



How to adequately represent biological processes in modeling multifunctionality of arable soils

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Abstract

Essential soil functions such as plant productivity, C storage, nutrient cycling and the storage and purification of water all depend on soil biological processes. Given this insight, it is remarkable that in modeling of these soil functions, the various biological actors usually do not play an explicit role. In this review and perspective paper we analyze the state of the art in modeling these soil functions and how biological processes could more adequately be accounted for. We do this for six different biologically driven processes clusters that are key for understanding soil functions, namely i) turnover of soil organic matter, ii) N cycling, iii) P dynamics, iv) biodegradation of contaminants v) plant disease control and vi) soil structure formation. A major conclusion is that the development of models to predict changes in soil functions at the scale of soil profiles (i.e. pedons) should be better rooted in the underlying biological processes that are known to a large extent. This is prerequisite to arrive at the predictive models that we urgently need under current conditions of Global Change.

Keywords Soil biology · Soil functions · Mechanistic modeling · Soil carbon · Soil nitrogen · Soil phosphorous · Soil structure

Introduction

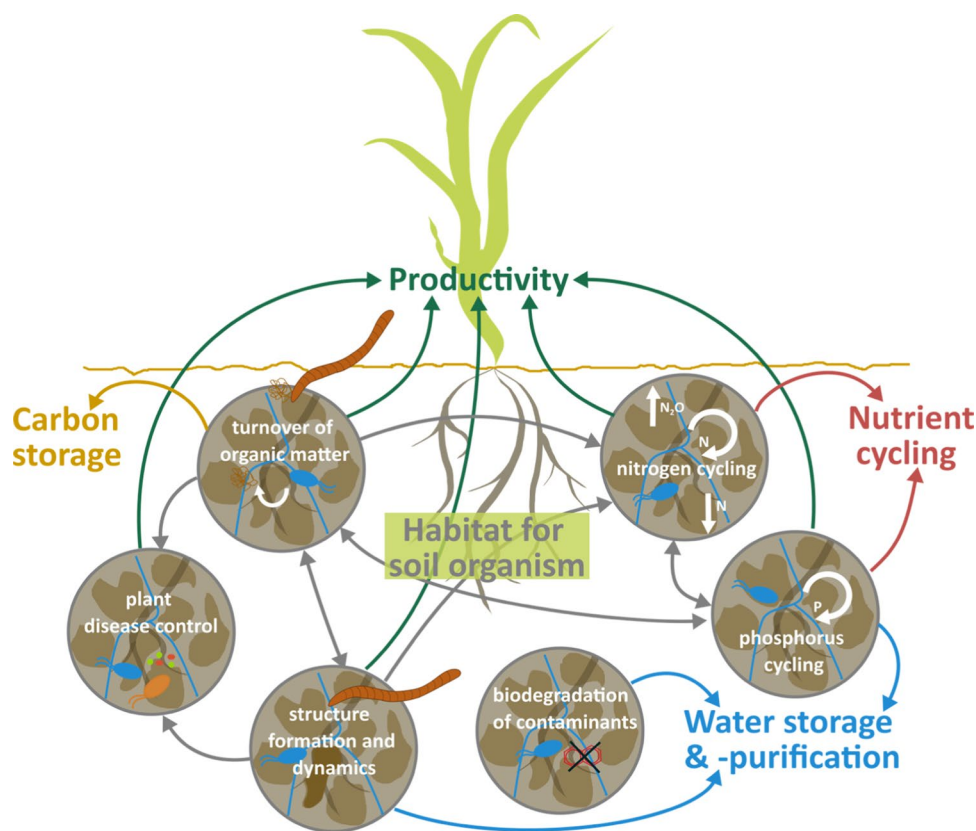
A current challenge in soil science is to understand, model and predict the dynamics of soil functions in response to external forcing brought about by different types of land use in general and by agricultural soil management in particular. In addition, the climatic boundary conditions of our planet are currently changing and this will have a significant impact on the functioning of soils in the future.

Soils are to a large extent biologically driven systems (Gardi and Jeffery 2009; Haygarth and Ritz 2009; Bardgett and van der Putten 2014) and virtually all soil functions that are relevant to the functioning of terrestrial ecosystems depend on biological processes, which, however, are rarely considered explicitly in soil and crop models. A reason for this is certainly the enormous diversity of biological actors and the complexity of their interactions. The five central soil functions that are predominantly biologically controlled are i) plant productivity, ii) water storage and purification, iii) C

storage, iv) nutrient cycling and, finally, v) being the habitat for the biological agents themselves (Fig. 1).

The underlying biological processes are accomplished by a myriad of organisms interacting within complex food webs in a habitat that is highly heterogeneous in terms of its physical and chemical properties. Relevant spatial and temporal scales of these processes span orders of magnitude. This heterogeneity provides a multitude of niches and, thus, allows the establishment of an overwhelming biodiversity in soils (Bardgett 2002; Nielsen et al. 2015). Such niche diversity can lead to the development of a considerable overlap in the contribution of different species to various soil functions, contributing to the functional resilience of soils under highly variable environmental conditions or agricultural soil management. Soil is surprisingly resistant with respect to biological functions such as C turnover (Griffiths et al. 2000). Nevertheless, perturbations due to soil management and/or current shifts in climatic boundary conditions may pass critical thresholds for soil functioning. Therefore, we need models that better reflect the key biological processes and help

Fig. 1 Soil functions and biologically driven process-clusters (circles) that are interconnected and considered to be highly relevant for the soils' capacity to fulfill these functions. The central function "habitat for soil organisms" is relevant for all the process-clusters



to predict critical transitions and shifts in functions under different environmental drivers.

During the last decade, our technical capabilities to identify and characterize the soil biome have increased enormously. Yet, it is not obvious or trivial how this information can be used to gain a more profound understanding of how soil functions may change in response to perturbations caused by agricultural soil management and/or climate change. Our knowledge about the role of soil biodiversity in soil functions is often limited to general principles, while the availability of detailed data regarding site- and species-specific roles is still highly insufficient and still treated as a black box. The present studies on microbial diversity give merely potential indications of soil functions because they are based on the detection and not on the expression of genes.

The dilemma of scale mismatch was recently described by Smercina et al. (2021). They note that biological processes and their interactions can be understood at the scale of the microscopic habitats while measures that quantify soil functions (such as C storage, CO₂ fluxes, cycling of nutrients, degradation of contaminants, filtration of water) are only accessible and relevant at the scale of soil samples much larger than the microscopic habitats, soil horizons, or soil profiles. At this scale the microscopic structure of micro-habitats is typically ignored and hardly accessible.

Also, the soil biome is typically investigated using bulk samples incubated under optimal conditions which masks the underlying structure. For this reason, soil structure and function appear to be disconnected (Smercina et al. 2021).

An open question and an ongoing matter of debate is how and to which level of detail biological processes and interactions can be and need to be represented in models of soil functions (Baveye et al. 2018). Recent examples of explicit modeling of the organisms involved in C stabilization are Romul_Hum (Komarov et al. 2017) and the KEYLINK concept (Deckmyn et al. 2020) that consider soil structure formation and food webs in conjunction. Critical questions are: which taxon-specific details need to be incorporated? How can soil organisms be summarized into functional guilds? Which spatio-temporal scales are relevant to capture biological soil functions? And how to parametrize such biological details? Is it at all possible to account for biological processes and communities without considering their spatial heterogeneity? In a recent review of Pot et al. (2022) the question of relevant scale is clearly challenged while acknowledging the unresolved issue of how to obtain the required data to bridge the scale between microscopic soil architecture and macroscopic functioning.

This problem might be tackled from top down by asking, which and to what extent can complex biological processes be adequately captured or lumped into simplified

process descriptions and how should such simplified models be parameterized? Addressing these questions is a formidable scientific challenge. It relates to upscaling biological processes from detailed interactions at the pore scale to soil functions at the scale of pedons. In this paper we intend to address these questions in a joint effort of empirical soil ecologists and modelers. The required detail and complexity of a model always depends on what is to be modeled. Our focus is on the relevance of biological processes for the dynamics of the five soil functions: productivity, C storage, nutrient cycling, water storage and purification, and being the habitat for soil organisms. What we are aiming for is modeling these soil functions based on an appropriate representation of the underlying biological processes.

We have aggregated the multitude of biological processes that contribute to these functions into six process clusters: i) turnover of organic matter, ii) N cycling, iii) P cycling, iv) biodegradation of contaminants, v) plant disease control, and vi) structure formation and dynamics. The soil functions and the governing biological process clusters are illustrated in Fig. 1.

In the following, we analyze the various biologically driven process-clusters in separate sections. For each process-cluster we discuss the relevant processes that should be either explicitly or implicitly considered in modeling approaches. This is followed by a short review on the state-of-the-art of how these process-clusters are actually represented in modeling approaches. Based on the identified limitations of today's model concepts we then discuss possible ways forward including actual knowledge gaps and data requirements. In the final conclusions we synthesize the results obtained for the different process-clusters towards a systemic modeling of soil functions based on an adequate representation of biological processes.

Organic matter turnover

Soil organic matter (SOM) has an essential role in controlling ecosystem functions. It is of biological origin and closely associated with soil chemical and physical properties (Cotrufo and Lavelle 2022). SOM increases the capacity of soils to sustain food security, and buffer environmental impacts. Soil organisms mediate most of the ecosystem services delivered by soils, and the majority depends on organic matter as substrate. Accordingly, fauna and microorganisms closely interact during SOM formation and turnover. This includes the incorporation of SOM into the mineral soil, litter comminution and mineralization (Frouz 2018), the formation of microbial necromass and the protection of SOM by occlusion within the soil matrix (Wolters 2000).

Biological processes relevant for SOM turnover

Biological processes that are highly relevant for the formation and turnover of SOM are: i) the efficiency by which plant litter, roots and rhizodeposition are decomposed, mainly determined by microbial stoichiometry and C use efficiency and supported by faunal comminution, ii) the priming of stabilized SOM related to the stoichiometry of added C sources, iii) mixing of SOM with and binding to mineral soil, occlusion of particulate organic matter (POM), and spatial collocation of SOM and organisms by bioturbation and physical structure formation affecting SOM accessibility. Models combining all, or including some of these processes would allow to identify the most essential drivers for SOM formation and turnover under specific site conditions. The appropriate scale of such modeling approaches should include macroscopically homogeneous areas in terms of the major structural components such as soil horizons and, if necessary, higher spatial detail in the case of the rhizosphere or the drilosphere.

Microbial stoichiometry and C use efficiency

Microbial **stoichiometry** uses elemental ratios to characterize physiological limits for the incorporation of C and growth-limiting nutrients from substrate inputs into microbial biomass (Sinsabaugh et al. 2009; Marklein and Houlton 2012; Mooshammer et al. 2014b). Depending on stoichiometric relations of mainly C, N and P, the ratios of living microbes, microbial necromass and available C sources may change dynamically (Drake et al. 2013; Buchkowski et al. 2015, 2019). The stoichiometric relations further determine the ratio between C losses through dissimilation and the temporal C assimilation within the microbial biomass, acting as a buffer for soil C and nutrients. Accordingly, the processing of soil C could be derived from stoichiometric considerations. It has been assumed that mineralization of SOC would be most effective when the nutrient demand of the microbes is met (Hessen et al. 2004). However, there is strong evidence that the stoichiometry of microbial biomass in soils behaves homeostatic to the *available* C and nutrients in soil and not to the total C: nutrient pool (Griffiths et al. 2012; Clayton et al. 2021). Consequently, also elevated C mineralization in N-deficient soils has been observed (Hagedorn et al. 2003; Craine et al. 2007), which can be explained by the microbial N mining theory. It assumes that microbes may use labile (i.e. available) C as an energy source for the decomposition of stable SOM, which contains the required N (Craine et al. 2007), so that decomposition of SOM is enhanced at low N supply or, in turn, additional N availability might inhibit the mineralization of previously stable SOC (Craine et al. 2007; Spohn 2015). The underlying processes

may change over time as microbes might compensate for initial limitations in soil N (Meyer et al. 2017).

The C incorporated into microbial biomass is partitioned between **catabolic processes** (respiration) and **anabolic processes** (biomass production) and extracellular expenditures (e.g., production of exoenzymes, extracellular polysaccharides, organic acids). Besides temperature, the substrate C:Nutrient ratio mainly determines the efficiency by which microorganisms convert utilized substrate C into microbial biomass C characterized by CUE, the ‘carbon use efficiency’ (Keiblinger et al. 2010; Manzoni et al. 2012). It is noteworthy that the CUE differs among fungi and bacteria, the main microbial decomposer groups in terrestrial systems, allowing soil fungi to grow more efficiently than bacteria on e.g. plant litter with wide C:N ratio (Malik et al. 2016; Wei et al. 2022). Assuming that with increasing microbial biomass more necromass is produced and subsequently stabilized as mineral-associated organic matter (MAOM), it was postulated that substrate inputs of matching stoichiometric microbial demands favor a high microbial CUE and, consequently, promote a faster replenishment of the stable MAOM pool in soils (Castellano et al. 2015; Buchkowski et al. 2019). In soils with high organic matter content, however, stoichiometric relationships are complicated by the priming effect.

Priming effect, stoichiometric constraints and microbial dormancy

Relatively small inputs of readily available C substrates can both increase or retard the subsequent decomposition of SOM by a phenomenon known as ‘**priming effect**’ (Kuzyakov et al. 2000; van der Wal and De Boer 2017). In agricultural soils the magnitude of priming mainly depends on the C:N ratio of soils and plant litter (Mo et al. 2022; Parajuli et al. 2022). There is a critical transition of microbial C-limitation to nutrient-limitation which is determined by the **threshold elemental ratio** of substrate C:Nutrient (Cherif and Loreau 2007; Mooshammer et al. 2014a). As an approximation, Hodge et al. (2000) calculated stoichiometric requirements for bacteria and fungi in soil and concluded that soil microbes start releasing N below a critical substrate C:N ratio of 12.5 and sequester N above a substrate C:N ratio of 30.3, while at intermediate C:N levels (C:N 12.5–30.3) fungi already release and bacteria still sequester N. In analogy, the turnover of SOM components is expected to be slowed down during nutrient limitation (Kuzyakov and Cheng 2004; Parajuli et al. 2022) while it is accelerated when small amounts of readily available C trigger a disproportional high consumption of less available C (i.e. ‘positive priming’)(Dijkstra and Cheng 2007; Kuzyakov 2010).

The soil microbiome is generally characterized by short periods of growth and longer periods of pure maintenance

and dormancy, so that microbial long-term maintenance requirements prevail over short-term gains during growth phases. Microbial maintenance respiration is given by the specific metabolic quotient (qCO_2), calculated as the ratio of basal respiration to unit biomass C (C_{mic}) (Anderson and Domsch 1985b, a). Stoichiometric mismatch requires higher maintenance respiration (Griffiths et al. 2012; Clayton et al. 2021) and can lead to a gradual decline of soil microbial biomass if C is not constantly supplied (Anderson and Domsch 1985a; Blagodatsky and Richter 1998).

Bioturbation, aggregation and occlusion

Unarguably, soil fauna plays major roles in the fragmentation and comminution of litter and their subsequent incorporation into the mineral soil through **bioturbation** (Anderson 1988; Wilkinson et al. 2009; Filser et al. 2016) mainly accomplished by earthworms. De Wandeler et al. (2016) recently identified specific threshold ratios of forest soil pH ($pH > 4$), litter traits (cellulose content $< 17\%$, LMA $> 16 \text{ cm}^2 \text{ g}^{-1}$) and soil and litter stoichiometry (soil C:N < 12 , litter C:P < 200) that must be attained for earthworms to occur. An indication for the bioturbation capacity of soil fauna is given by data from temperate deciduous forests where earthworms with a biomass of $10 \text{ g dry wt m}^{-2}$ annually translocate the total yearly litter fall of $5 \text{ t dry wt ha}^{-1}$ into the mineral soil (Scheu 1987a; Schaefer and Schauerermann 1990). In comparison, 2–8 g dry wt m^{-2} earthworm biomass were reported from arable fields with integrated management (Didden et al. 1994) while earthworm biomass in temperate meadows may reach $16 \text{ g dry wt m}^{-2}$ (Ellenberg et al. 1986).

