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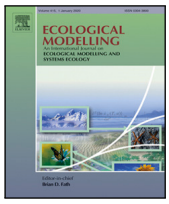

Buzy-pop: Multi-objective budget optimisation for constitutive and adaptive enzymatic activities of microbe populations

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ABSTRACT

Enzyme production is a key concept of the metabolism of microbe populations. Extracellular enzymes are notably responsible for the decomposition of the Particular Organic Matter (POM) in order to feed the Dissolved Available Matter (DAM) from where microbe populations and plants assimilate carbon (C), nitrogen (N) and phosphorus (P) based nutrients required for respiration and growth. The resource allocation theory tend to show that the production of enzymes by microbes dynamically adapts to the current needs of the population and to the composition of the POM and the DAM. @ However, it would be unrealistic to simulate all possible enzymes species, and the exact chemical composition of a real world POM and DAM is assumed unknown. In order to evaluate the decomposition of the substrate by a microbe population in this context, we propose the definition of generic *enzymatic actions* in a model called Buzy-pop. The notion of an *enzymatic budget* that can be allocated to each action allows to represent both constitutive and adaptive enzymatic activities according to the resource allocation theory. A multi-objective optimisation algorithm allocates the budget to available actions according to microscopic environmental conditions and life strategies of microbes, efficiently representing the decisions of microbe populations as the result of a compromise between sometimes contradictory objectives. The Buzy-pop model finally allows to dynamically compute quantitative decomposition rates of labile and recalcitrant C, N and P over time in any POM and DAM composition, and is configurable thanks to a carefully chosen set of meaningful parameters that could be calibrated to fit results to real world cases. Because of its low input parameters requirements and its extensibility, Buzy-pop could be used in many contexts. Calibration is provided for a set of life strategies (Opportunists, Foragers and Minimalists) as an use case example. Experimental results prove its consistency with theoretical expectations about the behaviour of microbe populations according to the proposed life strategies.

1. Introduction

Soil organic matter (SOM) is a reservoir of carbon (C), nitrogen (N) and phosphorus (P), which plays a vital role both in climate regulation (Ågren, 2010) and in plant production, and therefore in food security. There is a real challenge in modelling the dynamics of the decomposition of these organic materials in order to predict its evolution in response to the different components of global change. The decomposition of the SOM in classic models representing C/N/P cycles (Achat et al., 2016) is generally described using first-order kinetics to describe fluxes between matter compartments (as in CENTURY (Parton et al., 1988), RothC (Coleman and Jenkinson, 1996), DNDC (Gilhespy et al., 2014), Ecosys (Grant et al., 2001), CASA-CNP (Wang et al., 2010), N14CP (Davies et al., 2016)...). Such method cannot be used to represent the complex microbial dynamics at the local scale to understand interactions between soil processes (Lehmann et al., 2020). For example, such models implicitly include in their decomposition parameters phenomena still not understood as the priming effect (PE). This approach implies that the PE is fixed in space and time and do not depends on microbial parameters, an hypothesis partly invalidated in numerous works, as highlighted in the review of Bernard et al. (2022). Several scientists predict that PE will play a major role in how C balances are affected by global changes (Hungate et al., 2009; Terrer et al., 2021). In order to understand and quantify soil processes such as PE, it is necessary to explicitly represent them as a consequence of microbial, physical and chemical processes instead of just considering them implicitly. More generally, we lack clear theoretical frameworks that link the micrometric scales where the transformation processes of organic materials take place under the action of microorganisms and the interactions with their environment and the scales where we are in capacity to manage organic matters (Lehmann et al., 2020).

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Several models have been recently developed to offer a more realistic view of microbial decomposition of organic materials, by taking into accounts, trait-based extracellular enzymes (Allison, 2012; Traving et al., 2015), microbial functional guilds (Allison, 2012; Kaiser et al., 2014; Song et al., 2017) and spatialised interactions (Allison, 2012; Kaiser et al., 2014). All these models challenged the traditional view that organic matter decomposition and nutrient recycling depended only on the imbalance between the stoichiometry of the substrate and microbial biomass.

Models such as C-STABILITY (Sainte-Marie et al., 2021) switch from a compartmental to a continuous representation of organic matter. However, it is still not enough to represent the adaptation of microbe behaviours to their environment and the decomposition of N and P. Hence the efforts of the scientific community to develop models (Allison, 2012; Kaiser et al., 2014) that include key characteristics of microbial metabolism such as dynamic organic matter decomposition to be able to test and simulate significant ecological hypotheses.

On a dynamic level, the fresh organic matter which enters the soil mainly originates from plants (aerial and root parts), the animal contribution being relatively low (Kögel-Knabner, 2002). Heterotrophic microorganisms, bacteria and fungi are the first decomposers of SOM. All of them are represented as *microbe populations*, defined in our context as spatially confined aggregates of microbes with their own functional characteristics. They break down plant, microbial or animal residues (i.e. Particulate Organic Matter, or POM) by producing extracellular or membrane-bound enzymes that will depolymerise large compounds to release smaller compounds into the soil solution, to form Dissolved Organic Matter (DOM). Only molecules less than 600 Da, produced by the action of enzymes, can be transported through microbial walls and membranes (i.e. Dissolved Assimilable Matter, or DAM) to be assimilated there (Lehmann and Kleber, 2015). Intracellular enzymes are also used in the nutrient assimilation processes, but are not explicitly considered in this study since they have no direct influence on the flows between microbes, the DAM and the POM.

Microbes can produce a wide diversity of extracellular enzymes in order to establish various decomposition strategies. The quantity of each enzyme produced can be *constitutive* — i.e. continuously produced in constant quantity by the microbe, without any adaptation to the environment—, or *adapted* to the current needs of the microbes, the composition of the decomposed substrate (POM) and the nutrients already available (DAM), according to the resource allocation theory. The adaptation of microbes is especially relevant in the context of increasing N and P inputs in soils due to human activities (Schleuss et al., 2021). Strategies implemented by microbes are however very complex and hard to predict. For example, the study of Chen et al. (2018) shows that high mineral N availability produces a decrease of the activity of *glycine aminopeptidase*, an increase of the activity of *urease* and no impact on the activity of *leucine aminopeptidase*. On the other hand, considering the resource allocation theory, we might expect at a first glance that their activity should globally reduce due to an increase of available mineral N. This tend to show that the production of N extracting enzymes cannot be driven by a single parameter such as N availability, but also by other criteria such as C and P availability (Schleuss et al., 2021), the chemical composition of the substrate and the nutrients uptake strategies of populations (Geisseler et al., 2010).

