immediately around the fertilizer pellet (ranging from 0.9 to 3.8 mm depending on soil moisture status), causing a major loss of soil biological activity by up to 90%. This model demonstrates the importance of pore-scale processes in regulating N movement in soil with special capability to predict the effects of fertilizers on rhizosphere-scale processes and the root microbiome.