Litter consumption and bioturbation are coupled to the occlusion of particulate organic matter (POM) in faecal aggregates (Didden 1990; Marinissen and Didden 1997; Bossuyt et al. 2004, 2006; Bottinelli et al. 2015; Frouz 2018), but it is surprisingly difficult to predict the resulting extent and direction of the impact of soil fauna on SOM turnover (see excellent reviews by Frouz (2018) and Wolters (2000)). This is because two contrary processes are simultaneously affected by the soil fauna. On the one hand, fresh cast materials of earthworms and enchytraeids are hot spots of microbial activity and lead to a transient increase of decomposition rates of SOM (Scheu 1987b; Van Vliet et al. 2004; Frouz et al. 2014), but after drying, aged cast aggregates provide long-term physical protection of occluded POM from further microbial degradation (Scheu and Wolters 1991; Marinissen et al. 1996; Marinissen and Didden 1997; Wolters 2000; Bossuyt et al. 2005). Mechanistically, occlusion of POM in earthworm cast and cross-linking of calcium ions with SOM on negatively charged clay surfaces explains the stabilization of OM in these biogenic soil structures (Shipitalo and Protz 1989). Accordingly, the

balance of mineralization and stabilization determines net-effect of soil fauna on POM formation.

The main feature of mixing processes such as bioturbation is the change of spatial collocation of SOM and microorganisms. Substrates can be adsorbed, occluded or can be brought into closer contact with the microbiome. The potential relevance of the microscopic collocation of substrate and microorganisms for macroscale SOC decomposition was recently demonstrated through numerical experiments by Chakrawal et al. (2020). The net-effect may change along the vertical length of a soil profile. In upper soil layers at high SOM contents and high biological activity both processes might be balanced while in deeper soil layers biological activity is typically concentrated on hot spots such as root and earthworm channels. Some evidence for the vertical stratification of biological processes was provided by Sokol and Bradford (2019) who explicitly differentiated between above-ground or below-ground applications of dissolved organic C (DOC) for the formation of MAOM. DOC inputs into the deeper mineral soil through artificial roots led to high conversion rates of DOC via microbial biomass into MAOM, while above-ground inputs were mostly respired by microbial communities in the litter layer.

State of the art in modeling SOM dynamics

Traditional models associate the build-up and persistence of SOM in soils with the slow degradation of a ‘humified’, recalcitrant’ fraction of SOM. Resulting models on SOM turnover assumed a bipartite SOC pool, with one humified, recalcitrant and thus stable, and a second, i.e. labile SOM pool (Jenkinson et al. 1995; Sollins et al. 1996; Mikutta et al. 2006). However, high decomposition rates of ‘recalcitrant’ organic matter increasingly raised doubt about the traditional assumptions underlying the idea of ‘humification’ through the condensation of large molecules from decomposition products (Hammel 1997; Marschner et al. 2008; Sinsabaugh 2010; Schmidt et al. 2011; Sinsabaugh and Follstad Shah 2011; Guenet et al. 2012). Recent research emphasized microbial residues (i.e., microbial cell wall fragments composed of fatty acids and amino sugars) as main contributors to stable SOM (Joergensen 2018; Liang et al. 2019), while another fraction of fine POM is being stabilized by occlusion within the soil matrix and faunal casts (Angst et al. 2019; Baumert et al. 2021; Witzgall et al. 2021), for details see section on soil structure further below. Together, this led to a radical reconsideration of the build-up and maintenance of SOM stocks (Kindler et al. 2006; Miltner et al. 2012; Kallenbach et al. 2015; Kästner et al. 2021). The persistence of organic matter in soils is now considered to be an emergent property derived from biological processes and the physico-chemical boundary conditions of the

surrounding soil environment (e.g., parent rock material, soil depth, climate) rather than being dependent on the intrinsic chemical properties of SOM itself (Schmidt et al. 2011). Biological processes have thus become central to SOM research, raising the question of how SOM models should adequately represent them (Filser et al. 2016). In modelling, the quality of decomposing organic substrates, which affects the persistence of the SOM, should be taken into account from the point of view of molecular diversity, as this in turn determines the energy expenditure required by the microorganisms to break up the organic matter (Lehmann et al. 2020; Chakrawal et al. 2022).

The recent conceptual framework, formalized as ‘microbial carbon pump’ (Jiao et al. 2010; Liang et al. 2017), assumes that after microbial death, with each iterative turnover of the microbial biomass, a fraction of its necromass (here used as a summary term for microbial residues) is being stabilized by the mineral soil matrix, leading to the gradual accrual of SOM until the mineral soil matrix is saturated (Chenu and Stotzky 2001; Kögel-Knabner et al. 2008; Liang et al. 2017). Though the idea of microbial biomass turnover as a primary driver of SOM formation is not completely new (see for example models by Bosatta and Ågren (1991, 1997)), it finally became generally accepted. Cotrufo et al. (2013) summarized the new evidence in what they termed the ‘microbial efficiency matrix stabilization’ (MEMS) framework. It is based on the two principles that i) soil organic matter (SOM) stabilization mainly occurs through its stable sorption to mineral surfaces and to a lesser extent through occlusion in dense parts of the soil matrix (Six et al. 2002; von Lützow et al. 2007; Kögel-Knabner et al. 2008), and ii) mineral-associated soil organic matter (MAOM) is of microbial origin (Kindler et al. 2006; Simpson et al. 2007; Miltner et al. 2009, 2012; Kallenbach et al. 2015).

Based on findings that the soil clay fraction represents the main reactive mineral surface for the stabilization of microbial residues as reviewed in Kögel-Knabner et al. (2008), Stewart et al. (2007) put forward their ‘soil carbon saturation concept’. They confirmed in a number of successive experiments that a soil’s capacity to retain microbial residues in a stabilized MAOM pool has an upper limit mainly constrained by a soil’s physicochemical characteristics related to clay content and mineralogy, e.g. content of Al and Fe oxides (von Lützow et al. 2006; Gulde et al. 2008; Stewart et al. 2008b, a, 2009; Barré et al. 2014; Doetterl et al. 2015; Angst et al. 2018). Based on this, Castellano et al. (2015) finally proposed a two-pool model, with a protected SOM pool mainly composed of MAOM and to a lesser extent by occlusion of < 20 POM fragments, and a non-protected, potentially accessible SOM pool primarily composed of plant litter inputs.

Accordingly, classical SOM models today, such as RothC (Jenkinson 1990) and CENTURY (Parton et al. 1987), consider these pools (i.e. fresh organic matter, available SOM and stabilized SOM) and rate parameters describing the transition from one pool to the others. Thereby, microbial biomass is part of the available SOM and is not considered explicitly. Conceptually the idea of chemical stabilization was replaced by mechanisms of matrix stabilization (MAOM) and physical occlusion of POM (Hassink et al. 1993; Schmidt et al. 2011; Lehmann and Kleber 2015). Substantial differences between models arise by considering an upper threshold for the saturation of the protected SOM pool (Saidy et al. 2013), while the non-protected SOM pool does not saturate (Stewart et al. 2007; Kimetu et al. 2009; Castellano et al. 2015). However, the limited capacity of soil for MOAM depending on soil texture was recently questioned by Schweizer (2022). Using various chemical imaging techniques, he showed that the distribution of MOAM is patchy and piled up at a minor part of mineral surfaces rather than covering them homogeneously. Thus, the capacity of C sequestration appears decoupled from the extension of mineral surfaces. Recently, several alternative model approaches stemming from experimental data linking soil heterogeneity and pore structure with biologically-driven decomposition (Strong et al. 2004; Ruamps et al. 2011; Kravchenko and Guber 2017) were proposed, extending the basic concept of physical protection of SOM (Balesdent et al. 2000; Pot et al. 2021; Pagel et al. 2020; Mbé et al. 2022).

Models that explicitly describe the dynamics of soil microbial biomass appeared nearly 50 years ago (Parnas 1976), and in recent decades a newer generation of such models (Wieder et al. 2015; Huang et al. 2021; Sulman et al. 2014; Abramoff et al. 2018) became a mainstream in the SOM modeling research. In contrast to models with implicit representation of microbial activity they are capable of describing priming effects, microbial acclimation to temperature change, and respiration pulses caused by drying-rewetting of soil (Lawrence et al. 2009; Allison et al. 2010; Wutzler and Reichstein 2013; Luo et al. 2016). Currently, there is an increased interest in the application of the life strategy theory with the following formalization of the microbial functional properties in the models (e.g. Fierer 2017; Pagel et al. 2020; Ho et al. 2017; Krause et al. 2014). The classical concept of life strategies (Pianka 1970), which considers copiotrophs (fast-growing, low-yield *aka* r-strategists) and oligotrophs (slow-growing, high-yield *aka* K-strategists), was implemented e.g., in the soil biogeochemistry MIMICS model (Wieder et al. 2014). Alternatively, a three-dimensional microbial life strategy approach based on the trade-offs between growth efficiency, resources acquisition and stress tolerance (Malik et al. 2020) of soil microorganisms was applied in the DEMENT model and tested

against experimental data (Allison and Goulde 2017; Wang and Allison 2021).

There are few model concepts linking SOM turnover to the soil food-web and soil structure dynamics. An example is KeyLink, which was recently developed by Deckmyn et al. (2020). It includes the effect of fauna acting as ecosystem engineers, as well as the corresponding effect of soil structural changes on soil hydrology and on the accessibility of SOM or prey to predators. Applied to different test cases, the model predicted i) shifts from a more bacterial dominated to a more fungal dominated system based on input quality, ii) switching from an arbuscular mycorrhizal to an ecto-mycorrhizal dominated system based on N content, and iii) excluding predators or excluding earthworms influences soil hydrology and C content and partitioning (Flores et al. 2021). Overall, KeyLink shows an approach to simulate the linked effects of biopore formation, hydrology, and aggregation on soil functioning. Other models simulate reversible occlusion of SOM by aggregate formation and decay (Segoli et al. 2013; Jha et al. 2023). While the interaction of SOM with mineral surfaces is known as a relevant mechanism process of SOM stabilization, the consideration of aggregates as functional units is not obvious (Vogel et al. 2022). Meurer et al. (2020b) abandoned the idea of building a model based on the concept of single aggregates. Instead, within a dual-porosity framework, changes in SOM alters the total porosity and pore size distribution. In this model, soil structure affects SOM stabilization via slower mineralization rates for SOM stored in the microporous region.

Challenges and missing data

Models of Drake et al. (2013) indicate that root exudate stoichiometry may significantly affect microbial C use efficiency (CUE) and must be given greater consideration. Accordingly, in terrestrial stoichiometric models, where poorly accessible C has been partitioned into MAOM and occluded POM, also the accessible SOM pool must be subdivided into an accessible POM pool containing structural carbohydrates metabolized only after enzymatic degradation, and dissolved, readily available C (DOC) directly disposed for microbial uptake (e.g., root exudates). The incorporation of different pools of C for microbial uptake in SOM models, in particular the dynamic nature of readily available C, which may cause negative or positive priming of soil organic C, is a challenge. A general, critical question is if it is sufficient and appropriate to lump microbial processes into some effective microbial pool while considering stoichiometry and spatial heterogeneity. Or, if this black box needs to be opened and if crucial features must be explicitly addressed such as i) microbial traits related to community composition

that affect CUE and the decomposition rates of SOM, such as copiotrophic/oligotrophic growth strategies, bacterial/fungal ratio, ii) enzymatic activity and enzymes turnover in soil with the description of both abiotic and biotic interactions, (iii) microbial necromass, which eventually can be stabilized as MAOM by organo-mineral associations (Vogel et al. 2014; Kopittke et al. 2020), (iv) spatial representation of microbial energy expenditure for enzyme production vs. energy return as modeled for marine bacteria by Vetter et al. (1998) and discussed in Lehmann et al. (2020), and v) dormancy, a metabolic state far exceeding the short periods of microbial growth.

In particular microbial dormancy can be considered as an alternative modeling concept expanding the model flexibility with respect to simulation of soil microbiome response to substrate limitations or unfavorable environmental conditions. Dividing the total microbial biomass pool into active and dormant microorganisms facilitates the description of SOM and microbial dynamics in terrestrial environments (Joergensen and Wichern 2018), as exemplified in several models that applied this approach (Blagodatsky and Richter 1998; Blagodatsky et al. 2011; Wang et al. 2015; Stolpovsky et al. 2016; König et al. 2020). Recent advances in the experimental methods to distinguish active from dormant microbial biomass in soil based on genomic and transcriptomic community analyses (Bowsher et al. 2019; Alteio et al. 2021), combined with stable isotope probing (Papp et al. 2018), could strengthen the validity of this type of model.

Complex systems describing biological processes, such as SOM formation by microbial activity, typically do not have a single model structure capable of adequately predicting all processes. On the contrary, multiple solutions may be equally successful in describing microbial and SOM dynamics. One advantage should be that these approaches can be tested on data with better parameterisation capabilities. Thus, the recently developed process-based microbial-mineral models were compared with observational data gathered in field manipulation experiments, considering warming effects and long-term detritus input and removal (Sulman et al. 2018). The conclusion was not very encouraging: due to the high variability in the data sets, no clear answer could be given to the advantages of the proposed model structures, as no model was able to capture all observed effects. Sulman et al. (2018) like other authors of similar recent comparative studies (Wieder et al. 2018; Georgiou et al. 2021), concluded, that microbial-based models should be further elaborated. Nevertheless, some conclusions about preferences of specific model features can be drawn after rigorous statistical testing on a wide range of data, as for example in the publication of Abramoff et al. (2022) advancing the Millennium v2 model. There, for example, the authors found that the combination of reverse (for OM depolymerization) and forward (for microbial uptake of DOM) Michaelis–Menten

kinetics was superior to the linear kinetics and equilibrium chemistry approximation (Tang and Riley 2019).

The magnitude of bioturbation may be estimated by earthworm biomass. However, the importance of bioturbation is less apparent in disturbed agricultural systems, like tilled soils, while it is more prominent in perennial systems, such as grasslands, plantations or agroforestry systems (Wachendorf et al. 2020). Therefore, effects on bioturbation may be considered by implementing threshold values above which earthworm activity will considerably change SOM turnover. The dual role of soil fauna, which accelerates decomposition on the one hand, but also enhances occlusion and stabilization of SOM in casts, is a challenge for modeling the net effect of soil fauna on SOM turnover. It also depends on the ecological types of earthworms (Bouché 1977; Lavelle 1988), thus affecting the location of casts along the soil profile.

Conclusions for modeling SOM turnover

In summary, models considering ecological stoichiometry and threshold elemental ratios (e.g. Kyker-Snowman et al. (2020) appear most promising to reflect the biological processes which regulate the turnover of SOM and the conversion of substrate C into microbial biomass, microbial respiration and stabilized C fractions. Considering stoichiometry implies that the dynamics of microbial biomass, including active and dormant pools, need to be an integral part of SOM modeling concepts besides C pools of different quality. Also, such models likely need to be expanded for exceptions, when nutrient mining causes deviations from mere stoichiometric considerations on SOM turnover.

The biological processes leading to the conversion of plant biomass into SOM and its sequestration in the soil profile are determined on the one hand by substrate stoichiometry in concert with clay content and mineralogy. On the other hand, bioturbation determines the contact of SOM with mineral surfaces and the occlusion of particulate organic matter within the soil matrix. These processes should be represented in mechanistic and process-based models to gain predictive power. By considering the mismatch of SOM and microbial stoichiometry the efficiency of substrate use can be predicted. The interaction of the quality of organic inputs (litter, roots, rhizodeposition), stoichiometry, faunal and microbial activity should be considered by implementing threshold values explaining C dynamics in soils under different management. However, these threshold values for different climate and soil conditions remain to be defined. Also, the capacity of soils to stabilize C depending on texture and mineralogy can be readily implemented in models. The impact of mixing processes including diffusion of DOC, however, is by far more challenging because the effects may vary widely between top and subsoils, with

the C-saturation deficit and soil structure dynamics as main differences between both habitats. Thus, spatial interactions along the soil profile deserve by far more attention.

Nitrogen cycling

Agriculture is an important driver of N₂O emissions and N leaching. Both have negative impacts on climate and water quality. Nitrous oxide emissions and nitrate leaching are attributable to farming activities such as reactive N inputs from organic and mineral fertilizers, plant residues and biological N fixation by legumes as well as soil conditions controlling soil N turnover and associated losses into the atmosphere and hydrosphere. N losses to the environment result from the still low N use efficiency of global croplands with only half of the N additions taken up by plants (Dobermann 2005; Lassaletta et al. 2014).

Global human-induced N₂O emissions increased by 30% over the past four decades to 7.3 (4.2–11.4) tera-grams of N per year (Tian et al. 2020b). The recent growth in N₂O emissions exceeds some of the highest projected emission scenarios (Gidden et al. 2019), underscoring the urgency to mitigate N₂O emissions. Additionally, with excessive input of chemical N fertilizers, nitrate N leaching into water bodies is a serious threat for drinking water and biological environments (Wang and Li 2019). Nitrate leaching from different sources and contamination of surface and groundwater with exceeding the threshold of 50 mg L⁻¹ set by the World Health Organization (WHO) is a global phenomenon that has prompted social and political pressure to reduce nitrate leaching and contamination of water bodies (Padilla et al. 2018).