Such complexity is a strong motivation to implement a flexible enzymatic activity model to allow soil experts to easily test and adapt different hypotheses. Considering the high diversity of microbes, enzymes and strategies, it is required to choose a minimalist set of significant parameters to keep the model tractable and easy to configure in each context.

Moreover, modelling flows of C/N/P in soils at local scales in terms of space (μm to mm) and time (hours to days) is required to understand the soil mechanics at the landscape level, as the microbe populations occupy less than 1 % of the bulk soil, concentrating their activity in *hotspots* (Kuzyakov and Blagodatskaya, 2015). Modelling population dynamics at this scale requires to be able to model local decisions performed by microbe populations as they dynamically adapt to their environment. Considering variations in the metabolism of microbes and the compositions of the POM and the DAM at a time scale of one hour implies to quantitatively estimate the microbial decomposition of C/N/P compartments at such a small time step. Moreover, the resource allocation theory tends to show that enzymatic activities of microbes must dynamically adapt to properly represent the dynamics of populations according to their evolving environment.

In the following sections, we propose the definition of an innovative enzymatic activity model, Buzy-pop, to overcome the following constraints:

1. The model must simulate quantitative C/N/P flows between the compartments of POM and DAM.
2. The exact chemical composition of the POM and the DAM is unknown.
3. A part of the enzymatic activities of each population might be constitutive.
4. A part of the enzymatic activities of each population must adapt to the environment.
5. The spatial environment of microbes (POM and DAM) varies significantly over time at the local scale.

Even if some of the previously cited models solve part of those issues, no existing model can currently solve all of them. For example, DEMENT (Allison, 2012) and the model of Kaiser et al. (2014) propose to optimise enzymatic strategies of microbial communities thanks to a selection in a spatialised environment. Even if such propositions allow to represent adaptation at the level of a community, they do not account for adaptation at each population level (Traving et al., 2015) and do not explicitly include constitutive enzymatic rates. Models based on chemical speciation (Song et al., 2017) also limit the application of the model to complex soil systems (Lehmann et al., 2020). Its worse noticing Buzy-pop can but do not require to be included in a spatialised environment, thanks to the usage of a generic optimisation algorithm. The explicit and extensible goal-oriented specification of the model is also a significant advantage of Buzy-pop.

The design of the Buzy-pop model is an exploratory work that demonstrates how the proposed formalism and methods allow to accurately represent the enzymatic adaptation of microbes according to their strategies and local environment. Even if classical enzymatic kinetics models (e.g. Michaelis–Menten equations) allow to represent the activity of each enzymatic species, Buzy-pop is focused on (1) an aggregated representation of a real soil system that can include hundreds of enzymatic species and (2) the adaptation of microbes according to the resource allocation theory . Agent based modelling (ABM) notably allows to consider microbe populations as active entities who perceive and adapt to their environment, what seems particularly adapted in the context of our study. This leads to several contributions:

1. definition of a set of generic *enzymatic actions* and equations to evaluate the associated C/N/P flows.
2. definition of the *enzymatic budget* formalism, that allows to represent constitutive and adaptive enzymatic activities according to the resource allocation theory.
3. a multi-objective method to optimise the enzymatic budget according to microscopic environmental conditions and life strategies of microbe populations.
4. an example application to calibrate and test the model from qualitative characteristics of the proposed O-F-M strategies (Opportunists, Foragers and Minimalists).

The usage of an agent oriented optimisation method is particularly adapted to the previous constrains compared to other mathematical modelling techniques, as the latter would require lots of specific data

Table 1
Nutrient compartments entities.

Entity	State variables		
Recalcitrant OM	C_{recal}	N_{recal}	P_{recal}
Labile OM	C_{labile}	N_{labile}	P_{labile}
Dissolved Organic Matter (DOM)	C_{dom}	N_{dom}	P_{dom}
Dissolved Inorganic Matter (DIM)	N_{dim}	P_{dim}	

to be calibrated, while the former can be theoretically validated as it directly represents the expected logical behaviour of microbe populations. The agent oriented method is also expected to better adapt to complex and unexpected environmental conditions.

2. Model and methods

The description of Buzy-pop — including the enzymatic actions, the enzymatic budget and the optimisation method — is provided in this section using the Overview, Design concepts and Details (ODD) protocol (Grimm et al., 2020), allowing a logical, readable and reproducible specification of the model. The ODD protocol also allows a progressive level of abstraction of the model, from general purpose and patterns to detailed equations provided in submodels. This scheme is particularly efficient in the current interdisciplinary context. Experimental results obtained from the calibration of the model for O-F-M life strategies are provided in Section 3. A complete model implementation is available within the CAMMISOL project (Breugnot et al., 2024).

2.1. Purpose

The objective of the model is to quantitatively predict exchanges of matter within the POM and the DAM implied by the enzymatic activity of a single microbe population.

Results of the model represent (1) flows of C/N/P from the POM to the DAM induced by the enzymatic activity of the microbe population (decomposition), and (2) the adaptation of the enzymatic activity of the population according to the POM, the DAM and the characteristics of the population (optimisation).

2.2. Entities

2.2.1. Matter compartments (POM and DAM)

The model contains four passive entities (Table 1) that represent matter compartments used to represent C, N and P cycles. Quantities are expressed in grams, but other units could be used as long as the consistency of units is preserved.

The POM is divided in two compartments: *Recalcitrant OM* and *Labile OM*. The exact chemical composition of each compartment is assumed unknown.

The recalcitrant OM is composed of macromolecules of variable C, N and P composition that includes bonds that are hard to break such as lignin, tannins or phytate. It also includes long molecules whose fragmentation does not directly provide a return on investment for the population producing the enzyme, such as cellulose, fatty acids or chitin. The decomposition of recalcitrant OM to labile OM thus requires specialised enzymes that are not available to all decomposers. Recalcitrant matter can more generally be defined as matter which decomposition presents a low return on investment due not only to the structure of molecules but also to their spatial and temporal diversity (Lehmann et al., 2020). Users of Buzy-pop are free to feed the recalcitrant matter pool according to their own criteria.

The DAM is also divided in two compartments: the DOM and the DIM. The DOM contains small-sized organic matter molecules (< 600 Da) assimilable by the microbe population. The DIM represents mineral N and P in that same solution, also assimilable by the microbe population.

Table 2
Microbe population entity.

State variable	Description
C_M	Active structural C. It represents the size of the awoken population.
$C{:}N_M$	Structural C:N ratio.
$C{:}P_M$	Structural C:P ratio.
$\tau_{e,min}, e \in [e_r, e_C, e_N, e_P]$	Constitutive activity rate of each enzyme.
$\tau_{e,max}, e \in [e_r, e_C, e_N, e_P]$	Maximum activity rate of each enzyme.
$\tau_e, e \in [e_r, e_C, e_N, e_P]$	Current activity rate of each enzyme.

