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Mechanistic modelling of soil organic-inorganic carbon dynamics

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Abstract: Soil carbon is the largest terrestrial carbon pool globally, exceeding the carbon stored in the atmosphere, and is therefore central to climate change mitigation. This has driven a large effort in studying soil organic carbon (SOC), aimed at improving our understanding on its composition, decomposition pathways, and response to, and effect on increased atmospheric CO_2. In contrast, soil inorganic carbon (SIC) has received far less attention, attributed to its longer turnover time under natural conditions, more stable inorganic mineral form and prevalence in semi-arid and arid regions. Yet globally, SIC stocks rival those of SOC and, in regions such as Australia, can even exceed them. However, its abiotic nature can be disputed as it appears highly interlinked with organic soil processes. Field and laboratory studies have revealed a range of interactions between SIC and SOC, such as the incorporation of SOC respired carbon in SIC, and the mutual effect on, and response to soil pH. Ignoring SIC will therefore lead to an incomplete understanding of SOC and vice versa. Further, the idea that SIC is stable at short time-scales and therefore contributes little to atmospheric carbon appears outdated. This raises questions on SIC stability, and the potential sensitivity to changing rainfall, temperature and management practices due to climate change and anthropogenic activities. Mechanistic modelling can help to improve our understanding of the drivers behind soil biogeochemical process, thereby revealing the relevance of SIC to atmospheric CO_2 concentration and SIC-SOC interactions over large spatial and temporal scales.

To this end, we developed, calibrated and validated a reaction network, replicating SOC and SIC dynamics under controlled microbially-induced carbonate precipitation (MICP) experiments in four soil columns (San Pablo et al. 2020). The reaction network describes kinetic and equilibrium reactions including microbial growth on organic substrates. Decomposition of yeast extracts, acetate and urea by bacteria provide carbon and nitrogen for microbial growth. The resulting respiration of CO_2 and changes in H^+ concentration drive calcite ($CaCO_3$) precipitation following the injection of Ca^{2+}. The reaction network was tested in the BRTSim solver (Maggi, 2024), hence called the BRTSim-MICPv1 model. BRTSim is a general-purpose solver, describing the main soil biogeochemical processes including the flow of water, gas and energy, advective-dispersive-diffusive transport, chemical kinetics and equilibrium, and microbial composition over space and time.

BRTSim-MICPv1 was able to capture soil hydraulic properties near perfectly (NSE > 0.98, and NRMSD < 4.5%) and showed strong performance for SOC decomposition and calcite precipitation (SIC formation) (NSE > 0.51, and NRMSD < 22.5%). Generally, BRTSim-MICPv1 captured the SIC dynamics from microbially produced CO_2 well and was able to provide valuable insights into the interplay between SIC and SOC. Up to 74% of the injected Ca^{2+} was incorporated into SIC over the duration of the experiments, while nearly all respired carbon, mainly originating from urea degradation, precipitated as SIC. The model accounted for all dissolved inorganic carbon (DIC) species, which was dominated by bicarbonate and CO_2(aq) following neutral to slightly acidic pH. For future research into soil carbon cycling and SIC deposits this reaction network can be coupled with a complete reaction network for soil organic carbon, and deployed at larger scale, in order to investigate how SIC and SOC will change in variable environmental conditions.

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