Modeling of N cycling, associated N₂O emissions, nitrate leaching, and assessment of mitigation options from agricultural soils requires a certain degree of complexity. This is particularly true since N₂O emission and nitrate leaching budgets are mainly driven by hot moments (e.g., rewetting, heavy precipitation, freeze–thaw events). These hot moments are still not sufficiently captured by comprehensive field measurements but likely will increase in frequency due to climate change. Also, climate change induced warmer and wetter conditions are expected to enhance soil N turnover and associated emissions into the environment (Griffis et al. 2017).

Nitrogen cycling and atmosphere-biosphere-hydrosphere exchange

Modeling ecosystem N turnover and associated atmosphere-biosphere-hydrosphere exchange of N compounds is extremely complex. This is mainly due to the wide

variety of N forms and spatial and temporal variability of numerous biotic and abiotic processes driving N turnover in soil–plant–microbe systems. Most biogeochemical models consider biotic processes like biological N₂ fixation, ammonification, nitrification, denitrification, microbial immobilization, plant N uptake and plant litter production (Butterbach-Bahl et al. 2013) as well as abiotic processes such as NH₃ volatilization and NO₃ leaching (Chalk and Smith 2020). However, there are large differences in how processes are described, parametrized and linked to environmental controls governing different steps of N turnover in the soil–plant–microbe system. Next to mineralization/ammonification (see section on SOM turnover), aerobic nitrification and anaerobic denitrification are of central importance in biogeochemical models, because these processes regulate soil N availability, competition with plants and N losses into the atmosphere (NO, N₂O, N₂) and hydrosphere (mainly NO₃).

Thereby, the current level of detail of process description does not reflect the wealth of microbial metabolic pathways and their interactions as there are (Butterbach-Bahl et al. 2013):

- heterotrophic nitrification (by fungi or bacteria)
- autotrophic nitrification (two steps: ammonia and nitrite oxidation, one step: complete ammonia oxidation: comammox)
- coupled nitrification–denitrification (production of nitrate by nitrite oxidizers, which is immediately denitrified in situ by denitrifiers)
- nitrifier-denitrification within the same nitrifying microorganism
- denitrification conducted by bacteria capable of using N oxides as alternative electron acceptors under O₂-limiting environmental conditions
- fungal denitrification
- co-denitrification of organic N compounds with NO
- nitrate ammonification or dissimilatory nitrate reduction to ammonium

In addition to the complexity and interaction of different N processes (list above) there can be further complexity originating from different microorganisms driving the same N process but preferring different ecological niches. For example, ammonia oxidation can be performed by ammonia oxidizing archaea and bacteria (Rütting et al. 2021) as well as comammox, i.e. the conversion of ammonia directly to nitrate by a single microbial taxon belonging to *Nitrospira* (Van Kessel et al. 2015; Mehrani et al. 2020). Besides performing similar reactions, they differ in kinetics and preferred environmental conditions such as pH, O₂ and substrate availability. The discovery of comammox bacteria further broadens the environmental niche for nitrification processes,

but also bears the potential to reduce nitrification related N_2O emissions, as comammox bacteria release hydroxylamine, which is only abiotically converted to N_2O , but this happens to a much lower extent than the conversion to N_2O , e.g., via nitrifier-denitrification (Han et al. 2021). Additionally, the impact and drivers of heterotrophic nitrification are still poorly understood. There is increasing evidence of the importance of oxidation of organic N to nitrate especially in croplands (see review from Gao et al. 2023). However, disentangling whether nitrate originates from organic or inorganic sources is still methodologically difficult.

Also, for denitrification, a high diversity exists in terms of genetic capability to produce the respective enzymes controlling actual process rates. Around two third of bacteria have a truncated denitrification pathway (Graf et al. 2014; Lycus et al. 2017), and very often different denitrification steps are performed by different phylogenetic groups and functional genes can be exchanged by horizontal gene transfer. All of these have significant influence on transformation rates, environmental impacts and the predictability of process rates based on the abundance/activity of different functional groups. For example, two clades of nitrous oxide reductase containing bacteria exist, which seem to differ in N_2O affinity (Jones et al. 2014; Yoon et al. 2016) and gained growth yield (Yoon et al. 2016), both of which seem to be higher for clade II *nosZ*, and in response to fertilizer addition (Xu et al. 2020). However, both *nosZ* clades are hampered by pH below 6.5 (Bergaust et al. 2010; Liu et al. 2014), which explains higher N_2O emissions in acidic soils (Šimek and Cooper 2002).

In addition to nitrification and denitrification, the ambivalent role of biological N fixation in terms of a N_2 sink and a NH_4 source is only rudimentary represented. Especially if considering the symbiosis of N_2 fixers with legumes compared to other plant functional groups. Thus, the composition of the plant community can significantly determine soil N input and might directly affect N_2O emissions as symbiotic diazotrophs often exhibit a truncated denitrification pathway (Basaglia et al. 2007; de Diego-Diaz et al. 2018).

Microbiome analyses are more and more advancing our process understanding of soil N cycling and its dependency on the abundance and activity of soil microbes and environmental controls. Nevertheless, current biogeochemical models still lag behind. They generally use more simplified routines especially for describing the dynamic separation and interaction of coexisting nitrification and denitrification and their multiple variants listed above. Even though an increasing number of data are becoming available on actual gross turnover rates of, e.g., mineralization, nitrification and denitrification and its correlation to microbial gene and transcript abundance (Wang et al. 2016), those studies are still low in number and are outcompeted by studies performing net and potential activity measurements, which only reflect

capacities under optimal conditions. Furthermore, these molecular studies often lack representation of the variability at temporal and spatial scales, which is still the main limitation for improved parameterization, calibration and validation of biogeochemical models. A further drawback is that the kinetics (e.g., Michaelis–Menten) of underlying processes of soil N transformation are still mainly based on studies with pure cultures of microorganisms under controlled laboratory conditions. Therefore, it still remains a major challenge to transfer this knowledge to the field scale, where microbial functional gene abundance and N process rates do not necessarily correlate (Duffner et al. 2021). This is mostly caused by the complexity of natural microbial communities and the fact that many studies and models do not distinguish between active, alive, dormant or intact bacterial cells (Ascher et al. 2009; Ceccherini et al. 2009), which might significantly alter the abundance and composition of microbial functional groups (Carini et al. 2016).

Modeling soil N turnover and associated atmosphere-biosphere-hydrosphere exchange by biogeochemical models

Within the past decades, a large number of process models (e.g. DayCent (Parton et al. 2001; Del Grosso et al. 2020), ExpertN (Klier et al. 2011), LandscapeDNDC (Haas et al. 2013; Kraus et al. 2015), DNDC (Li et al. 1992; Li 2000), Daisy (Abrahamsen and Hansen 2000), ECOSSE (Bell et al. 2012), APSIM (Thorburn et al. 2010; Li et al. 2022), FASSET (Chatskikh et al. 2005), NOE (Hénault et al. 2005), WNMM (Li et al. 2007), Coupmodel (Norman et al. 2008)) have been developed for simulating soil N processes and associated N_2O emissions and nitrate leaching. The strengths, limitations and applications of commonly used field-scale N_2O emissions models (e.g., DayCent, DNDC, NLOSS, ecosyss, Expert-N, FASSET, WNMM, and CERES-NOE) have been reviewed by Chen et al. (2008). More recently, Giltrap et al. (2020) reviewed APSIM, DayCent and DNDC. Overall, models can be classified depending on their degree of complexity of descriptions of the main biogeochemical N turnover processes (i.e. mineralization, nitrification, denitrification) and trace gas production, consumption and emission processes.

More simplified models follow the concept of calculating potential N turnover rates, e.g., for nitrification and denitrification which are subsequently modified to actual denitrification rates. This is done by applying a set of reduction factors that depend on actual environmental conditions and N substrate availability, e.g., conceptually introduced with the “hole in the pipe model” (Firestone and Davidson 1989) with N substrate passing through the pipe and N_2O emission released through holes which size are controlled by environmental conditions such as soil temperature, moisture, pH.

These reduction functions are often semi-empirical, derived from field and laboratory experiments, thereby lumping together different driving factors for microbial processes but do not explicitly consider growth and death of microbial biomass and subsequent enzymatic steps of denitrification.

Thus, in simpler models (e.g. DayCent, Apsim) microbial impacts are implicitly represented by assuming that, e.g., denitrifier activity is correlated with environmental conditions such as soil NO_3 concentration, water content (Del Grosso et al. 2020) and the fraction of N_2O produced from denitrification described as a fraction of the total denitrification flux (NO , N_2O , N_2). Therefore, these models may be used to reasonably predict the seasonal or annual pattern of N trace gas emissions and leaching from soils for a given site, while their capability for higher temporal resolution (e.g., sub-daily) and transferability to other sites is generally poor (Butterbach-Bahl et al. 2013).

Among environmental drivers, soil moisture plays a crucial role since it controls together with soil physical properties (soil texture and porosity) the diffusion of oxygen into the soil. The availability of oxygen is of decisive importance as main control for the contribution of aerobic nitrification and the onset of mostly anaerobic denitrification processes, the latter stepwise reducing oxidized N compounds to N_2O and N_2 . The central role of the soil oxygen status for controlling N turnover via nitrification and/or denitrification has been acknowledged and has led to more explicit descriptions of soil hydrology and soil gas transport mechanisms in complex ecosystem N cycling models (Butterbach-Bahl et al. 2013). A more detailed description of oxygen diffusion and consumption processes during decomposition of SOM (as discussed above) allows the estimation of the oxygen concentration in a given soil layer which is subsequently used as proxy to dynamically divide the soil into coexisting aerobic and anaerobic microsites, e.g., represented by the anaerobic volume concept (e.g., in DNDC, LandscapeDNDC and the Coupmodel). The explicit consideration of gas diffusion also for N trace gases allows to simulate emissions into the atmosphere based not only on production but also on transport and consumption processes. For example, NO or N_2O produced by nitrification can in the next time step either be consumed by denitrification or diffuse to the next soil layer before gases are finally emitted to the atmosphere. In APSIM and DayCent N_2O production equals N_2O emission into the atmosphere, irrespective of the soil depth where N_2O is produced. Nitrous oxide consumption is considered in the version of APSIM modified by Xing et al. (2011), DNDC, FASSET and WNMM, while other models do not consider a consumption of N_2O via denitrification (Xing et al. 2023).

The well-documented, high short-term dynamics of N transformation and associated episodic N_2O emission and nitrate leaching are driven by temporally and spatially dynamic complex interactions of microbiological, plant and

physico-chemical processes. To simulate such events, more complex, diffusion-based models may need to include and better describe microbial abundance and activity of particular groups involved in different nitrification and denitrification steps and the respective activity dynamics by simulating the sequential biochemical reactions of nitrification and denitrification. Thus, more detailed models (e.g., DNDC, Coupmodel, LandscapeDNDC) simulate the full denitrification enzyme chain ($\text{NO}_3\text{-NO}_2\text{-NO-N}_2\text{O-N}_2$) with the relative intensity of each step originating from the respective abundance and activity of the soil microbiome, as controlled by oxygen concentration (O_2) or redox potential (E_h), soil moisture, temperature, pH, concentration of N oxides and dissolved organic C (DOC). In this respect, soil microbial analysis linked to environmental controls and turnover rates can play a crucial role, but still are underrepresented with respect to spatial and temporal coverage of measurements.

Measurements of N_2O fluxes report net emissions without attributing the N_2O production to the most relevant microbial processes of nitrification and denitrification. Recent advances in stable isotope techniques have highlighted the contributions of various microbial groups to N_2O emission from soil. These include both enrichment and natural abundance (^{18}O , ^{15}N , site preference) approaches (Baggs 2008). While the total ^{15}N content of N_2O is reported as bulk ^{15}N content ($\delta^{15}\text{N}_{\text{bulk}}$), the predominance for ^{15}N substitution in the central position is reported as site preference (Toyoda and Yoshida 1999). Enrichment approaches have been used in fertilized systems, allowing the quantification of N_2O and N_2 produced during nitrification and denitrification following, e.g., addition of $^{15}\text{N-NH}_4$ and/or $^{15}\text{N-NO}_3$ to soil (Bateman and Baggs 2005; Mathieu et al. 2006). While most of these analyses were carried out on mass spectrometers and are low in temporal resolution, more recently continuous measurements on the $\delta^{15}\text{N}$ and site preference (central or outer position of ^{15}N) have been established, the latter even allowing for source partitioning between N_2O originating from nitrification and denitrification processes (Ibraim et al. 2019, 2020). Currently, in all models N_2O emissions from nitrification are calculated by an emission factor (EF) applied to gross N turnover rates. However, there is only scarce data and mostly from pure cultures available how this EF varies depending on environmental conditions. Overall, studies report a wide range of the EF from 0.006 to 29.4% with a median value of 0.19% (Inatomi et al. 2019). As reported by Xing et al. (2023) the EF is a constant in APSIM, DayCent and DNDC (Li 2000; Parton et al. 2001; Thorburn et al. 2010) while it is varied by soil moisture in NOE (Khalil et al. 2004), and by temperature and soil moisture in FASSET and WNMM (Chatskikh et al. 2005; Li et al. 2007).

Using the potential of emerging stable isotope data, process-based biogeochemical models were recently extended

such as LandscapeDNDC by SIMONE, an external ^{15}N isotope module, which can be applied for simulation of soil and plant natural abundance signatures and for following ^{15}N tracer applications in the soil–plant–microbe system (Denk et al. 2019). In addition to full ecosystem models, conceptual tools such as Ntrace have been developed for the analysis of emerging experimentally based ^{15}N tracing datasets to quantify simultaneous gross N transformation rates in terrestrial ecosystems (Jansen-Willems et al. 2022). This numerical analysis must account for simultaneous dilution and enrichment of ^{15}N pools and has the potential to quantify not only gross production and consumption rates, but also pathway-specific rates, such as the split between autotrophic and heterotrophic nitrification (Gao et al. 2022). In this way, this analysis can provide important information and guidance on how to refine N transformation processes in often less complex ecosystem models.

Requirements to further advance our understanding and description of N turnover in soils

Overall, the limited availability of detailed spatial and temporal representative measurements as compared with the complexity of simulated ecosystem N processes is a general problem for the calibration and validation of mechanistic biogeochemical models (Del Grosso et al. 2020). Although oxygen (O_2) is accepted as a key controlling factor of nitrification/ denitrification by the modeling community, soil moisture content is still mostly used as a proxy for controlling soil N turnover. Using oxygen instead of water content as critical model parameter has a high potential to improve simulation of co-occurring nitrification and denitrification processes and respective enzyme steps. Oxygen concentration could be also key for improved simulation of C and N decomposition, respectively. However, up to now there are hardly any measurements of soil oxygen concentration available and concentrations may vary significantly at smaller scale (Rohe et al. 2021). However, simulation of soil moisture and likely soil oxygen concentration can be biased since models are too simplistic and often fail in correctly representing root development and associated N and water uptake, respiration and root exudation in the soil profile over time. Thus, better description of the rhizosphere has a high potential to improve also simulation of soil N cycling and associated N trace gas emission (Uksa et al. 2014). Next to biological dependencies, improved representation of soil structure (see later) plays a further key role in simulating diffusion of atmospheric O_2 into the soil and associated occurrence of anaerobic microsites. As denitrification can be C limited at elevated nitrate concentration, which can be a particular feature of arable soils, explicit description of soil DOC dynamics (as already discussed) would allow for better stoichiometry dependent representation of denitrification.

Overall, soil microbial DNA and RNA indicators may have the potential for improved parameterization of respective enzyme steps of nitrification and denitrification as well as biological N fixation. Though studies reveal significant relations of N process rates and fluxes with the abundance and/or activity of microbes, still the translation into model process description is hampered due to the lack of measurements with the desired spatial and temporal resolution. It is particularly difficult to quantify the activity of certain functional groups (e.g. RNA level) under *in-situ* field conditions. On transcription level, there would be the need for incubation experiments under controlled conditions to understand which key microorganisms are key drivers of N cycling processes under which conditions, and if pure abundance is correlated to activity or not. Under the assumption that intact bacterial cells are able to quickly adapt to changing environmental conditions, the use of techniques which discriminate relic DNA might be a good compromise (Carini et al. 2016; Schulze-Makuch et al. 2018). Using total microbial biomass as proxy for microbial processes is difficult or would result in low precision, because bacteria and archaea strongly differ in their physiology and functional diversity. In particular the diversity of nitrifying microbes is very low compared to denitrifiers, thus their correlation with microbial biomass is weak. While nitrification is an essential process for nitrifiers to gain energy, denitrification in soil is often facultative and only occurs under specific conditions when aerobic respiration is not possible.