2.2.2. Microbe population

The *Microbe population* (Table 2) is the only active entity of the model. Microbes in a population do not necessarily belong to a common species, but rather share a common functional behaviour, represented by parameters defined at the scale of each population (Song et al., 2017). The enzymatic activity generated by each microbe population is assumed proportional to the active weight of the population. Its needs are represented by required C:N and C:P ratios, that might vary over time. The capacity of the population to decompose the POM is represented with constitutive and maximum activity ratios. The nature and usage of those ratios are described in Section 2.3.

Characteristics of each population can notably be set to reflect the behaviour of microbes at the scale of aggregated populations according to identified life strategies such as *r*- and *K*- strategies, C-S-R (Fierer, 2017; Krause et al., 2014; Ho et al., 2017) or *Y-A-S* (Malik et al., 2020). An instantiation of parameters reflecting our own *O-F-M* strategies and associated experiments are proposed in Section 3.

2.2.3. Spatial and time scales

The model is intended to work at time scales in the order of 1 hour to 1 day. However, the mathematical specification of the model allows to estimate enzymatic activity over an arbitrary duration. In consequence, the model might be used on smaller or bigger scales, as long as equations and hypothesis seem consistent at the considered scale. This allows the Buzy-pop model to be applied both for low definition simulations with a very small optimisation time step and for large scale simulations that can be based on static results of Buzy-pop obtained in a generic context.

It is more adapted to deal with weight scales rather than spatial scales in our context, as spatial characteristics are not explicitly considered. The model is designed to work at the scale of a microbe population, ranging from the order of 10^{-9} g to 1 g, what corresponds to soil dimensions in the order of 1 µm to 1 cm. The decomposed POM and DAM are assumed to be represented at the same scale as the microbe population.

2.3. Process overview and scheduling

Before describing the processes that occur in the model, we propose to introduce the notion of *enzymatic actions*.

2.3.1. Enzymatic actions

Inspired from the methodology of the Y-A-S classification (Malik et al., 2020), we propose to group enzymes into *families of enzymes* with a generic *action* on the decomposed substrate, as already proposed in the context of the C-STABILITY model (Sainte-Marie et al., 2021) where enzymes are represented by type of actions (depolymerisation of C in the context of C-STABILITY) on the substrate rather than by chemical species.[1] Enzymatic actions proposed in the current model are represented on Fig. 1. The set of enzymatic actions could be refined

[1] [(Sainte-Marie et al., 2021)][]"e.g., combined action of endoglucanase, exoglucanase, betaglucosidase, etc., on cellulose will be reported as cellulolytic action"

as required in future developments of the model, without altering its global structure.

The first enzymatic action considered is the *recalcitrant cleavage* action (e_r), which consists in breaking coarse recalcitrant C based molecules into smaller and more labile compounds, but not yet assimilable. This action brings together the activities of numerous enzymes such as laccases, peroxidases, cellulases, tannases, lipases, endoproteases, endochitinases, and endonucleases. Doing so, trapped N and P is released in the *Labile OM* in addition to C according to the C:N and C:P ratios of the recalcitrant OM. Actually, even if lignins and tannins are not constituted of N and P themselves, other N and P enriched molecules can be trapped in their complex structures. Therefore, we assume that recalcitrant cleavage on such C-enriched molecules can release N and P in the *Labile OM*. In order to model the special action of phytases, a small fraction $\alpha^P_{e_r}$ of the released P is directly sent to the DIM, modelling the first P extracted from recalcitrant phytic acid molecules. The rest of the molecule is released into the *Labile OM*. The parameter $\alpha^P_{e_r}$ depends both on the ability of microbe populations to produce phytases, but also on the phytic acid concentration in the recalcitrant OM, a parameter assumed unknown.

The labile OM is assumed to be constituted by a pool of polypeptides, carbohydrates, polynucleotides and aliphatic compounds smaller than recalcitrant matter but too big to be assimilated, in unknown proportions. Contrary to recalcitrant matter, labile molecules are assumed to be independent, i.e. enzymes can target specific molecules that are not trapped in bigger ones. Three more types of actions can then be defined from labile OM to DAM:

1. Decomposition of sugars, carbohydrates, proteins and fatty acids (*CNP extraction*, e_{CNP}): reduces the size of carbon based polymers (depolymerisation) using endocleaving and exocleaving enzymes. Produces C/N/P compounds with C:N and C:P ratios corresponding to the C:N and C:P ratios of labile OM.
2. Decomposition of polypeptides and amino sugars (*N extraction*, e_N): extracts assimilable amino acids from polypeptides or N-acetyl glucosamine — which is the building block of chitin molecules — from amino sugars. Represents the grouped actions of aminopeptidases and N-acetyl glucosamidase. The C:N ratio μ_{CN} of the decomposed matter is expected to represent the distribution of amino acids and N-acetyl glucosamine in the decomposed matter.
3. Mineralisation of P (*P extraction*, e_P): extracts P into the DIM. Represents the decomposition of phosphate groups by the combined action of phosphomonoesterases and phosphodiesterases.

Detailed explanations and schemes of each enzymatic action are provided in the *decomposition* submodel (Section 2.7.1).

Mineralisation of N is currently not considered in the model, assuming N uptake is only performed from organic compounds (direct route). Future works might however include the mineralisation of N to the set of enzymatic actions, as it might represent an adaption of the population to the environment (Geisseler et al., 2010).

Each enzymatic action e is associated to an enzymatic activity rate, τ_e. Values of τ_e are expressed in grams of substrate s per gram of active structural microbial C per day ($g_s\, g_M^{-1}\, d^{-1}$). The nature of the substrate attacked by each enzymatic action (Table 3) is important to consider when defining values of enzymatic rates. For example, all the labile C can be attacked by *CNP extraction* even if quantities of labile N and P are very low, while only C grouped with N (respectively P) according to a μ_{CN} (respectively μ_{CP}) ratio can be attacked by *N extraction* (respectively *P extraction*).

The amount of resources invested in each enzymatic action is represented in Buzy-pop introducing the concept of *enzymatic budget*, explained in detailed in the *decomposition* submodel (Section 2.7.1). This formalism is a key contribution of the Buzy-pop model design, as it allows to represent both the constitutive and adaptive enzymatic activities using an explicit set of parameters and equations. Moreover, the approach could be easily adapted or extended to other enzymatic actions.

