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# Modelling decomposition, intermolecular protection and physical aggregation based on organic matter quality assessed by 13C-CPMAS-NMR

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Modelling organic matter decomposition is fundamental to predict biogeochemical cycling in terrestrial ecosystems. Current models use C/N or Lignin/N ratios to describe susceptibility to decomposition, or implement separate C pools decaying with different rates, disregarding biomolecular transformations and interactions and their effect on decomposition dynamics. We present a new process-based model of decomposition that includes a description of biomolecular dynamics obtained by 13C-CPMAS NMR spectroscopy. Baseline decay rates for relevant molecular classes and intermolecular protection were calibrated by best fitting of experimental data from leaves of 20 plant species decomposing for 180 days in controlled optimal conditions. The model was validated against field data from leaves of 32 plant species decomposing for 1-year at four sites in Mediterranean ecosystems. Our innovative approach accurately predicted decomposition of a wide range of litters across different climates. Simulations correctly reproduced mass loss data and variations of selected molecular classes both in controlled conditions and in the field, across different plant molecular compositions and environmental conditions. Prediction accuracy emerged from the species-specific partitioning of molecular types and from the representation of intermolecular interactions. The ongoing model implementation and calibration are oriented at representing organic matter dynamics in soil, including processes of interaction between mineral and organic soil fractions as a function of soil texture, physical aggregation of soil organic particles, and physical protection of soil organic matter as a function of aggregate size and abundance. Prospectively, our model shall satisfactorily reproduce C sequestration as resulting from experimental data of soil amended with a range of organic materials with different biomolecular quality, ranging from biochar to crop residues. Further application is also planned based on long-term decomposition datasets from different natural and agro-ecosystems.