Multi-disciplinary field studies linking environmental controls (e.g., O_2 concentration, DOC, organic and inorganic N concentration), nitrification and denitrification gene abundances and expressions and fluxes including ^{15}N stable isotope based N_2O source partitioning (Ibraim et al. 2020) have the potential for advanced calibration and validation of N cycling processes. Considering that N losses such as N_2O emissions and nitrate leaching are eventful, it would be also important to focus more on hot moments and extreme events, e.g., storms, high soil moisture, rewetting after drought, and freeze–thaw events.

Phosphorus cycling

Phosphorous (P) makes up about 0.2% of plant dry biomass (Schachtman et al. 1998). It is an important macronutrient element since it is a component of key molecules like for example ATP, which plays a key role in photosynthetic activity. A major function of agricultural soils is thus the supply of P for crop growth. According to (Turner et al. 2013) up to 40%, and according to Schachtman et al. (1998) between 20 to 80% of soil P is bound organically and thus not immediately available for plants. The mineralization of organically bound P involves processes that

are mainly driven by soil organisms and therefore involves a multitude of biological processes and biochemical reactions (e.g. Bünemann 2015). The biologically driven processes of nutrient cycling, especially the connected transformations of N- and P-compounds, has been increasingly better understood in recent years, which opens up new ways for abstraction and modeling. This section provides an overview of models of P cycling and summarizes recent developments in the process understanding of direct biotic effects on P mobilization,—transfer, -uptake, and -storage and indirect biotic effects via alterations of physical soil parameters and transport pathways. Finally, knowledge gaps and missing process understanding are highlighted, pointing to research needs for better modeling approaches.

Biological processes in P cycling

Biological processes in P cycling in soil have a much smaller dimension compared, e.g., to N cycling, caused by the predominating abiotic controls, such as mineral composition (e.g., Ganta et al. 2021a, b; Gypser et al. 2021; Siebers et al. 2021), soil pH (e.g., Ahmed et al. 2020) and redox status (Shaheen et al. 2022). Nevertheless, biotic P cycling in soils is essential for the phosphate supply to soil microorganisms and terrestrial plants because of their limited direct access to phosphate from the soil solution. Processes summarized as “biotic P cycling in soil” comprise mobilization (solubilization and mineralization), transfer and uptake by microorganisms and plants, and indirect effects through changes in soil physical properties. Such biological soil P processes are involved in directly controlling P leaching by storing a labile P pool (temporal immobilization) and indirectly through the biotic impact on relevant soil physical properties (e.g., soil structure stabilization, biopores) which greatly affect the soil solution movement. These processes are discussed in more detail in the following paragraphs.

Biotic phosphate mobilization

Since the concentration of plant-available P in the soil solution is generally low, biotic phosphate mobilization is essential for soil microorganisms and plants. In case of very large C:P ratios in SOM, the microbial P demand may lead to immobilization and temporary binding of P in organic compounds (as discussed above for microbial stoichiometry). Under such conditions, microbes take up phosphate from the soil solution, which subsequently can be remineralized. Many isotopic studies have quantified microbial turnover rates of organic P and P bound in the microbial biomass as summarized in the review by Bünemann (2015). Several studies stress the relevance of the amount of soil microbiome

(e.g., Stewart and Tiessen 1987; Liebisch et al. 2014) as the microbes represent a sort of bottleneck where all organic P must pass through in the mineralization process. On the other hand, Spohn and Kuzyakov (2013) found evidence that P mineralization is driven by the demand for C, i.e., the microorganisms most abundant in the rhizosphere feed on phosphorylated organic compounds, but do not incorporate the P. Root C exudates stimulate organic P mineralization by associated non-mycorrhizal microorganisms, which again increases mineral P availability to plants (Hinsinger 2001). Here, the structure and C:N:P-stoichiometry of exudates determine the strength and stimulation of P mineralization (Spohn et al. 2013). However, the site-specific bacterial potential for P mobilization was assumed to be relatively stable independent of C input by fertilization (Grafe et al. 2018). Recently, it was indicated that oligotrophic bacteria play a pivotal role in the early phase of litter decomposition, but oligotrophic bacteria dominate sites with low bacterial diversity (Chiba et al. 2021). Mixed intercropping of plant species can promote the phosphate solubilizing bacteria in roots and rhizosphere (Koczorski et al. 2022). Ongoing research is directed to select soil microorganisms that are highly capable of mobilizing phosphate (Chiba et al. 2022), which potentially can be applied to new P recycling products such as bone char.

Biotic phosphate transfer

Fungal hyphae in general and especially symbiotic associations between plants and mycorrhizal fungi are leading controls of the phosphate transfer from soil to plants (Behie and Bidochka 2014). Over 90% of all plant species form symbioses with fungi (Bonfante and Genre 2010) and more than 70% of the total P uptake of the host plant can be provided by the transfer of associated fungal partners (Smith et al. 2011; Yang et al. 2012). The mutualistic exchange of C from the crop in return for P can increase P uptake by a factor of 3 to 5 (Schachtman et al. 1998). The utilization of mycorrhizal symbioses was assumed to be one of the most promising options for developing resource-saving and sustainable agricultural systems (Kobae 2019). Mycorrhizal fungi link the topsoil with the subsoil and contribute therefore to a reduced need and more efficient use of fertilizers (Sosa-Hernández et al. 2019).

Endophytic fungi, like, e.g., *Piriformospora indica*, can be also highly capable of phosphate transfer to plants (Yadav et al. 2010). Recently, it was demonstrated that the fungal contribution to the P cycling can be promoted by increased vegetation diversity using, e.g., tolerance of weeds (Zacher et al. 2021), catch crops in the rotation (Vitow et al. 2021), or mixed growth of different plant genotypes (Baum et al. 2018; Shaheen et al. 2022).

Biotic phosphate uptake and storage

The P uptake by plants is the dominating biotic process, driven by a diffusive mechanism since the concentration of plant-available P in the pore water is low but the inorganic P concentration in the root cytoplasm is high and the plant membrane potential is characteristically negative. Thus, an energized transport across the plasma membrane is required, presumably a cotransport with one or more protons (Schachtman et al. 1998). Between pH 6.5 and 7.5 dihydrogen phosphate is the dominating P form, which is preferably taken up by plant roots since, in relation to other P species, the lowest amount of energy is required for uptake. The diffusive root uptake is generally limited by a rather low diffusion coefficient of phosphate in water of about $0.036 \text{ cm}^2 \text{ h}^{-1}$ (Kirk 1999).

The microbial biomass is an important storage pool that can account for 2 to 6% of the total P in the topsoil of arable sites (Peine et al. 2019). With respect to the plant-available P in soils, up to 20% can be stored in the biomass of mycorrhizal fungi (Hou et al. 2021). In the case of P limitation, a dynamic response of root architecture was observed, where growing root tips sense sites of low local mineral P availability. The response was a reduction of meristematic activity and cell elongation at low P sites and an increased growth of root hairs and lateral roots, compensating for the limited P uptake by an enlarged absorptive surface (Hoehenwarter et al. 2016). Further, crops can also adaptively respond to P limitation by conservation and remobilization of internal P resources, e.g., by reusing P from phospholipids (Lin et al. 2014). This may cause a marginal P starvation having no or very limited effect on crop growth. Furthermore, P limitation promotes enzymatic P mobilization in the rhizosphere (Tarafdar and Jungk 1987), mycorrhiza formation in host plants (Peine et al. 2019), and plant recruitment of fungi and bacteria in the rhizosphere of non-mycorrhizal hosts (Zuccaro 2020).

Stoichiometry

Microorganisms have the potential to control the induction or repression of genes coding enzymes that catalyze different processes in P, N, and C mobilization, uptake, and storage (Santos-Beneit 2015). However, to do so, they need a stable intracellular nutrient stoichiometry explaining a stable microbial C:N:P ratio of about 60:7:1 on the global scale (Cleveland and Liptzin 2007; Griffiths et al. 2012). There is a cross talk of P, N, and/or C metabolisms (McGill and Cole 1981; Peng et al. 2022). For example, excess P can cause the expression of genes involved in urea degradation, repression of glutamine synthesis, ammonium uptake, or the inhibition

of gluconeogenesis and glycogen catabolism (Ljungdahl and Daignan-Fornier 2012). Under inorganic P and C limitations the expression of the *ugp* operon in *Escherichia coli* is induced, being involved in utilizing glycerol-3-phosphate and glycerophosphodiester (Kasahara et al. 1991; Robichon et al. 2000; Rodriguez et al. 2020). Thus, a change might occur from a limitation of energy (C) to a limitation of P and N depending on the C:N:P ratio of the surrounding, e.g., fertilizers, organic matter, or soils (Allison 2012; Kaiser et al. 2014; Zechmeister-Boltenstern et al. 2015).

The C:N:P stoichiometry of system compartments (i.e., fertilizers, SOM, microorganisms) is mainly not considered in the models reviewed in this chapter. An exception to this is SWAT that also considers the C:N and C:P ratios of the fresh residue organic P pool to estimate the mineralization and decomposition rates.

Indirect biotic effects by soil physical impact

SOM interacts with mineral surfaces. There are a number of different binding forces that increase the mechanical stability of soil structure (Totsche et al. 2018). The resulting organic-mineral associations are composed of phyllosilicates, Fe-(hydr)oxides, remnants of microbes and other organic molecules from soil solution, where especially the pedogenic oxides are important P binding partners. As a consequence of the heterogeneous binding forces, soil disintegrates into aggregates of different size and stability when exposed to mechanical loads (Díaz-Zorita et al. 2002). Smaller aggregates are more stable and include smaller pores which results in a lower accessibility for microorganisms and enzymes, also resulting in a slowed down P turnover (Siebers et al. 2018). Changes or disturbance of soil structure by tillage or natural soil processes can lead to the release of mobile soil colloids known to be carriers for P (Gottselig et al. 2017) and thus affect P pool dynamics (e.g., Siebers and Kruse 2019; Baumann et al. 2020). This is the same process as discussed earlier for the physical protection of SOM.

The contribution of colloidal P transport in nutrient cycling is still scarcely explored. Fine colloids (<450 nm) are highly mobile in soils and the colloid-facilitated transport of elements is highly dynamic as the transport is closely connected to water movement in soil (Koch et al. 2019). Thus, losses of nutrient elements due to particulate transport are a rising concern, especially for P (Siebers et al. 2023). Even though colloidal transport has been intensively studied over the last decades (e.g. DeNovio et al. 2004; Wang et al. 2020), there is still a lack of understanding processes and transport pathways of natural soil colloids with different chemical compositions and characteristics under changing soil water contents (Wang et al. 2020).

State-of-the-art in modeling P cycling

In modeling N cycling, single species like ammonia or nitrate concentrations are accounted for, whereas for the P cycle, only overall mineral P concentrations are simulated, usually grouped in mineral P pools. The reason behind this is the diverse species composition, mainly driven by soil pH, of about 170 mineral P species (Holford 1997). This also explains that in many models the sorption behavior

is not simulated with a classical sorption isotherm involving a partition coefficient, but with one or more pools of sorbed mineral P, often characterized by a sorption kinetic with fast sorption and slower desorption. An in-depth discussion of P sorption modeling approaches is provided in the review by Lewis and McGechan (2002).

The present review considers the following P models: APSIM-SoilP, DSSAT, 2D_CycP, ANIMO, APEX, APLE, DAYCENT, EPIC, GLEAMS, RZWQM2-P, SWAT,

Table 1 Overview of models for P transformation and transport processes in soil

#	Model	Full name	Mineral P		Organic P			Plant P uptake	
			Sorption	Total pools	Pools	Link to C/N	Immob	Demand	Stress
1	APSIM-SoilP	Agricultural Production Systems Simulator	1 pool; unavailable	2	4	yes	yes	organ-specific	yes
2	DSSAT	Decision Support System for Agrotechnology Transfer	2 pools, reverse rates differ	3	5	yes	yes	organ-specific	yes
3	2D-CycP	-	Freundlich	2	2	no	no	organ-specific	no
4	ANIMO	Agricultural Nitrogen MOdel	2 pools + precipitated pool	4	4	yes	yes	grassland or arable	yes
5	APEX	Agricultural Policy/Environmental eXtender	2 pools, reverse rate 0.1	3	2	no	no	entire plant	yes
6	APLE	Annual P loss estimator	2 pools, reverse rate 0.1	3	1	no	no	user-specified	no
7	DAYCENT	-	2 pools + occl. + weathering	5	5	yes	yes	shoot and root	yes
8	EPIC	Environmental Policy Integrated Climate	2 pools, reverse rate = sorp rate	3	2	no	no	entire plant	no
9	GLEAMS	Groundwater Loading Effects on Agricultural Management Systems	2 pools, reverse rate 0.1	3	2	no	no	entire plant	yes
10	RZWQM2-P	Root Zone Water Quality Model 2	2 pools, reverse rate 0.1	3	2	yes	no	organ-specific	yes
11	SWAT	Soil and Water Assessment Tool	2 pools, reverse rate 0.1	3	3	yes	yes	entire plant	yes
12	Hydrus-1d	-	Linear	-	-	no	no	user-specified	no
13	MACRO	-	Freundlich	-	-	-	-	user-specified	yes
#	C:N:P	Exports				Unsaturated	Time step	Reference	
	Stoichiom	Leaching	Runoff	Tile drains	Particulate	Transport			
1	no	no	no	no	no	no	day	Delve et al. (2009)	
2	no	no	no	no	no	no	day	Dzotsi et al. (2010)	
3	no	yes	yes	no	no	no	year	Li et al. (2019)	
4	no	yes	yes	yes	no	CDE	day or week	Groenendijk and Kroes (1999)	
5	no	yes	yes	yes	yes for runoff	Convective	day	Williams and Izaurrealde (2005)	
6	no	yes	yes	no	yes (sediment)	yes, empirical	year	Vadas et al. (2012)	
7	C:N	yes	yes	no	erosion	no	day	Parton et al. (1998)	
8	no	yes	yes	yes	no	no	day	Wang et al. (2022)	
9	no	yes	yes	no	Yes (sediment)	Convective	day	Knisel et al. (1993)	
10	C:N	yes	yes	yes	yes	no	day	Sadhukhan et al. (2019)	
11	yes	yes, at 10 mm	yes	no	yes for runoff	no	day	Chaubey et al. (2007)	
12	no	yes	no	yes	yes (colloidal)	dual-permeability	day	Gupta et al. (2021)	
13	no	yes	no	yes	yes	CDE also particulate	< hour day	McGechan et al. (2002)	

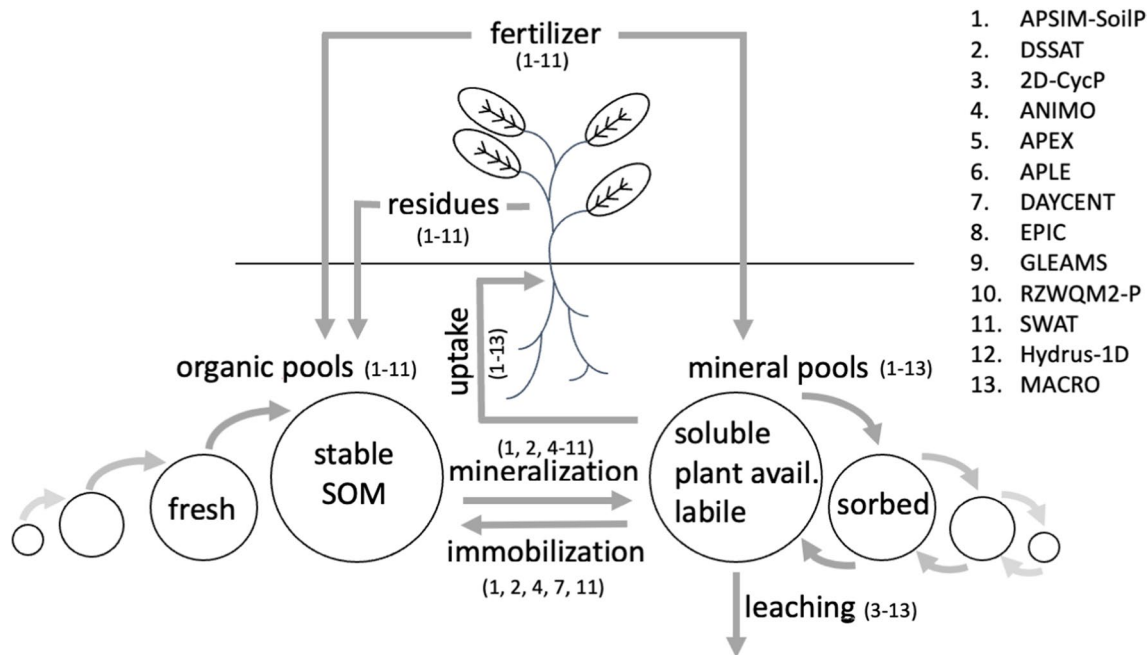


Fig. 2 Main processes and pools (circular shape) of the P cycle implemented in models (1. to 13.) reviewed in the present study. The numbers at the processes represent the models that consider these processes (see Table 1)

Hydrus-1D, and MACRO. References and full names are given in Table 1, where rather the most recent application than the paper describing the original model development are cited.