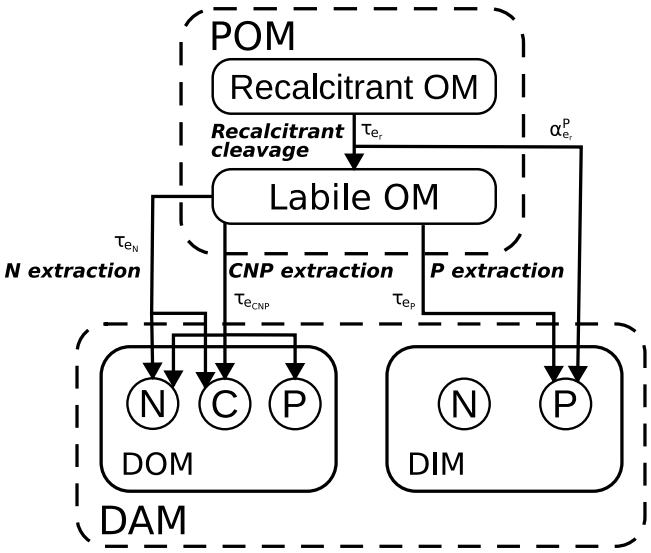


Fig. 1. Enzymatic actions.

Table 3
Substrate attacked by each enzymatic action. $C_{N,labile}$ denotes the quantity of labile C grouped with labile N included in polypeptides and chitin (amino acids and N-acetyl glucosamine), $C_{P,labile}$ represents sections of carbon polymers (of size μ_{CP}) bound to a phosphate group.

Enzyme	Substrate
e_r	C_{recal}
e_{CNP}	C_{labile}
e_N	$C_{N,labile}$
e_P	$C_{P,labile}$

2.3.2. Decomposition and optimisation

Two processes occur in the model.

Decomposition. Represents the passive decomposition of matter that occur at each time step according to the current activity of each action, τ_e. Equations used to compute the flows of C/N/P at each time step are described in the *decomposition* submodel (Section 2.7.1).

Optimisation. Action triggered by the microbe population to optimise the enzymatic activity of each action according to its needs, the POM and the DAM. More details are presented in Section 2.4.5 and in the *optimisation* submodel (Section 2.7.2).

2.3.3. Scheduling

The *decomposition* process occurs at each time step in order to update the composition of all matter compartments according to the current enzymatic activities. External inputs and outputs to the POM and the DAM might occur between each decomposition cycle, as model inputs. Flows of C/N/P can be computed at each time step from equations proposed in the *decomposition* submodel.

In order to update activity rates, the *optimisation* process can be used. Conditions to trigger this action is left to the modeller, and might be considered as a parameter of the model. *Optimisation* could for example occur at each time step, every 10 h, when the quality of the available nutrients reaches a given threshold, or only at the initialisation of the model from a default POM and DAM composition.

2.4. Design concepts

2.4.1. Basic principles

The enzymatic activities of the *Microbe population* result from the optimisation of the enzymatic budget allocation x with a generic optimisation algorithm according to a set of objectives that should reflect the biological behaviour of microbe populations. Multi-objective optimisation allows to represent the fact that several objectives might be contradictory considering the constrained enzymatic budget, so that compromises should be made, as detailed in Section 2.4.5.

The proposition is consistent with the resource allocation theory that states that microbes adapt their production of enzymes to their environment to best fit their needs (Mooshammer et al., 2012; Chen et al., 2018; Schleuss et al., 2021).

2.4.2. Emergence

Strategies established by the *Microbe population* in each environmental condition are an emergent behaviour, as corresponding enzymatic activities result only from simpler rules to specify:

1. The effect of each *enzymatic action* (*decomposition* submodel, Section 2.7.1).
2. The optimisation of explicit and simple objectives, defined from the expected behaviours of microbe populations (Section 2.4.5).

2.4.3. Adaptation

The optimisation of enzymatic activities is an adaptation of the *Microbe population* to the current POM and DAM. It might for example be expected than when N or P are limited in the DAM, the microbe population should invest more in *N extraction* or *P extraction*. On the contrary, less should be invested in those actions if N or P are in excess in the DAM. Moreover, when C, N and P are limited in the labile OM compared to the maximum enzymatic activity of the population, the population should decompose the available recalcitrant OM to feed the labile OM, if it has the ability to do so.

2.4.4. Learning

No learning process is involved in the model.

2.4.5. Objectives

An objective is defined as a function $f_i : X \to [0, 1]$, associated to a weight ω_i. The purpose of optimisation algorithms is to find values of x that minimise f_i, i.e. so that the value of $f_i(x)$ is as close as possible to 0 in this case.

The following objectives are defined:

1. *MaxLabileC*: Maximises the quantity of produced labile C.
2. *MaxC*: Maximises the quantity of produced available C.
3. *CapCN*: Minimises the C:N ratio of available nutrients so that it is at most equal to the target C:N ratio. A smaller C:N ratio is assumed to satisfy the needs of the microbe population, as it represents an excess of N. On the other hand, a bigger C:N ratio reflects a lack of N compared to the available C.
4. *CapCP*: Analogous to *CapCN*.

Mathematical expressions of each objective and their associated weights are described in Appendix A, Table A.8.

The consideration of those objectives reflects the complexity of microbe populations strategies, that must find compromises between all of them. Maximising the availability of C notably contradicts the *CapCN* and *CapCP* objectives because it increases the available C:N and C:P ratios. Investing in *recalcitrant cleavage* also implies to reduce energy invested in other actions. However, all those objectives are useful for the microbe population. Moreover, *CapCN* and *CapCP* objectives tend to increase available N and P production until the required ratios are reached. Combined with the *MaxC* objective, that tend to maximise the production of available C, the complete set of objectives tends to maximise the production of available C/N/P nutrients, while keeping available C:N and C:P ratios acceptable.

In consequence, the budget should be optimised as a *multi-objective optimisation problem*, detailed in the *optimisation* submodel (Section 2.7.2).

Notice that other objectives might be designed as extensions of the model, for example to make available C:N and C:P ratios tend to exact values and not only cap them.

2.4.6. Prediction

The optimisation process is made possible considering that the *Microbe population* can use the decomposition equations introduced in the *decomposition* submodel (Section 2.7.1) to predict the quantity of nutrients they could receive if they implement a possible enzymatic budget allocation x. Objectives can then be applied to the predicted compositions of compartments to evaluate the quality of the budget allocation x.

2.4.7. Sensing

The *Microbe population* perceives the composition of the recalcitrant OM, labile OM, DOM and DIM at the current time step. The model thus assumes that the population always has a perfect perception of its environment.

2.4.8. Interaction

In practice, several *Microbe populations* might cohabit and try to decompose a common substrate. No direct interaction occurs between populations, and the current study is voluntarily limited to the case where only a single *Microbe population* exists. However, Buzy-pop can easily account for mediated interactions, applying the decomposition model on a substrate shared by microbes populations that independently optimise their enzymatic activities. See possible extensions presented in Appendix C.1 for more detailed explanations.