Most basic P cycling concepts have common features (Fig. 2). Almost all models account for mineral and organic P fertilization, plant root uptake, one or more organic P pools, and one or more mineral P pools. The organic P pools often comprise at least one pool for fresh organic P with a fast turnover and one with a slower turnover, usually referred to as humic material or humus. The mineralization of organic material always feeds the mineral P pools. In all model concepts, one of the mineral P pools is characterized as either soluble P, plant-available P, or labile P. This always represents the P pool available for plants and from which P can be leached. Many of the models do not account for the convective/dispersive unsaturated transport of P (e.g., APSIM-SoilP, 2D-CycP, APLE, DSSAT, DAYCENT or EPIC). However, they do account for the leaching of P (see Table 1), which can be achieved by implementing an empirical approach. For example, the APLE model estimates the leachate/precipitation ratio from a log-linear regression with soil layer depth. Almost all models referenced in this review account for a demand-driven P uptake by crop roots. This demand can either be specified by a dynamic crop growth module or be user-specified. Further, this demand can either be specific to the entire plant (e.g., by APEX, EPIC, GLEAMS, and SWAT) or it can even be

organ-specific, which holds for the APSIM-SoilP, DSSAT, 2D-CycP, and RZWQM2-P model. The advantage of a dynamic growth simulation, as implemented in the models with a crop production background like APSIM-SoilP, DSSAT, and ANIMO, is that feedbacks between P uptake limitation and crop growth are reproduced and crop harvest/biomass P measurements are not required inevitably like, e.g., for APLE.

The simulation of the feedback from P stress to crop growth is very diverse. All the models discussed in this section differ with respect to the algorithm estimating how limited P availability affects crop growth. Model disparities could also be stated for the transport of particle-bound P, either through the soil profile (McGechan et al. 2002) or in runoff (Table 1). General P loss via runoff or tile drains is often accounted for (e.g., by RZWQM2-P and SWAT), which largely depends on how detailed hydrological fluxes are generally reproduced by the model (Radcliffe et al. 2015). Currently, there is a lack of process implementation, especially for colloidal P transport which, if at all, is mainly considered under constant flow conditions in P models. However, especially the transient flow is of importance, by resembling more closely the wetting and drying of natural soils in response to rainfall, snowmelt, or irrigation events being mainly responsible for colloid mobilization (Cheng and Saiers 2010). A special model group comprises the two solute transport models MACRO and Hydrus-1d. Both models were originally not designed to be used for the simulation

of the P cycle, however with some unconventional use of methods already implemented in the solute transport models, they can be used. For example, the root uptake of P missing in MACRO can e.g. be mimicked with a contaminant decomposition rate (McGechan et al. 2002). Even though MACRO and Hydrus-1d have some gaps in the P cycle as the organic P part and mineralization/immobilization are completely missing (Lewis and McGechan 2002; Gupta et al. 2021) the strength of both models is to capture the dual-domain transport of particle-bound P and dissolved P, and the less conceptual description of physicochemical sorption with a Freundlich isotherm. Depending on the model target, this represents a valid approach.

An interesting timeline for the mineral P sorption/desorption pools was observed. Out of the ten models that apply a pool concept instead of a physicochemical sorption isotherm, seven models are based on a 3-pool concept (Table 1), comprising one labile pool and two sorption pools, namely active and stable. This approach was suggested by Jones et al. (1984) and was originally implemented in the EPIC model, a precursor of the CREAMS model, which again is a precursor of GLEAMS. Only ANIMO, APSIM-SoilP, and DAYCENT are based on their own original mineral sorption pool concept.

How well are biological processes of P turnover already represented in model approaches and what should be improved?

The models accounting for organic P turnover consider one (APLE) to five (DAYCENT) organic pools. Each pool is characterized by an optimum decomposition rate constant, which is scaled with rate modifiers for soil temperature and soil water content, except for the APLE approach. Some of the organic pool cycling concepts take microbial biomass P into account, but only in the sense that organic P is stored in the microbes without having a functional effect on the partitioning or the decomposition rate of the other organic P pools. An example for this is the DAYCENT active organic P pool, which comprises the organic biomass P (Parton et al. 1998). This demonstrates the close link between the turnover of organic P and the turnover and organic C and N. Some models recently include microbial C pools regulating turnover through the production of extracellular enzymes, which increases the decomposition rates of SOM (Buchkowski et al. 2015). Using priming experiments Blagodatsky et al. (2010) developed and successfully tested a model explicitly including the effect of microbial biomass C. While such an approach may improve C turnover model performance under field conditions, it remains unclear, however, if this is also true for organic P turnover. Generally, considering the stoichiometric link between organic P and organic C and N is highly relevant, since P may limit microbial growth and mineralization and immobilization of P

which are controlled by associated C and N turnover (Lewis and McGechan 2002). A coupled simulation of organic C, N, and P turnover, as given for ANIMO, APSIM, DAYCENT, DSSAT, RZWQM2-P and SWAT, instead of an isolated simulation of organic P turnover is probably as relevant as including microbial biomass P, even though under field conditions it does not correlate with the concentrations of plant-available P (Liebisch et al. 2014).

In most P cycling models, the P-uptake by roots is described with a diffusive mechanism, however, none of the models simulates an active P uptake. Detailed 3-dimensional root architecture models that describe P uptake with the Michaelis–Menten kinetics do exist (Schnepf et al. 2012). An effective 1-dimensional process description derived from the more sophisticated 3-d approach, which could be applied to the plot-scale models as reviewed in the present study, is however lacking. The processes of root exudation, enhancing P uptake rates of roots, is also not considered in any of the models. This also holds true for the effects of mycorrhiza on plant P availability. The issue probably is that the mycorrhiza colonization frequency is crop-specific and driven by current overall soil nutrient status. Attempts to predict the degree of mycorrhiza formation for a specific site and time period do exist (Hempel et al. 2013) but are not specific to crops.

The relevance of bioturbation for the vertical translocation of P along the soil profile largely depends on the time scale considered. A rather conceptual diffusion-based approach is implemented in the 2D-CycP model, which was applied for 23 years (Li et al. 2019). Based on model tests without bioturbation implementation Li et al. (2019) concluded an improved performance for the model including bioturbation. While soil aggregate structure dynamics are not considered in P cycling models, Hydrus-1d attempts to simulate colloid transport and associated elements under transient flow conditions. The C-Ride module incorporates mechanisms associated with colloid and colloid-facilitated solute transport in variable saturated porous-media based on convection, diffusion, and dispersion. It also accounts for attachment/detachment processes to or from the solid phase, straining, and/or size exclusion describing colloidal and associated P movement between different phases (Šimůnek et al. 2016). Colloidal transport of P in macropores can also be simulated with the ICECREAM model, but due to the need of calibration for macropore flow and transport parameters options for a predictive application are limited (Larsson et al. 2007).

What data or mechanistic knowledge is missing and would be required to better represent the biological processes important for P cycling?

The effect of mycorrhiza on crop P uptake, generally accepted as an important P mobilization/transport

mechanism, is not considered in any of the reviewed model concepts. This is probably related to the fact that the mycorrhiza abundance is a result of the specific crop and soil combinations and as such hard to predict. A comprehensive and systematic inventory of mycorrhiza abundance covering a broad range of crops, soil, management, and climatic conditions could be a starting point for its future consideration in models.

Studies on the C:N:P stoichiometry of organic fertilizers, SOM, and soil microbial biomass (Tipping et al. 2016) exist for a subset of these components but do not cover all the typical crop management options. It is desirable to have such a complete set of stoichiometry data for modeling as this would make it possible to simulate the coupled nutrient turnover if any kind of organic matter is involved.

Even though colloidal transport has been intensively studied for decades, most laboratory and even modeling studies analyzed the colloidal transport only under constant-flow (saturated or unsaturated) conditions (e.g., DeNovio et al. 2004; Wang et al. 2020). However, especially the transient flow is of importance, as abrupt changes in soil water content, flow velocity, and pore water chemistry control the attachment and detachment of colloids at various interfaces, and thus the amount of colloids that are retained or mobilized in the soil (Wang et al. 2020). Furthermore, so far only engineered nanoparticles and colloids or pollutants of colloidal size (or being associated with colloids) were subjects of transport modeling in soil. Modeling of P associated with natural (in situ) colloid transport has not been done so far. The main problem with modeling natural colloids is their unknown source strength, a measure of the amount of colloids released by the soil matrix, as they can be continuously and simultaneously released into the pore water and immobilized through sorption onto the solid phase and precipitation processes. Understanding the controls of colloid transport is elementary to integrate particle transport into numerical modeling, which in turn is indispensable for more precisely describing and predicting P fluxes in ecosystems.

Biodegradation of contaminants

Biodegradation of contaminants like pesticides refers to the natural breakdown of organic substances. As already mentioned, this degradation process is commonly included in models of C turnover. However, soil microorganisms are also able to degrade xenobiotics. In this regard, biodegradation of pesticides is particularly relevant in agroecosystems because microorganisms in the vadose zone including soils can effectively attenuate the applied agrochemicals (Fenner et al. 2013) and, thus, minimize groundwater contamination (Holden and Fierer 2005). Therefore, this section focuses mostly on pesticide biodegradation, acknowledging that

the discussed processes and control factors apply similarly to the biodegradation and transformation of other organic chemicals and contaminants threatening soil functions such as plastics (Brodhagen et al. 2015; Amobonye et al. 2021), per- and polyfluoroalkyl substances (Sharifan et al. 2021), or pharmaceuticals (Jechalke et al. 2014; Thelusmond et al. 2018); although transport processes may differ significantly, for example for plastics (Lwanga et al. 2022).

Biological processes relevant for biodegradation

Biodegradation of pesticides in soil involves the complete breakdown (i.e., mineralization) and the partial transformation of parent compounds to metabolites by soil microorganisms (Leisinger 1983). Abiotic degradation pathways are not considered here. Soil microorganisms can principally transform pesticides in two metabolic modes, either via growth-linked metabolism or via so-called co-metabolism (Janke and Fritsche 1985). Growth-linked biodegradation requires pesticide-degrading microorganisms, which are often prokaryotic organisms (Fenner et al. 2013). They are capable of using pesticides as C, nutrient or energy sources and typically have evolved functional genes that encode for specific enzymes catalyzing the complete or the partial breakdown of individual compounds (e.g. Leveau et al. 1999; Zaprasis et al. 2010; Douglass et al. 2017; Zhan et al. 2018). In contrast, co-metabolic degradation implies the transformation of a non-growth substrate while the involved microorganisms rely on other C, energy or nutrient sources for growth (Horvath 1972). It is mediated mainly by fungi and proceeds due to the action of broad-spectrum enzymes that can catalyze the breakdown of multiple pesticide molecules (Harms et al. 2011). Growth-linked biodegradation by specific pesticide degraders often leads to complete mineralization and proceeds faster than co-metabolic transformations, which are often incomplete, hence, metabolites can accumulate (Leisinger 1983).

While co-metabolic pesticide transformation is an unspecific process that is carried out by many different organisms, growth-linked pesticide degradation can be considered as specific process that relies on metabolic pathways carried out by a specific phylogenetically constrained group of microorganisms (Schimel et al. 2005; Schimel and Schaeffer 2012). Due to the high functional redundancy of microbial communities carrying out unspecific processes, co-metabolic pesticide degradation is probably more robust against disturbances of soil systems triggered by multiple stressors (Schaeffer et al. 2016) than the specific process of growth-linked pesticide degradation because of its dependency on specific microorganisms. There is some experimental evidence that supports a potentially high susceptibility of growth-linked pesticide degradation to disturbance (Pesaro Manuel et al. 2004; Baker et al. 2010), but experimental

insights on stress compensation mechanisms, particularly in response to spatial and temporal disturbance characteristics, are still minimal (König et al. 2019).

Degradation pathways and the involved functional genes and enzymes have been identified and well-studied for some well-known compounds such as phenoxy acetic acid or triazine herbicides (Serbent et al. 2019; Chavez Rodriguez et al. 2022). Biochemical degradation pathways are typically unknown for recently introduced pesticides, such as the fungicide bixafen, which is highly persistent in soils and can form several metabolites during biodegradation (European Food Safety Authority 2012). New pesticide degradation pathways emerge and spread through evolution (Shapir et al. 2007; Udiković-Kolić et al. 2012). Evolutionary processes such as horizontal gene transfer (Nielsen and van Elsas 2019) controlling pesticide biodegradation are still widely undiscovered and not yet considered in pesticide fate models. In general, adaptation mechanisms of pesticide degrading microbial communities are challenging to describe in a mechanistic way, but the adaptation probability could be described as a function of pesticide application history given that the latter is well known.

The actual accessibility of pesticides for microorganisms determining biodegradation rates is strongly affected by soil minerals, porosity, and thus soil structure (Nunan 2017; Rillig et al. 2017; Tecon and Or 2017). Biodegradation occurs at interfaces of various organic and inorganic compounds closely attached to minerals. However, many of these interfaces are clustered frequently within a hierarchical network of pores of different scales and residence time. Sampling such pores may help validating hot spots of microbial habitats and pesticide accrual to understand the biodegradation potentials in pores of different sizes and characteristic interfaces (Totsche et al. 2018). Additionally, specific accessibility of certain biogeochemical interfaces contributes to controlling the bioavailability. Diffusion of xenobiotics into small pores and soil organic matter reduces the availability of the xenobiotic for desorption and bio-uptake; a process called “sequestration” (Lueking et al. 2000). It is the same mechanism as previously discussed for the physical protection of soil organic matter. When sequestration is detected via a decreased extractability of a compound with increasing contact time in soil, the phenomenon is termed “aging” (Alexander 2000). The situation is further complicated by the fact that the 3-dimensional arrangement of soil biogeochemical interfaces itself is not static but dynamic. Apart from anthropogenic disturbance such as tillage, both abiotic (e.g., shrinking and swelling) and biotic processes (e.g., bioturbation) contribute to the re-arrangement of soil particles (Six et al. 2004; Bronick and Lal 2005) and of its interfaces. Hence, understanding the role of biogeochemical interfaces for the biodegradation potential of soils should include modeling of their spatial arrangements and dynamics.

Due to the spatial heterogeneous soil structure, also soil microorganisms are heterogeneously distributed as well (Nunan et al. 2002, 2003). For instance, highest microbial activities have been found in pores with diameters of 30–150 μm (Kravchenko et al. 2019). This preference is attributed to better water availability, higher organic matter accessibility than in larger pores and fewer predators in this pore-size class. A correct assignment of biodegradation pathways to xenobiotics will have to consider these heterogeneities, e.g., by considering effecting pore size classes for biodegradation modelling.

The different processes of sorption of xenobiotics in soil have been distinguished into readily reversible (i.e., equilibrium sorption), slowly reversible (i.e., “aged” or “sequestered” residues, with kinetically hindered desorption), and irreversible (i.e., bound residues) sorption. Presumably, each fast equilibrium sorption is accompanied by a “slow” desorption process (rate-limited sorption; e.g., Altfelder et al. 2000), which reduces the relative proportion of readily desorbable substances in soil. Consequently, these aged residues are less available for leaching and biological uptake in soils and prevail in a less reactive and thus less (bio)degradable state (e.g., Chung and Alexander 1998; Barriuso et al. 2004). Bound and to some extent also sequestered and aged residues are not necessarily toxic because they become non-accessible and also not available for microbes, as e.g. reported for the antibiotics fluoroquinolones (Rosendahl et al. 2012). Substance sequestration in soils has been mainly attributed to i) sorption at a condensed, glassy form or high-surface-area carbonaceous fraction of SOM (Huang and Weber 1997; Chiou et al. 2000) exhibiting stronger/more specific sorption sites for xenobiotics (OMD model; Brusseau et al. 1991) or ii) retarded diffusion of xenobiotics in small pores, in part due to bottle-neck effects or organic matter coatings in fine pores (SRPD model; Wu and Gschwend 1986; Pignatello and Xing 1996). Experimental evidence supported both theories, making a combination of either effect on aging processes in soils probable (reviewed by Pignatello and Xing 1996). Aging/sequestration phenomena are especially relevant for soils rich in organic matter (Chung and Alexander 1998) but have also been shown for purely mineral sorbents due to diffusion into micropores (Farrell et al. 1999). Also, aggregation in soils has been shown to induce non-equilibrium sorption and aging of pollutants (Amellal et al. 2001; Nam et al. 2003; Villaverde et al. 2009). This effect apparently applies to a broad substance spectrum, as enhanced mineralization of the relatively polar cabaryl as well as the more hydrophobic phenanthrene was observed in pulverized soil relative to naturally aggregated ones (Hatzinger and Alexander 1995; Ahmad et al. 2004), which, thus, likely also applies for pesticides.

Substance aging in soils increases also with fluctuating soil moisture conditions. Shelton et al. (1995) observed for

atrazine a lower availability for desorption after drying and re-wetting of incubated soils. Similarly, enhanced phenanthrene sorption was found for short-term soil incubations (<60 d), which included drying-wetting cycles (White et al. 1998). However, when the soils already contained aged residues, wetting and drying cycles increased the mineralization and extractability of sorbed phenanthrene. Possibly, the higher biodegradation of phenanthrene was caused by the priming of microbial activity (see section on SOM), which is typical for the initial wetting phase after a dry period in soils (Kuzyakov et al. 2000). Shaw et al. (2002) demonstrated that the effect of soil drying on the aging of 2,4 dichlorophenol might be related to a water-tension controlled accumulation of substances in less bio-accessible soil micropores. Immediate immobilization is particularly observed when pollutants are added to soil in a moist matrix (Kuzyakov et al. 2000). Müller et al. (2013) described this effect as flash NER (NER = non-extractable residue) and concluded that its accurate description could be decisive for accurate fate modeling (Zarfl et al. 2009; Kasteel et al. 2010; Unold et al. 2010).

State-of-the-art in modeling biodegradation

Pesticide degradation models can be roughly classified regarding the applied scale: i) small scale models focusing on explicit microbial degradation of pesticide or other compounds at the pore scale and ii) larger scale pesticide fate models integrating simple degradation rates with physical transport processes while often neglecting detailed biological processes (Soulas and Lagacherie 2001; Dubus et al. 2003).

Small scale biodegradation models usually include an explicit representation of microbes and their processes (Banitz et al. 2011; Pagel et al. 2014; Vogel et al. 2015; König et al. 2017; Schmidt et al. 2018). Microbial growth is based on the specific pollutant as a C source described with simple Monod kinetics (Shelton and Doherty 1997). The parametrization of the model processes and rates is mainly based on laboratory experiments under controlled conditions, limiting the transferability to real soil systems. However, these models are very valuable to study the effect of bioavailability and contact probability under small scale spatial heterogeneity. This includes the effects of pore topology (Vogel et al. 2015) heterogeneous distribution of bacteria or target compound (Babey et al. 2017; Schmidt et al. 2018), or fungal hyphae acting as dispersal network (Banitz et al. 2011; Ellegaard-Jensen et al. 2014). Other studies analyzed indirect effects of spatial heterogeneity by varying microscale conditions, which are determined by the pore system, by water content or distribution of soil organic matter (Centler et al. 2011; Ghafoor et al. 2011). However, environmental conditions such as pH, water content or temperature are often

assumed to be constant, likely because the underlying rates were measured at constant conditions in the lab (Soulas and Lagacherie 2001). Some models also account for different degradation strategies (co-metabolic, growth-linked) where a second C source usually in the form of soil organic matter needs to be included in the modeling approach (Soulas and Lagacherie 1990; Pagel et al. 2014, 2016). While the microbial processes are often well described in the small-scale modeling approaches, other processes affecting pesticide fate such as the sorption behavior, leaching or physical degradation processes are often neglected. This can be explained by the different scales these processes are acting on. Microbial degradation models operating on larger scales tend to account for more physical factors such as sorption (Pagel et al. 2014) or leaching (Rosenbom et al. 2014). Generally, those models do not account for feedbacks with other soil organisms or compartments, which is again likely due to scaling issues and also observed in other microscale models not related to pesticide degradation (König et al. 2020).

Model approaches to simulate microbial evolution in soil have been outlined by Crawford et al. (2005). The authors envisioned a model approach that accounts for interaction between individual microbial cells with specific (evolving) traits. They pointed out that the model parameterization is challenging because of limited capabilities to measure traits of specific microorganisms and suggest using stochastic simulations that are validated against observable constraints of emergent community behavior. Trait-based models have been set up for C cycling (e.g., Wang and Allison 2022), but they do not yet consider evolutionary processes, particularly not specifically for pesticide degrading consortia. Certain microbial traits, such as maximum growth rates, might be constrained using genomic data (Valdivia-Anistro et al. 2016; Weissman et al. 2021; Malik and Bouskill 2022; Sokol et al. 2022). A Bayesian constraint-based model conditioning technique has been recently used to support the optimal design of experiments to distinguish between alternative models reflecting alternative pesticide degradation pathways (Chavez Rodriguez et al. 2022). Such a method could similarly facilitate constraining the simulated behavior of co-evolving pesticide degrading communities to observed patterns in genomic proxies of pesticide-degrading microbial consortia.

Models formulated using ordinary differential equations can include distribution processes like sorption or volatilization, dissipation processes like transformation and degradation, microbial population dynamics, or the spread of resistance genes. Alternative techniques that account for heterogeneities in soil rely on stochastic approaches (Volkova et al. 2013) or individual-based or agent-based models (Bora et al. 2017). These approaches usually include microbial population dynamics that differ between susceptible (or sensitive) and resistant bacteria. They do not yet account

for various contact options of microbes to mobile pollutants within a dynamic 3D soil matrix. However, there are novel approaches in place to consider, for instance, fluid dynamics and cellular automata modeling for describing soil structure dynamics (Ray et al. 2017; Zech et al. 2022a, b).

In contrast to the described microscale models, pesticide fate modeling approaches operating on profile to field scale have been developed since decades, motivated by the need to predict pesticide persistence and groundwater pollution (Boesten and van der Linden 1991; Diamantopoulos et al. 2017). They do not explicitly account for biology but describe biodegradation with simplified constant / first-order rates (Köhne et al. 2009) or using pedo-transfer functions (von Götz and Richter 1999). Often, 1D water flow models without any structural aspects are extended by sorption processes and first-order degradation rates, resulting in an estimate of pesticide leachate (Armstrong et al. 2000; Ma et al. 2012; Filipović et al. 2014; Diamantopoulos et al. 2017). Those models can be applied to specific compounds but need thorough fitting, which increases the uncertainty for predictions (Dubus et al. 2003). Here, dynamic environmental conditions and feedbacks to other compartments can be better represented since they act at a similar scale. Still, these large-scale models are not feasible for generic pesticide degradation modeling as the underlying mechanisms are not described, and the pesticide dynamics are highly dependent on the specific compound parameters.

In summary, a combination of the two types of existing pesticide degradation models is needed to integrate microbial controls at the profile or field scale, while accounting for feedbacks with physical and chemical factors and dynamic environmental conditions. More mechanistic knowledge is needed to develop such a combined model and to improve the assumptions building the basis for such a model approach.

What data or mechanistic knowledge is missing and would be required to better represent the biological processes important for biodegradation?

Overall, there have been recent huge advances in the modeling of microbial activity in heterogeneous soils and thus on the biodegradation potential for pesticides. Yet, data for model validation have been largely achieved by laboratory incubations, which frequently only account inaccurately for the prevailing climatic conditions (particularly under freezing conditions), related soil structure dynamics, and dynamic changes of C and nutrient stoichiometry to feed the biodegrading communities. Besides, high uncertainties exist on dose–effect relationships, because i) both microbes and pesticides are allocated in certain hotspots that do not always overlap, ii) effect concentrations and biodegradation

potentials are usually co-affected by site factors such as temperature, C supply, water content or pH, and iii) system behavior is not necessarily linear but may show synergistic or antagonistic effects that do not only depend on substance concentration. The latter can become particularly complex when dealing with compound mixtures, that are rarely covered in the models but are common in reality. More complexity is added when microorganisms have started to adapt to environmental stressors so that their role in biodegradation potentials has changed with multiple pesticide applications. This might even be coupled with other stresses as recently discussed in concepts of xenoresilience (Schaeffer et al. 2016).

Thus, generic model approaches for predicting biodegradation of different pesticides in various soils at the pedon scale need to represent the response of microbial degrading communities and their activity to dynamic changes in environmental conditions, soil structure and to regimes of pesticide application. The consideration of bioenergetics of pesticides in soil biodegradation models constraints growth yields as well as energetic limits of pesticide degradation and thus also the formation of remobilizable and irreversibly bound non-extractable residues (Trapp et al. 2018; Thullner and Regnier 2019). Hybrid multiscale methods effectively bridge multiple scales by combining representations of processes at pore-scale in parts of the domain while the rest of the domain is represented at the continuum scale (Molins and Knabner 2019). This could represent biological and physical processes affecting biodegradation of pesticides at appropriate scales. Such pore-scale biodegradation models can use measured pore characteristics obtained by X-ray computed tomography and explicitly describe the localization of microorganisms in the pore network and their accessibility to substrates (Pot et al. 2022). Alternatively, implicit approaches utilize calibrated stochastic spatial statistical models to reflect pesticide degrader distributions in continuum scale models (Schwarz et al. 2022). Predicted biodegradation rates by both approaches can be calibrated and validated against measurements at macroscopic scales (soil cores or pedons). Measurements of biodegradation rates under field conditions could be achieved with long-term lysimeter studies using compound-specific isotope labeling (Melsbach et al. 2020). While the outlined approaches are limited to individual case studies, they could facilitate the improvement of pedotransfer functions (e.g., von Götz and Richter 1999) for predicting biodegradation rates based on physical and biological soil characteristics and pesticide properties under specific environmental conditions.

Modeling approaches for predicting biodegradation at pedon scale need to distinguish between growth-linked and co-metabolic degradation because the degradation mode determines how fast pesticides are degraded. The relative importance of growth-linked versus co-metabolic

metabolisms depends on the chemical characteristics of the degraded compound and whether specific degradation pathways have been evolved. In general, growth-linked and co-metabolic biodegradation scales with microbial activity and can be considered to become more relevant at high rates of C and energy supply via fresh organic matter input. Model approaches should reflect evolutionary adaptation mechanisms and ecotoxicological effects in response to pesticide mixtures due to their impact on biodegradation potential and rates. To account for the different degradation pathways, a model could distinguish the two processes by different maximum biodegradation rates and environmental dependencies. Growth-linked degradation is defined with a higher maximum degradation rate, while the actual degradation rate highly depends on environmental conditions. This will result in a stronger reduction of the degradation rate in case of unfavorable conditions. It could be also coupled to an application memory, where an increased number of applications is equal to an enhancement in environmental conditions. Co-metabolic degradation is defined with a lower maximum degradation rate, but with a broader definition of “favorable conditions” and a direct dependency to the overall microbial activity, as the whole microbial community can be assumed to be active in this.

Overall, the soil function of biodegradation should likely not be assessed for individual hot-spots but at the scale of pedons. This will also allow to account for former adaptation potentials of microbial communities to pesticides loads, irrespectively whether metabolic or co-metabolic degradation pathways dominate. It does not allow, though, to explain variations in ecotoxicity, as the latter depends on contact times, and thus bio-accessibility and availability of additional growth supporting substrates. Yet, the modeling of these processes will likely continue to be different from those of modeling the fate of soil organic C, which can i) be continuously replaced by plants and microbes, and which ii) includes other size ranges such as stabilization of particulate organic matter that reacts with soils by other mechanisms than relevant for individual xenobiotics. However, describing the immobilization of xenobiotics in analogy to the formation of mineral-associated organic matter (MAOM) driven by diffusion of dissolved or low molecular weight organic matter into smaller pores might be sufficient as a simple approach. To improve this, more process knowledge is needed on mechanisms of how xenobiotics become inaccessible to microbes and solvents, previously described as the NER effect.

Yet, the modeling approach depends – as always – also on the specific research question. If the focus is on understanding the dynamics and transport of a specific pesticide, the simulated pathway and the parametrization should be adapted to this pesticide, provided that the data is available. Here, also possible metabolites and their dynamics should be

included for a full picture. If pesticide fate is not the focus, but, for instance, the effect of other management practices on microbial activity and the related soil functions; a simple ‘generic’ model approach distinguishing the two degradation pathways with some general parameters correlated with the microbial activity as described above might be sufficient. An example might be comparing tillage with no-till farming systems, where the differences in pesticide applications are a consequence of the soil management, and thus can have an additional effect on the microbial activity and processes; however, the specific compound applied is not important in this case.

Plant disease control

Soil fertility and health depend strongly on the composition and activity of soil microbial communities including bacteria, oomycetes and fungi. Agricultural management practices affect the ratio between and within these groups as well as the relative abundance of individual microbial taxa, among them known soil-borne pathogens (Thiet et al. 2006). As an example, we will focus in the following on soil-borne pathogens as for some of them there is information on propagation and survival in soils as well as movement/spread of propagules within the soil. For other beneficial organisms like plant growth promoting bacteria our mechanistic understanding is much more limited. This is true in respect to the mechanisms of interaction with the plants, be it direct (e.g., providing nutrients like P or Fe), or indirect (e.g., protection against pathogens). However, this applies even more so in respect to the interaction within the microbial community, i.e. whether there is competition for resources or even facilitation. The specific and well-known examples for symbioses between plants and microorganisms, i.e. symbioses between legume family and rhizobium on the one hand and symbioses of arbuscular mycorrhiza and crop plants (except lupine and *Brassicaceae*) on the other hand, are not covered here. The latter is addressed in the section on P cycling.

Soil-borne fungal pathogens

Soil inhabiting fungi can be divided into three functional groups: i) species participating in organic matter decomposition and transformation, ii) ecosystem regulators, and iii) biological controllers (Swift 2005; Gardi and Jeffery 2009). Because soil fungi are capable of producing various extracellular enzymes, they are able to break down a variety of organic compounds, contributing to the balance of C and nutrients (Žifčáková et al. 2016). Saprophytic fungi are pivotal for decomposition of plant residues and contribute to soil organic matter formation (Treseder and Lennon 2015). In addition, ectomycorrhizal fungi also have

the ability to oxidize organic material (Lindahl and Tunlid 2015). Ecosystem regulators are involved in formation of soil structure by contributing to the stabilization of soil aggregates (enmeshing of particles by hyphae) and likewise by facilitating transport of other soil organisms like bacteria in the soil environment (Fraç et al. 2018; Jiang et al. 2021). The group of biological controllers regulate growth of other organisms including plant growth such as mycorrhizal fungi that can improve availability of nutrients (Bagyaraj and Ashwin 2017; Almeida et al. 2019). Soil-borne fungal pathogens that cause diseases are examples for negative impacts on the plant within the group of biological controllers. We will here use the example of soil-borne fungal pathogens as a placeholder for any microbial taxa associated with a specific soil function as detailed above, to illustrate how the biology of individual organisms can be explicitly addressed in models. Fungal pathogens are the most prevalent plant pathogenic organisms and responsible for more than 80% of crop diseases (Tian et al. 2020a). Important soil-borne fungi and oomycetes (e.g., *Fusarium* spp., *Rhizoctonia solani*, *Sclerotinia sclerotiorum*, *Pythium* spp.) belong to the most aggressive pathogens that threaten food security (Van Bruggen and Semenov 2000; Ghini and Morandi 2006; Fiore-Donno and Bonkowski 2021). In general, plant pathogens (e.g., fungi, protists, oomycetes, bacteria, viruses) are responsible for about 16% of global yield losses annually and it has to be expected that this will increase due to climate change (Newbery et al. 2016). It would be critical to gain more insight into the ability of the soil ecosystem, and in particular its biome, to suppress plant pathogens and to identify the key factors (e.g., density and type of inoculum, distribution of inoculum, soil microbiome, external factors) that control this ability. For example, plant viruses often use soil borne microbial and nematode vectors as transmitters (e.g. Barr 1979; Bertioli et al. 1999). Waterfilms are essential for the spread of bacteria, and of the flagellated zoospores of protistan plant pathogens, while fungal pathogens infect plants via hyphal mycelia which can spread also at dryer soil conditions (Boswell et al. 2003). Such basic knowledge might allow us to model disease dynamics and related management options in soil systems.

General aspects in plant disease epidemics of soil-borne pathogens

Plant disease epidemic is a progress of disease in time and space. The interaction between a pathosystem and environmental conditions determines the structure of each epidemic and the respective temporal dynamic and spatial patterns (van Maanen and Xu 2003). An improved knowledge about temporal and spatial changes during epidemics caused by a plant pathogen population is required including the impact of the environment on disease progress. Based on this

knowledge it will be possible to develop suitable control strategies.