2.4.9. Stochasticity

Because metaheuristics such as simulated annealing provide approximate solutions, results of the model might depend on random features used internally by the optimisation algorithm. This is however a side effect that is only due to approximation, since perceptions and actions used in the model are completely deterministic.

Although it is very unlikely to occur in practice, the objective function could mathematically be minimised by several budget allocations. In this case, the solution can be considered as chosen randomly by the simulated annealing algorithm. Due to approximations, the fact that many budget allocations might result in objective values close to the theoretical optimum increases the variability of the results.

2.4.10. Collectives

No collective organisation is currently considered in the model, although considering the dynamics of *Microbe population* collectives would be interesting for model integration in other systems. See possible extensions presented in Appendix C.1.

2.4.11. Observation

The main observation of the model is the enzymatic activities of the *Microbe population*. The decomposition of the POM and DAM resulting from those activities can be observed as an output of the *decomposition* submodel.

2.5. Initialisation

Each instance of the model is created by initialising a *Labile OM*, a *Recalcitrant OM*, a *DOM* and a *DIM*, by specifying the initial C, N and P quantities of each entity (Table 1).

Then, a single *Microbe population* entity (Table 2) is initialised specifying values for the following parameters:

- C_M;
- Structural C:N$_M$ and C:P$_M$ ratios;
- $\tau_{e,min}$ and $\tau_{e,max}$ for each enzymatic action.

τ_e values do not need to be initialised, as they are set by the *optimisation* action. See B for a method to define $\tau_{e,min}$ and $\tau_{e,max}$ from a single *base* set of enzymatic activities.

The model is designed for an iterative application: the state of the model at each time step can be reinitialised from the previous time step. In consequence, considering dynamic needs and enzymatic capacities of the *Microbe population* is a valid use case of the model. When it is relevant, the current time step at which the model is initialised is denoted by t. The *decomposition* then consists in evaluating the updated composition of compartments at time $t + 1$.

Other parameters are required for the usage of the *decomposition* submodel, and are detailed in the dedicated section.

2.6. Input data

No input data is used by the model to represent time-varying processes. The evolution of input POM and DAM compartments due to external processes could however be used as input data.

2.7. Submodels

Detailed explanations and equations about the *decomposition* and *optimisation* processes are provided in this section as submodels.

2.7.1. Decomposition submodel

The purpose of this model is to compute the flows of C/N/P between the POM and the DAM given their initial composition and enzymatic activities.

A *decomposition problem* is defined from values of $\tau_{e,min}$ and $\tau_{e,max}$. $\tau_{e,min}$ represents constitutive enzymatic rates, so that $\forall e, \tau_e \geq \tau_{e,min}$. $\tau_{e,max}$ is then defined so that $\tau_e = \tau_{e,max}$ if and only if the population dedicates all its enzymatic capacity to the action e, and $\tau_e < \tau_{e,max}$ otherwise. The resource allocation theory indeed states that all τ_e cannot be equal to each $\tau_{e,max}$, so that a compromise should be made to invest energy in each enzymatic action e.

In order to model the allocation of energy to each action, we assume that the population owns an *enzymatic budget*, that must be shared between enzymatic actions. For each enzymatic action e, τ_e is equal to $\tau_{e,max}$ if and only if all the budget is invested in e, and $\tau_e \in [\tau_{e,min}, \tau_{e,max})$ otherwise. The problem then consists in computing possible τ_e values. To do so, we define the enzymatic budget allocation (x_r, x_{CNP}, x_N, x_P) and the solution set X as:

$$X = \{(x_{e_r}, x_{e_{CNP}}, x_{e_N}, x_{e_P}) \in [0,1]^4, x_{e_r} + x_{e_{CNP}} + x_{e_N} + x_{e_P} = 1\} \quad (1)$$

Each $x \in X$ is considered a *solution* of the *decomposition problem*, as it can be used to compute values of τ_e that are compliant with the previous constraints, using the following equation:

$$\tau_e = \tau_{e,min} + x_e(\tau_{e,max} - \tau_{e,min}) \quad (2)$$

Examples of enzymatic activities resulting from various budget allocations are provided on Fig. 2.

The quantity of each substrate nutrient $j \in [\mathrm{C}, \mathrm{N}, \mathrm{P}]$ *requested* by each enzymatic action e is noted $\delta^j_{e,x}$ where x is the current enzymatic budget. Since each enzymatic action can only attack a single compartment (*labile* or *recalcitrant*), the labile or recalcitrant origin of j is implicit. For convenience, the notations δ^j_e will be used when the value of x does not need to be explicit. $x_e = 1$ might also be used as a value for x to denote the single possible budget allocation $x \in X$ such that the allocated budget is 1 for e and null for all other enzymes.

The quantity of nutrient j on which e can finally perform its action, i.e. the quantity *decomposed* by e, is similarly noted $\Delta^j_{e,x}$ or Δ^j_e. δ^j_e is used to compute Δ^j_e, but Δ^j_e is not necessarily equal to δ^j_e. Indeed, several actions can *request* a common substrate, but since a substrate section can only be *decomposed* by one enzymatic action, the quantity *decomposed* by each enzymatic action will correspond to a fraction of what they *requested*.

Parameters specific to the decomposition submodel are presented on Table 4. Their usage is detailed in following explanations.

Table 4
Parameters specific to the decomposition model.

Parameter	Domain	Description
μ_{CN}	$\mathbb{R}^*_+$	C:N ratio of matter produced by *N extraction*.
μ_{CP}	$\mathbb{R}^*_+$	C:P ratio of matter requested by *P extraction*.
$\alpha^P_{e_r}$	$[0, 1]$	Rate of P mineralised by *recalcitrant cleavage*.
β_{e_i,e_j}	$[0, 1]$	Concurrent enzymatic action rates.

In the general case, the quantity of substrate s requested by e can be computed with

$$\delta^s_e = \min(C_M \tau_e \Delta t, S) \quad (3)$$

where S is the quantity of substrate and Δt is the period of time over which the decomposition should be calculated.

The *recalcitrant cleavage* action is the only one to decompose recalcitrant matter. Decomposed quantities can then be expressed as follows:

$$\Delta^C_{e_r} = \delta^{C_{recal}}_{e_r} = \min(C_M \tau_{e_r} \Delta t, C_{recal}) \quad (4)$$

$$\Delta^N_{e_r} = \Delta^C_{e_r} \frac{N_{recal}}{C_{recal}} \quad (5)$$

$$\Delta^P_{e_r} = \Delta^C_{e_r} \frac{P_{recal}}{C_{recal}} \quad (6)$$

The quantity of C requested by *CNP extraction* can be computed directly applying Eq. (3), assuming the following hypothesis.