The ecology of soil-borne pathogens has distinctive features that differ from epidemics caused by foliar pathogens. Whereas foliar pathogens have to contend with various external factors such as wind, radiation and varying temperatures, the effects of these factors are limited in soil. In the soil, pathogens have to contend with a completely different quality of factors. The most notable differences are the propagule/inoculum reservoir in soil affected directly and indirectly by biotic (e.g., soil microbial community composition, soil fauna) and abiotic soil environment (e.g., physico-chemical factors, soil type). The soil environment influence processes such as propagule survival, dispersal, and germination (MacDonald 1994). A further important point is the role of the host plant (e.g., susceptibility, growth and development, root architecture, plant-soil feedback) in contacting and spreading of pathogen inoculum (Gilligan 1983; Anguelov et al. 2019), and co-infections affecting virulence of the pathogen (Williamson and Gleason 2003). The soil structure formed by physical and biological processes affect to a large extent both the pathogen and the plant and their interaction and thus disease incidence and severity. The complex structure and processes in the soil environment need an improved understanding. The components affect each other and can have positive and negative (suppressive) effects on soil-borne pathogens. The modeling of all the processes such as inoculum density, spatial pattern of pathogen inoculum in the soil, latent and infectious periods and spread impacted by soil biotic and abiotic soil variables is a challenge. Modeling aims at predicting future incidence and severity of plant diseases in agricultural systems. For this purpose, knowledge about the pathogen life cycle, the current pathogen distribution and environmental factors (e.g., soil structure, nutrient cycle and turnover, as described in other sections of this review) influencing them is required.

State-of-the-art in modeling of plant diseases

Mathematical and statistical models are important in epidemiology of plant diseases to describe spatio-temporal dynamics to improve the understanding of disease development (Cunniffe et al. 2014). There are two main groups of plant disease models (Donatelli et al. 2017). The first group is inspired by epidemiological models used for human and livestock diseases (Cunniffe et al. 2014). The second group focuses on the consequences of the host–pathogen interactions and hence on the physiology and resulting yield loss. In the past, plant disease models were dominated by short-term tactical questions such as the support to schedule scouting or pesticide use (Magarey et al. 2002; Isard et al. 2015). These models usually focus on specific host–pathogen systems in a

distinct environment. Multi seasonal observations to receive robust empirical relationships between local weather variables and disease progress caused by a specific pathogen on a host are traditionally the basis of these models (Madden et al. 2007). Alternative approaches are models like phenology models (Welch et al. 1978) and infection models (Gilligan 1995) based on parameterization from independent experiments under controlled conditions focused on identification of pathogen and plant responses to a range of environmental factors (Zadoks 1971; Magarey et al. 2005). Note that this type of models is more difficult to establish for soil-borne diseases because the models do not consider the impact of soil state variables (e.g., soil structure, organic matter, nutrient status, water content) due to the difficulty of obtaining the respective input data (Roget 2001). For above ground diseases (leaf diseases), the key factors are (i) availability of a susceptible host, (ii) presence and amount of inoculum (propagules), and (iii) environmental conditions such as rainfall, humidity, temperature, the situation is more complex for soil-borne pathogens. Here additional knowledge is required on soil microbial activity (including disease suppressiveness), soil water or more general any soil or root parameter affecting pathogen motility, survival and dispersal (Gilligan 1983; Bekker 2018). Relevant controls and relevant processes related to soil-borne pathogens are plant residues and soil management (affecting density of propagules and their dispersal), the microbial activity and microbiome composition regulating the breakdown of residues (containing propagules) in general and specifically suppressing individual organisms and finally crop rotation defining phases of host and non-host presence. One of the few examples for a decision support system for soil-borne diseases is the study of Roget (2001) providing a case study for take-all disease (*Gaeumannomyces graminis* Ggt) in which inoculum density in the soil was derived from DNA probes. Inoculum density of Ggt decreases during phases with high microbial activity (e.g., at rainfall events), addressing the fact that Ggt is a poor competitor during the saprophytic phase. In addition, crop rotation has been included, i.e. dividing the system in host and non-host phases. More recently plant disease modeling is moving towards the use of more process-based mechanistic models and seeking the integration into crop models. A roadmap for this has been provided by Donatelli et al. (2017).

Perspective for the integration of plant diseases into process-based models – the bottleneck of data availability

In principle the approaches of existing models, in particular the relatively simple decision support system for Ggt could be easily implemented into a process-based model. The shortcoming is the availability of data, i.e. inoculum density and not just relative abundance of a pathogen within the soil

microbiome. For some soil-borne fungi and even more so for plant growth promoting microorganisms there is a lack of mechanistic understanding about factors that affect their activity, how they might disperse in soil, and how they interact with the plant and other members of the soil/rhizosphere microbiome under consideration of environmental factors. In general, parameters which were indirectly included in the modeling like crop rotation (periods with host and non-host plants), soil organic matter and soil management (fate of propagule containing material) may be valid for any pathogen. Deriving further progress in disease process-based models, a link to models of biological soil processes is required.

Structure formation and dynamics

Soil structure refers to be the spatial arrangement of mineral particles of different size (i.e. soil texture), organic material and pore spaces in soil (Dexter 1988). It is formed on the one hand by physical processes such as swelling/shrinking, freezing/thawing and the translocation of material with moving water. But, on the other hand, it is formed to a large extent by biological processes, which is the focus of this section. Besides these natural processes some tillage practices in agriculture are designed to optimize soil structure for plant germination and growth. During the last decades, our tools for the quantitative description of soil structure have developed considerably, both in terms of available techniques (Rabot et al. 2018) and the analysis of 3D images of undisturbed soil structure (Schlüter and Vogel 2016) which is a prerequisite for linking soil structure and functions. The key role of soil structure for soil functioning is increasingly recognized (Fatichi et al. 2020; Sullivan et al. 2022). Soil structure is the major control of how much water can be stored, how it can flow through soil, how gases can diffuse and how many pore-solid interfaces are available to exchange elements and compounds. Moreover, soil structure provides the habitat for the myriad of organisms living in soil including plant roots. Consequently, all biological processes discussed in this paper depend in one way or another on soil structure. There are a number of different biological processes that have an immediate impact on soil structure in terms of the formation of the pore space, the mixing of organic and mineral compounds and its mechanical stabilization. These processes are discussed in the following before we examine how biological formation of soil structure can be modelled.

Biological processes forming soil structure

Formation of biopores by roots

Roots create cylindrical bio-pores when growing and decaying in soil (Kautz 2015). Some plants form deep and thick

taproots such as alfalfa and are used specifically to access the subsoil for subsequent crops (Sun et al. 2008). In contrast, it is mainly the fine roots with a diameter of 0.1 to 0.2 mm that often form a dense network of biopores. Lucas et al. (2019a) showed for a reclaimed soil that roots can create an extensive biopore system in less than a decade. The biopores are potentially stabilized by the formation of CaCO_3 or CaSO_4 in the rhizosphere (Hinsinger et al. 2009). For the reclaimed soils investigated by Lucas et al. (2019a) chemical conditions for CaCO_3 formation were favorable. Root channels provide thus the pathways for water and gas but also for other plants to explore the soil volume especially in deeper horizons. There is evidence that plants reach the subsoil almost exclusively through preexisting biopores if they encounter a compacted layer further up (White and Kirkegaard 2010; Gao et al. 2016). In loose topsoil of low bulk density generated by earthworm activity or tillage, roots typically use the existing pore space so that cylindrical root channels are less frequent and roots do not compact the surrounding soil matrix during growth (Lucas et al. 2019b). However, root growth also affects the connectivity of the pore space in loose topsoils. Analysis of pore connectivity as a function of pore size revealed that the pore space is getting continuous as soon as pores with a diameter of 0.1 mm and smaller are taken into account. This threshold corresponds to the typical diameter of fine roots (Lucas et al. 2021). Larger pores between soil clods created by tillage in arable fields are often isolated while pore connectivity is provided by the growth of roots.

Formation of biopores by earthworms

Among the soil macrofauna, earthworms have the most impact on soil structure formation, at least in temperate humid regions. Earthworm burrows are typically cylindrical in shape with a diameter in the range of millimeters. Hence, their burrows are mostly air-filled and promote the gas exchange with the atmosphere. However, during heavy rainfall they provide efficient drainage pathways and an improved infiltration capacity. It was found that anecic species such as *Lumbricus terrestris* produce fewer but more continuous and more vertical burrows as compared to endogeic species (Bastardie et al. 2005). This is explained by the different life forms (Bouché 1977). Anecic species feed at the soil surface and their burrows mainly serve as shelter from predators and drought, while endogeic species eat their way through the soil, living on the organic matter they absorb. Hence, the endogeic species tend to refill their burrows with their casts. This is expected to be similar for enchytraeids but it has been shown that they can also produce pores in the size range of their bodies (Porre et al. 2016). Anecic species often drop their casts at the soil surface leaving their burrows open. As a consequence, anecic

species have a higher potential to lift the soil surface and thus reduce soil bulk density while endogeic species and enchytraeids have a higher potential for bioturbation within the upper soil horizon where they are active.

Formation of bio-aggregates

Besides biopore formation, soil fauna contributes to soil structure formation by casting and the formation of faecal aggregates. In mineral soils this is most evident for earthworms and enchytraeids. The porosity inside casts has been shown to be substantially lower compared to the surrounding soil while their mechanical stability is higher (Jouquet et al. 2008). It was found that the overall soil bulk density is either higher or lower or not affected at all. This was demonstrated by Barré et al. (2009) who showed that a compacted soil is loosened and a loose soil is compacted by earthworms. Hence, the pore size distribution is changed and the soil is homogenized in terms of structure that is formed by relatively dense bio-aggregates (i.e., casts) and relatively large inter-aggregate pores. The resulting crumbly structure is typical for grassland soils with high earthworm activity where the entire topsoil material is going through an earthworm gut about once a year at high bioturbation rates (Ellenberg et al. 1986). The formation of casts can accelerate C turnover shortly after casting but, as already discussed, organic matter inside the casts can be physically protected from further decay at longer time scales (Frouz 2018). This occlusion of particulate organic matter is a protective means against microbial decay (Lubbers et al. 2017). The intensity of bioturbation was quantified by Capowiez et al. (2021) using luminophores as a tracer to calculate a mean displacement distance per time. They confirmed that endogeic species are much more effective for bioturbation as compared to anecic species as was already demonstrated by Scheu (1987a).

Stabilization of soil structure by biological activity

In addition to direct structure formation, biological activity has a considerable impact on the stabilization of soil structure and thus on the maintenance of pore connectivity, habitats and biogeochemical interfaces as well as on the vulnerability of soils to erosion. This function is mainly provided by microorganisms and less by soil fauna (Lehmann et al. 2017). During microbial decomposition of organic matter extracellular polymeric substances and low molecular weight organic matter are produced that are quite mobile within the soil solution in the form of dissolved organic matter (Kaiser and Kalbitz 2012). In this way organic molecules come in close contact to mineral surfaces where they increase the binding forces in different ways (Totsche et al. 2018). Furthermore, fungi stabilize the soil structure through their network of hyphae, which spreads in smaller,

but also in larger air-filled pores enmeshing the solid phase (Chenu and Cosentino 2011). The stability of soil structure is expressed in the measurement of aggregate stability. With increasing mechanical stress, the soil breaks down into smaller and smaller fragments with smaller internal pore size and increasing stability which is related to the organic glue from microbial origin (Chenu and Cosentino 2011; Miltner et al. 2012). Hence, microbial activity and the interaction between organic matter and mineral particles leads to heterogeneous binding forces at the microscopic scale while the disintegration into fragments of different stability is the macroscopic manifestation of this heterogeneity (Vogel et al. 2022). When referring to aggregates, the different formation processes should be distinguished, which can be either natural biological aggregation (e.g. casts), natural physical aggregation (sharp-edged aggregates by swell-shrink processes) or artificial fragmentation along zones of weakness (e.g. by dry or wet sieving).

Even if a stable structure has formed under constant boundary conditions, the various structure-forming processes lead to the fact that soil structure may change steadily at any point within the soil volume. At the same time, however, macroscopic structural properties such as bulk density, pore size distribution and pore connectivity may stay rather constant in time, or may seasonally fluctuate around some relatively stable state due to oscillating biological activity or physical processes such as swell-shrinking with changing water content or freezing and thawing cycles. As a consequence of the internal dynamics, the microscopic configuration and the accessibility of organic matter for soil organisms is continuously changing, having an impact on process rates.

State of the art in modeling soil structure dynamics

Modeling of soil structure has long focused on the abiotic processes of soil compaction by heavy machinery in agriculture and forestry (Kuhwald et al. 2018; Duttmann et al. 2022). This was and still is motivated by the fact that soil compaction has an extremely critical impact on soil water dynamics and soil as habitat for organisms and herewith on many soil functions (Nawaz et al. 2013). More recently, however, biological processes that can promote the recovery of disturbed soil structure have come more and more into focus. There is experimental evidence that some soil properties such as the infiltration capacity may recover relatively fast due to the formation of biopores while, for example, the recovery of bulk density after compaction seems to be a much slower process (Keller et al. 2021). Despite the known importance of biological processes for the formation of soil structure, relatively few modeling approaches have been developed so far to represent these processes. Some of them are briefly discussed below.

Root channels

It is well known that root systems have the capacity to alter soil structure either directly by shaping soil pores or indirectly through the supply of organic matter to fuel biological activity in the rhizosphere or by extracting water (Gregory 2022). Catch crops, especially the deep-rooted ones, are specifically used to improve the structure in deeper soil layers (Lucas et al. 2022). Despite this importance, there are no models yet that are capable of describing these processes and their impact on soil properties for different plant species under different site conditions. The reason for this is probably the many interacting factors that influence root growth such as soil moisture and mechanical stability. A complicating aspect is probably the fact that roots may use the existing pore system (White and Kirkegaard 2010) especially in compacted soil layers. Recently, it was shown by Phalempin et al. (2022) that the reuse of existing pores is less effective in non-compacted soils. However, in the subsoil, pre-existing soil structure can be very stable and may originate from times when a different vegetation shaped the structure formation (Schlüter et al. 2011). Modeling root growth can be a valuable approach to describe structure formation by roots and more detailed knowledge on soil mechanics and the physical interactions at the root tip will help in building such models (Kolb et al. 2017). Meurer et al. (2020a) suggested a model approach describing the effect of root growth and earthworm activity on the pore size distributions where the required ‘pore-change’ factors are based on plausible assumptions. There is an increasing number of 3D single plant root architectural models (Pagès et al. 2014; Schnepf et al. 2018). They can be parameterized to represent root growth in the field also for a consortium of plants. Such models could potentially be used for modeling biopore formation in crop rotations, however, data on biopore reuse in the field for the calibration of such models are scarce (Landl et al. 2019).

Earthworm burrows

Especially the large continuous earthworm burrows have long been a subject of research in the field of water and solute transport and the phenomenon of preferential flow. The number of such biopores is highly relevant for the infiltration capacity but also as pathways for roots to reach the subsoil. This is why modeling the number density of mainly vertical, continuous earthworm burrows is an essential task. It has been shown that there is a clear relation between earthworm abundance and the number of such burrows (Van Schaik et al. 2014; Bouché and Al-Addan 1997) however, the number of burrows per individual may vary considerably (Pérès et al. 2010). There are no reliable models yet to link site characteristics to earthworm abundance and macropore

density but the increasing number of field data might provide a clearer picture in the future.

Bioturbation

Modeling bioturbation was developed mainly in benthic systems. As an example, Gerino et al. (2007) used a classical advection–dispersion model where local mixing is covered by the dispersive part while the transport by organisms over larger distances is covered by the advective part. For soil systems an equivalent model concept was presented by Jarvis et al. (2010) which was successfully applied to the spreading of ^{137}Cs from the fallout of the Chernobyl accident. It distinguished between local mixing (dispersive part), thought to be brought about by endogeic earthworm species, and non-local mixing (advective part) induced by anecic species feeding at the soil surface and egesting their feces partly deeper down as tapestry in their burrows. Although obviously successful, these models have not been further developed since then. One reason for this is probably the need for suitable tracers to determine the model parameters. Bioturbation in terms of mixing efficiency, induced by different behavioral types of earthworms was modelled by Blanchart et al. (2009) using an agent-based, spatially explicit, 3-dimensional model (SWORM). This allowed to demonstrate the impact and efficiency of individual earthworms on bulk density and mixing. However, it is not obvious how to parameterize this type of model for a given soil.

Aggregate formation

The modeling of aggregate formation, beyond the biological formation of casts as discussed above, has developed in recent years (e.g. Segoli et al. 2013). Thereby, the focus is less on structure formation per se but rather the inclusion of organic matter in these aggregates and thus the physical protection against biological degradation. There is a current discussion on the extent to which such aggregate formation through the agglomeration or some kind of self-organization of organic and mineral components actually takes place (Vogel et al. 2022). Direct observations in natural soils are still lacking and it is not obvious which biotic or abiotic processes should lead to the local reorganization of organic and mineral particles. What is undisputed is that the binding of organic matter to mineral surfaces makes an important contribution to stabilizing soil structure (Totsche et al. 2018). The fact that the soil typically disintegrates into aggregates of different size and stability when mechanically stressed is a direct consequence of the heterogeneous binding forces within the soil matrix. Hence the critical process to be considered in future model concepts is the mixing of organic compounds with mineral particles as e.g. bioturbation or the diffusion of dissolved organic matter.