Hypothesis 1. All the labile C can be considered as substrate for *CNP extraction* (i.e. sugars, carboxylic acids or proteins).

This is a strong hypothesis, currently required by the fact that the composition of labile OM is unknown.

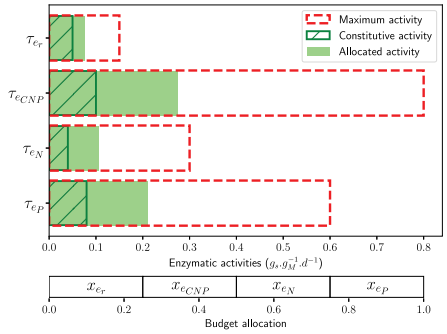
The composition of products of *CNP extraction* depends on the C:N and C:P ratios of the labile substrate. If N and P are scarce, *CNP extraction* might correspond to cellulolytic action as the products is almost only constituted by C, but if N and P are abondant, *CNP extraction* mostly corresponds to the depolymerisation of proteins by DNAases or RNAases. Grouping all those enzymatic activities as *CNP extraction* is a relevant and efficient simplification, as they are all based on the depolymerisation of carbon chains.

Then we can define:

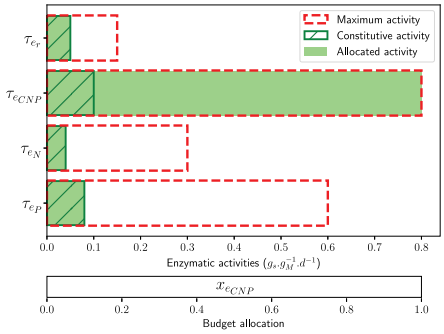
$$\delta^C_{e_{CNP}} = \min(C_M \tau_{e_{CNP}} \Delta t, C_{labile}) \quad (7)$$

For *N extraction*, we need to introduce an other hypothesis.

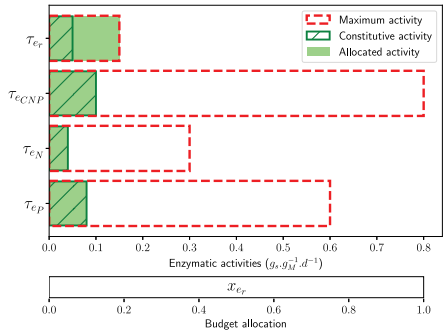
Hypothesis 2. All the labile C and N can be considered as substrate for *N extraction* (i.e. polypeptides and amino acids).



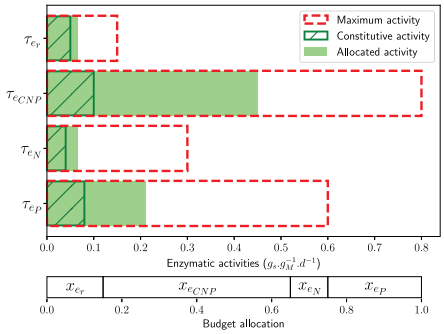
(a) Equal budget allocation for all enzymatic actions. Notice that this does not result in an equal activity for all actions.



(b) Activities resulting from the allocation of all the budget to *CNP extraction*. Even if no budget is allocated to other actions, constitutive rates are still included in allocated activities.



(c) Activities resulting from the allocation of all the budget to *recalcitrant cleavage*. The resulting absolute activity is completely different from case (b).



(d) Example of an arbitrary budget allocation.

Fig. 2. Examples of budget allocations.

The quantity of labile C included in amino acids and polypeptides is then defined as:

$$C_N = \min(C_{labile}, N_{labile}\,\mu_{CN}) \tag{8}$$

where μ_{CN} is the fixed C:N ratio of products of the *N extraction* action. Then comes:

$$\delta^C_{e_C} = \min(C_M\,\tau_{e_N}\,\Delta t, C_N) \tag{9}$$

A last hypothesis is finally introduced for *P extraction*.

Hypothesis 3. All the labile C and P can be considered as substrate for *P extraction*.

The quantity of C that can be considered bound to phosphate is computed as:

$$C_P = \min(C_{labile}, P_{labile}\,\mu_{CP}) \tag{10}$$

where μ_{CP} is the count of C in the polymer section bound to each P and attacked by *P extraction*. This quantity of C is requested, but not included in products as only the phosphate is extracted to the DIM.

Then we have:

$$\delta^C_{e_P} = \min(C_M\,\tau_{e_P}\,\Delta t, C_P) \tag{11}$$

Remark. Hypotheses 1 to 3 seem contradictory, since in reality a given amount of C/N/P cannot be a substrate for all enzymatic activities, as each substrate corresponds to a specific chemical species. However, since the composition of the labile OM is unknown, those hypotheses are considered satisfying for the current model. The contradiction could be solved in future works, either fixing a rate of the total C/N/P that can be considered substrate for each action, or explicitly considering the chemical speciation of C/N/P, what would significantly increase the number of parameters and the complexity of the model. The fact that results of the model rarely represent a situation where all the substrate is decomposed by a single action also moderates the impact of each hypothesis.

We now define β_{e_i,e_j} that represents the fraction of C *decomposed* by e_i when only e_i and e_j are *requesting* all the C of the substrate.[2] By definition, $\beta_{e_j,e_i} = 1 - \beta_{e_i,e_j}$. We can then compute the decomposition $\Delta^C_{e_i}$ values as follows:

$$\Delta^C_{e_{CNP}} = \delta^C_{e_{CNP}} - \beta_{e_N,e_{CNP}}\frac{\delta^C_{e_{CNP}}\delta^C_{e_N}}{C_{labile}} - \beta_{e_P,e_{CNP}}\frac{\delta^C_{e_{CNP}}\delta^C_{e_P}}{C_{labile}} \tag{12}$$

$$\Delta^C_{e_N} = \delta^C_{e_N} - \beta_{e_{CNP},e_N}\frac{\delta^C_{e_N}\delta^C_{e_{CNP}}}{C_{labile}} - \beta_{e_P,e_N}\frac{\delta^C_{e_N}\delta^C_{e_P}}{C_{labile}} \tag{13}$$

$$\Delta^C_{e_P} = \delta^C_{e_P} - \beta_{e_{CNP},e_P}\frac{\delta^C_{e_P}\delta^C_{e_{CNP}}}{C_{labile}} - \beta_{e_N,e_P}\frac{\delta^C_{e_P}\delta^C_{e_N}}{C_{labile}} \tag{14}$$