Challenges and possible ways forward

With regard to soil functions and the importance of biological processes of soil structure formation, two aspects appear to be of outstanding importance: i) the continuous internal dynamics of soil structure through biological activity without changing macroscopic properties and ii) the recovery of soil structure after some disturbance whereby macroscopic properties are reestablished. Along both lines we do not have suitable modeling tools yet that allow us to describe or even predict the relevant processes as a function of site conditions and the major drivers that are land use and climate.

Internal structure dynamics

The continuous reformation of soil structure induced by biological agents has considerable impact on SOM, N and P dynamics as discussed earlier. One critical prerequisite to address the internal structure dynamics is that tools are required to measure it. This is challenging since soil is opaque and macroscopic properties that can be measured in the field or at soil samples are a snapshot in time and do not change. Even the newly available techniques of 3D imaging of soil structure such as X-ray tomography do not help a lot since we typically look at just one point in time. To measure the structural dynamics, we need parameters such as the mean time it takes to move a soil particle from an accessible pore-solid surface to the inaccessible interior of the soil matrix or vice versa. Another characteristic parameter would be how long it takes for a point source to spread towards a randomized distribution in space. This could be used to quantify the intensity of the mixing that we expect to be important for stabilizing C or the retention of nutrients. In order to be able to measure such properties we need suitable tracers that can be visualized using existing tomographic techniques. Examples are dense particles visible by X-ray CT (Schlüter and Vogel 2016) or by analyzing subsamples as done by Capowiez et al. (2021) to analyze the spreading of luminophores as conservative fluorescent particulate tracer.

Another approach would be to analyze the natural distribution of specific soil components. For example, if the particulate organic matter is uniformly distributed within the soil matrix, this indicates a high mixing rate, because the input of these particles is typically spatially concentrated within the rhizosphere or, more generally, along larger pores. Similar concepts could be developed based on the distribution of mineral-bound organic matter presumed to have previously moved as DOC within pore systems. A first glimpse along these lines was recently shown by Schlüter et al. (2022) and there is room for further promising developments.

Once powerful tools to quantify bioturbation and mixing rates are available there is an obvious way forward. It can be assumed that bioturbation by earthworms is directly related to their biomass or abundance and their ingestion rates which depend on soil and site characteristics and the soil management. So far, this has been limited to qualitative observation, which could be put on a more solid quantitative basis in the future, paving the way towards better, mechanistic modeling. For example, the occurrence and ratio of different life forms of earthworms as a function of soil bulk density, pH, temperature, soil water content, organic matter or tillage can then be translated into something like a local and a non-local mixing rate.

Changes in macroscopic structural properties after disturbance

The potential of biological processes to improve a disturbed soil structure is well known. The disturbance and subsequent recovery of the structure can go in two directions. Either a settlement after loosening (by tillage) or a loosening after compaction (by too heavy vehicles). The two main candidates here are plant roots and, again, burrowing soil animals, mainly earthworms. While the process understanding is available to a large extent, there is a lack of empirical data necessary to parameterize these processes in appropriate models. However, there is a steadily increasing body of scientific work that is examining the effects of plants and soil biota on soil structure for various boundary conditions which is promising. Examples are the capacity of plants to improve structural properties of the subsoil (e.g., Lucas et al. 2019a), the capacity of earthworms to burrow through compacted soil layers (e.g., Capowiez et al. 2021), the contrast in soil structure between tilled and non-tilled soil (e.g. Schlüter et al. 2018) and the settlement of tilled soil layers (e.g. Geris et al. 2021). With that, the required experimental evidence will grow successively.

Integration of structure dynamic into soil models

Quantitative knowledge on how biological processes alter soil structure should ideally be integrated into more general soil process models since structure impacts important functional properties. This is not only true for flow and transport processes but also, as discussed in the previous sections, for the turnover of SOM and the cycling of N and P. It is a critical challenge to explicitly include changing pore size distribution and pore connectivity of a dynamic pore system. Considering the impact of soil structure dynamics on soil functions requires physical models that can cope with a non-rigid pore space dynamically changing at each time step. This remains to be a challenge for future developments.

Conclusions

The ultimate goal is to improve available model tools so that they are capable of predicting the impact of external drivers such as climate and soil management on soil functions and, herewith, to improve the scientific basis for sustainable soil management. Due to their complex interactions, an adequate representation of biological processes is the most critical challenge.

Interaction of biological processes

In this review six process clusters were distinguished that are mainly biologically driven and the key biological processes for each were identified. Regarding this analysis in overview of the different process clusters (Figs. 1 and 3), it becomes immediately apparent that many processes are directly involved in a number of different process clusters. This well reflects the close process interactions in soil. Figure 3 illustrates how external drivers impact relevant soil state variables and soil functions, mediated through biological processes.

Challenges for modeling

Besides identifying the relevant biological processes, this review shows the extent to which biological processes have already been considered explicitly or implicitly in modern approaches to modeling soil functions. This extent is different for the different process clusters. For example, in modeling soil N dynamics, the attempt has been made to represent individual processes such as nitrification and denitrification depending on local conditions in terms of water content, redox potential as well as quantity and quality of organic matter. In contrast, for other processes such as organic-matter turnover, individual processes are typically not distinguished but are lumped in a “black-box” approach by using some conceptual pools and effective parameters, such as ecological stoichiometry, threshold element ratios and life strategy theory. Examples are rate parameters for the transfer of C between different C pools, the importance of denitrification as a function of water content, the degradation of pollutants as functions of the overall biological activity, or the vulnerability of crops to fungal pathogens as a function of crop diversity. In view of the sheer number of processes involved, a black-box approach is indeed an appealing concept and a well justified method to reduce complexity. This is needed to render the model applicable in the sense that the number of required parameters remains limited and the model can be more easily calibrated to available observations.

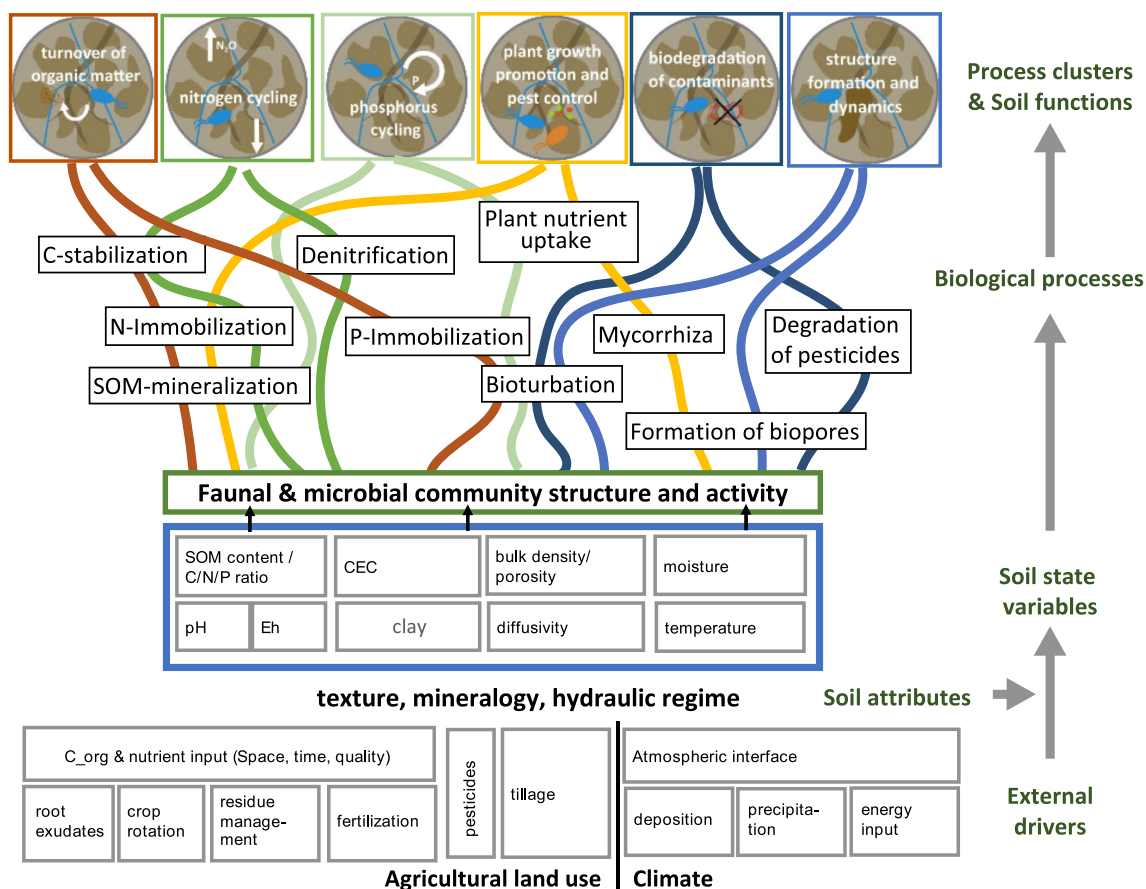


Fig. 3 The process clusters and related soil functions share a number of biological processes as indicated by the colored lines (the boxes of the processes are crossed by the lines of the process clusters to which they contribute). They depend on the structure and activity of the soil

biome which is sensitive to a number of soil state variables. These variables are sensitive to external drivers of land use and climate mediated by basic soil attributes

However, there are different shades of grey in these black-box approaches. The lumped effective parameters are tied to the underlying processes with varying degrees of rigor. In the simplest case, effective parameters are derived from state variables that are known to be well correlated with these parameters based on a statistical evaluation but without reference to the underlying processes. An example is the stabilization of organic matter which is assumed to be a fixed rate of some “active” organic pool as it is done in many models describing C turnover (Schimel 2023).

Ideally, our models should have predictive power and should react to changing boundary conditions in a realistic manner. To achieve this the model parameters need to be tied as closely as possible to the relevant processes. In this way, the models can be responsive to changing boundary conditions that have not yet occurred, such as climate change or can provide research into new management strategies for which solid observations are not yet available.

Strategies for upscaling and the right level of complexity

The key challenges are how to create model concepts that are closer to the actual processes and how detailed these processes need to be considered. The answers certainly depend on the purpose of the models and for which spatial and temporal scale they are designed for. For agricultural management, the target spatial scale is the soil pedon which can be considered as a functional unit representing an arable field. This is because soil processes are sensitive to the atmospheric boundary conditions and they interact vertically along the soil profile through water, matter and energy fluxes. These fluxes connect different horizons along the soil profile and are mainly vertical at the scale of pedons as long as the soil is not close to water saturation (Vogel 2019). Therefore, an upscaling of biological processes to the level of soil profiles is well justified and should be strived for. The central challenge is thus to describe the biological processes in as much detail as necessary so that the phenomena on the

pedon-scale can still be realistically represented. Concerning the temporal scale, the dynamics within a growing season should be addressed which leads to a required temporal resolution in the range of days or weeks.

It is well known that soils are heterogeneously structured at the various scales leading to micro- and mesoscopic hot spots and hot moments (Kuzakov and Blagodatskaya 2015; Thakur et al. 2020). Although there is considerable knowledge on biological processes at the scale of very local microbial and faunal communities and to some extent also on their interactions (Baveye et al. 2018), it seems, however, that it is prohibitive to obtain the required data for describing these processes at the individual or molecular level (Smercina et al. 2021). The problem is less the required computing power, but rather the fact that no means exist to measure the required initial conditions in terms of the spatial location and collocation of individual organisms and the nutrient resources (i.e. organic matter) on which they live. Another obstacle is the still incomplete understanding of the metabolic processes within heterogeneous microbial communities and the scale-dependent interactions with faunal populations. The obvious discrepancy in spatial and temporal scale between the ongoing processes and their macroscopic manifestation in terms of soil functions calls for appropriate strategies for upscaling.

Given the complex process interactions, upscaling strategies cannot be based on simple volume averaging. The various scales of spatial heterogeneity and the non-linear dynamics of individual processes (i.e. the switch from aerobic to anaerobic metabolism or the dormancy of microbes depending on soil moisture and resource availability) leads to a new quality of processes at the larger scales. Yet, to be able to well describe and model such emergent processes on the larger scale, it is certainly valuable to have a good understanding of the small-scale processes and their interactions. When it comes to organismic complexity, it is important to understand the processes at the scale of micro- and meso- habitats (Nunan 2017; Baveye et al. 2018) to come up with substantiated simplified descriptions at larger scales. A possible step towards upscaled model concepts appears to be the clustering of soil organisms into groups of similar guilds. This is also a widely used concept for a simplified description of food webs (Moore and Hunt 1988). However, it has been shown that in soil systems trophic chains are not directly linked to body size of the organisms as is the case for marine systems (Potapov et al. 2019). Yet, it is possible to assign certain functionalities to certain groups of organisms. Examples that were discussed in previous section of this paper are:

i) Burrowing animals such as earthworms (i.e. soil engineers) that generate macro-pores and mix soil components through bioturbation, while different activity rates

of life-form types, i.e. endogeic and anecic (Bottinelli et al. 2020), can be distinguished.

- ii) Mycorrhizal fungi which are able to massively expand the sphere of influence of root systems, both in terms of nutrient uptake and the release of organic compounds into the soil and soil organism food webs (Ryan and Graham 2018).
- iii) Saprophytic fungi that explore the entire soil volume and distribute inorganic nutrients via mycelial translocation (Tordoff et al. 2011) as well as organic matter within this volume in form of their necromass.
- iv) Groups of bacteria having different metabolisms in terms of, e.g., C use efficiency (Fierer et al. 2007).

To link these functionalities to the different guilds of organisms in modeling, much more knowledge is required about how these organism groups respond to external drivers such as climate change or land use. Increasing this knowledge could be an important step towards upscaling biological processes. With respect to C turnover and nutrient cycling there is some evidence that it might not be promising to distinguish functional guilds or organisms (Andr en et al. 1999; Griffiths et al. 2001). The enormous diversity of soil organisms contributes at various trophic levels and there is considerable redundancy with respect to the involved metabolic chains.

As discussed in the sections on C, N and P dynamics, ecological stoichiometry is considered to be a promising concept which has been well-established and successfully applied since quite a while in aquatic ecology (Anderson 1992; Elser and Urabe 1999). C use efficiency and nutrient cycling are sensitive to the stoichiometry of all the involved organisms and of the provided organic input. Hence, the dynamic interaction of litter quality, faunal and microbial activity can be modelled based on stoichiometric relations that are largely known. Together with the metabolic theory this would allow modeling of soil biological processes based on general laws of energy as well as C and nutrient constraints.

An appealing follow-up question would be whether the highly diverse (micro)biological communities might be reduced to some “effective” biome that reacts to boundary conditions such as temperature and moisture and, additionally, to the stoichiometric relations. There is some evidence that microbial metabolism has the potential to adapt itself to local conditions in terms of available substrates. For example, the ratio between microbial catabolism and anabolism is adapted but also the storage of energy and nutrients within living biomass to mitigate against stoichiometric imbalances (Mason-Jones et al. 2022). These features imply that also legacy effects and adaptation might be relevant for modeling. However, there are processes which can only be accomplished by a limited number of specialists and, thus, cannot be represented by some effective biome. Examples are the

denitrification to the final stage of N_2 , or the degradation of special classes of pollutants.

Besides the organismic complexity, also the soil structural complexity could be reduced by identifying characteristic spatial patterns of habitats or pore structural attributes. For instance, it has been demonstrated that a pore size range between 20 μm and 200 μm can be considered to be the “comfort zone” of microbial activity (Kravchenko et al. 2019). This is due to the simultaneous availability of water, O_2 and C sources in this pore size class. Based on X-ray CT, it is possible to characterize these pores in terms of volume and connectivity as potential indicators for microbial activity. Another structural indicator might be the density of large biopores originating from earthworms or plant roots that provide access for plants and soil organisms to deeper soil layers, improve aeration, and increase the infiltration capacity of the soils. In terms of soil aeration the mean distance of any point within the soil matrix to the next air-filled pore may serve as a valuable structural indicator which can be calculated using 3D x-ray CT images or the pore network (Rohe et al. 2021; Ortega-Ramírez et al. 2023).

The various concepts for upscaling leads to models in which the organisms driving the processes hardly appear as individual actors anymore. The main drivers are the changing state variables of the soils, which control the activity of the organisms. The concept “everything is *potentially* everywhere” shifts the focus towards external drivers and soil state variables, which then ultimately determine how the biological process clusters become established and stabilize. This is also illustrated in Fig. 3 where a relative limited number of soil state variables are the critical link between external drivers and the process clusters. Eventually, the processes need to be described as a function of the changing state variables that can either be directly observed or their dynamics can be modelled in response to the external drivers.

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Declarations

Competing interests None.

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