Decomposed quantities of N and P can then be deduced as:

$$\Delta^N_{e_C} = 0 \qquad \Delta^N_{e_N} = \Delta^C_{e_C}/\mu_{CN} \qquad \Delta^N_{e_P} = 0 \tag{15}$$

$$\Delta^P_{e_C} = 0 \qquad \Delta^P_{e_N} = 0 \qquad \Delta^P_{e_P} = \Delta^C_{e_P}/\mu_{CP} \tag{16}$$

A last effort is required to compute the flows of C/N/P obtained from the *decomposition* performed by each enzymatic activity, representing the quantities of *substrates* consumed by each enzymatic activity and associated *products*. For example, the P *decomposed* by e_r is $\Delta^P_{e_r}$, so

[2] For example, according to Eq. (12), $\Delta^C_{e_C} = \beta_{e_C,e_N} C_{labile}$ when $\delta^C_{e_C} = \delta^C_{e_N} = C_{labile}$ and $\delta^C_{e_P} = 0$.

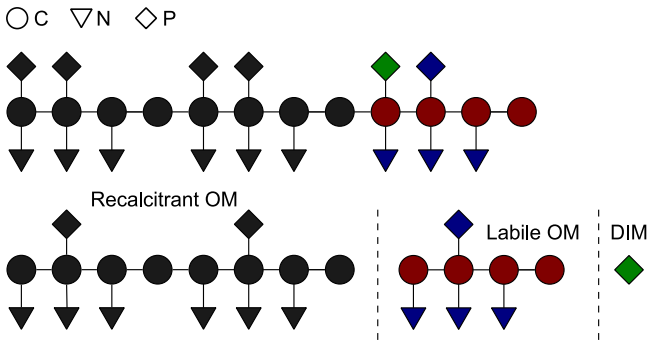


Fig. 3. Illustration of the *recalcitrant cleavage*. The considered substrate is all the recalcitrant C/N/P. $\Delta^C_{e_r} = 4$ units of C (represented in red) are *decomposed* to the labile OM. The associated quantities $\Delta^N_{e_r}$ and $\Delta^P_{e_r}$ of decomposed N and P are deduced from recalcitant C:N and C:P ratios. Among the decomposed P, a fraction $\alpha^P_{e_r} = 0.5$ is sent to the DIM.

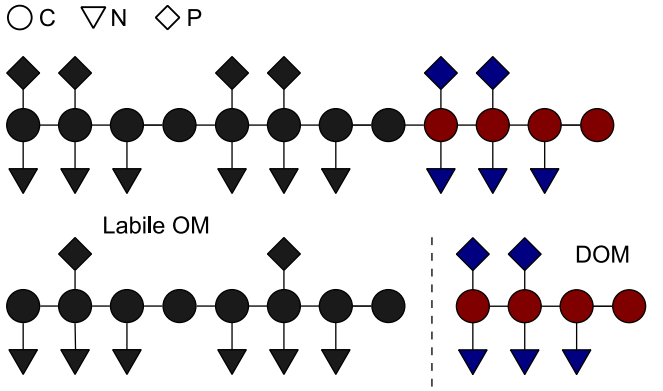


Fig. 4. Illustration of *CNP extraction*. The considered substrate is all the labile C/N/P. N and P are ignored (Hypothesis 1). $\Delta^C_{e_C} = 4$ units of C are *decomposed* to the DOM. The associated quantities $\Delta^N_{e_{CNP}}$ and $\Delta^P_{e_{CNP}}$ of decomposed N and P are deduced from labile C:N and C:P ratios.

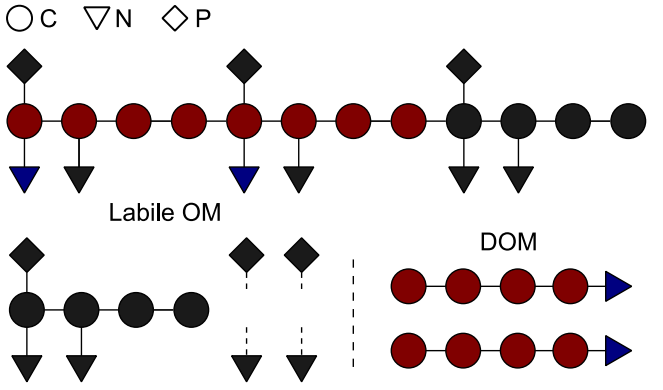


Fig. 5. Illustration of *N extraction*. The considered substrate is all the labile C and N that can be grouped with a $\mu_{CN} = 4$ ratio (Hypothesis 2, Eq. (8)). Other C/N/P is ignored and left in place. $\Delta^C_{e_N} = 8$ units of C are *decomposed* to the DOM (red), and $\Delta^N_{e_N} = 2$ units (blue) is deduced from μ_{CN}.

$\Delta^P_{e_r}$ is removed from $P_{recalcitrant}$, $\alpha^P_{e_r}\Delta^P_{e_r}$ is added to P_{dim} and $(1-\alpha^P_{e_r})\Delta^P_{e_r}$ is added to C_{labile}. This procedure must be applied to all compartments and all enzymatic activities to compute matter exchanges, i.e. the difference of composition between t and $t+1$. The effect of each action is illustrated on Figs. 3 to 6. It can be shown that the complete exchanges can be evaluated using Eqs. (17) to (27). The enzymatic budget allocation x it not represented for clarity, but all variables

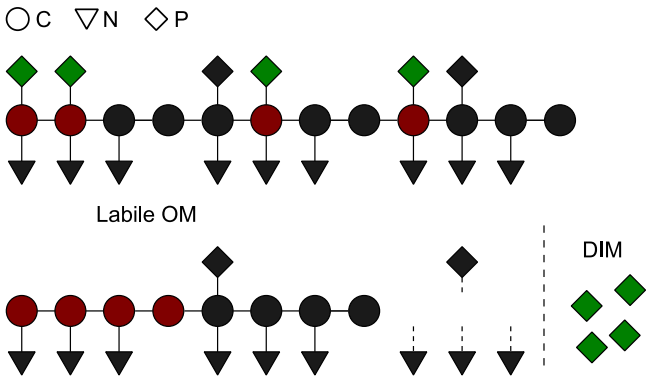


Fig. 6. Illustration of *P extraction*. The considered substrate is all the labile C and P that can be grouped with a $\mu_{CP} = 1$ ratio (Hypothesis 3, Eq. (10)). Other C/N/P is ignored and left in place. $\Delta^C_{e_P} = 4$ units of C are *decomposed* and $\Delta^P_{e_P} = 4$ units is deduced from μ_{CP}. $\Delta^P_{e_P}$ is sent to the DIM, and $\Delta^C_{e_P}$ is left in the labile OM.

depend on x. $\Delta^C_{e_P}$ is not included in fluxes as it is left in place. No N mineralisation is currently considered.

$$C^{t+1}_{recal} = C^t_{recal} - \Delta^C_{e_r} \tag{17}$$
$$N^{t+1}_{recal} = N^t_{recal} - \Delta^N_{e_r} \tag{18}$$
$$P^{t+1}_{recal} = P^t_{recal} - \Delta^P_{e_r} \tag{19}$$
$$C^{t+1}_{labile} = C^t_{labile} + \Delta^C_{e_r} - \Delta^C_{e_{CNP}} - \Delta^C_{e_N} \tag{20}$$
$$N^{t+1}_{labile} = N^t_{labile} + \Delta^N_{e_r} - \Delta^N_{e_N} \tag{21}$$
$$P^{t+1}_{labile} = P^t_{labile} + (1-\alpha^P_{e_r})\Delta^P_{e_r} - \Delta^P_{e_P} \tag{22}$$
$$C^{t+1}_{DOM} = C^t_{DOM} + \Delta^C_{e_{CNP}} + \Delta^C_{e_N} \tag{23}$$
$$N^{t+1}_{DOM} = N^t_{DOM} + \Delta^N_{e_{CNP}} + \Delta^N_{e_N} \tag{24}$$
$$P^{t+1}_{DOM} = P^t_{DOM} + \Delta^P_{e_{CNP}} \tag{25}$$
$$N^{t+1}_{DIM} = N^t_{DIM} \tag{26}$$
$$P^{t+1}_{DIM} = P^t_{DIM} + \alpha^P_{e_r}\Delta^P_{e_r} + \Delta^P_{e_P} \tag{27}$$

This set of equation is the result of the *decomposition* submodel, that can be used not only to simulate the *decomposition* process according to the current enzymatic budget allocation x of the microbe population, but also to estimate the quality of a possible budget x in the *optimisation* process using objectives presented in Section 2.4.5.

2.7.2. Optimisation submodel

This submodel provides useful details about the optimisation of the set of objectives introduced in Section 2.4.5, that must be optimised using a multi-objective optimisation problem. To do so, any global and continuous optimisation method can be used to minimise

$$f(x) = \sum_i \omega_i \cdot f_i(x)^2 \tag{28}$$

A classical *simulated annealing* method has been implemented with X (Eq. (1)) as the solution space. Optimising this single objective function with a classical simulated annealing algorithm has proved to yield satisfying results in our case although it would be worth studying other definitions of f and possible improvements towards algorithms more adapted to multi-objective optimisation problems (Amine, 2019). Considering the standard definition of the optimisation problem, other algorithms might indeed be used.

The squared value of f_i allows the algorithm to easily converge, as improvements made on an objective i in a state where f_i is close to the worse value is more valuable than in a state where f_i is already close to the minimum. See experiments in scenario 1 (Section 3) for possible biases that could be introduced by this method.

Contrary to the *decomposition* process that occurs at each time step, the execution of the *optimisation* routine is flexible. It could be called only at model initialisation to test a static decomposition problem. It can also be executed at a given period, or only when some conditions about the states of the environment and of the microbe population are met.

3. Experiments and discussion

Results of the model are presented in this section, to demonstrate the calibration of the model so that it can consistently represent the expected behaviour of our considered O-F-M life strategies. Our O-F-M classification is close to the Y-A-S classification proposed by Malik et al. (2020), with a particular focus on nutrients decomposition and assimilation:

- Opportunists (O strategists) correspond to the *Yield* strategy of the Y-A-S classification. They can decompose labile OM, but not recalcitrant OM, as they invest most of their metabolism in growth (assimilation and fixation) rather than in complex enzymatic systems. While enough nutrients are available, they grow rapidly and exponentially. But once not enough nutrients are available, they rapidly go dormant (sporulation). Their focus on growth is such that they cannot decompose as much nutrients as they can assimilate: as opportunists, they benefit from already available nutrients decomposed by other populations and amended to the soil.
- Foragers (F strategists) correspond to the *resource Acquisition* strategy of the Y-A-S classification. They grow slower than O strategists, to invest more of their metabolism in enzymatic systems. If not enough labile OM is available, they have the ability to forage recalcitrant OM, but only if it is necessary to maintain growth. They also go dormant once not enough nutrients are available.
- Minimalists (M strategists) only partly correspond to the *Stress tolerant* strategy of the Y-A-S decomposition. Indeed, we think that stress tolerance includes many different strategies also shared by Y and A classes. The *Minimalist* strategy is rather dedicated to strong oligotrophy, with an emphasis on a low cost metabolism. Such slow metabolism allows *Minimalists* to survive in poor environments, reducing competition for the available substrate with an high uptake efficiency optimised for environments with a low nutrient concentration (Coche et al., 2022). In order to limit the energy requirement of their metabolism, they do not have the ability to produce complex enzymes as it would require complex genomes that are costly to maintain: they can decompose simple labile compounds, but not recalcitrant OM. For the same reason, they do not have much adaptation capacity to the environment: they survive in any circumstance and never go dormant, but they have a limited capacity to adapt to the environment. In consequence, they will never grow rapidly, even if lots of nutrients are available.

It is then required to calibrate $\tau_{e,min}$ and $\tau_{e,max}$ values to instantiate O-F-M strategies, so they reflect the previously defined characteristics.

Values of parameters for each population strategy are presented on Table 5. Values have been chosen empirically, following the method presented in Appendix B.

This method leads to consistent values, but should not be considered exact. The purpose of this exploratory work is to demonstrate the potential of the model to consistently represent constitutive and adaptive enzymatic activities of a wide diversity of microbe populations. Calibration from field and laboratory experiments could then be performed to fit the model to real use cases.

Decomposition parameters have also been set empirically and are presented on Table 6.

Table 5
Enzymatic and structural parameters for each strategy. Enzymatic activities are expressed in $g_s g_M^{-1} d^{-1}$ where s is the substrate decomposed by the corresponding enzyme (C_{labile} for e_{CNP}, C_N for e_N, C_P for e_P, C_{recal} for e_r). ϵ has been set to 10^{-6}.

Strategy	O	F	M
$\tau_{e_{CNP},min}$	0	0	0.2
$\tau_{e_N,min}$	0	0	0.008
$\tau_{e_P,min}$	0	0	0.0016
$\tau_{e_r,min}$	0	0	0
$\tau_{e_{CNP},max}$	0.6	3	0.25
$\tau_{e_N,max}$	0.2	1	0.028
$\tau_{e_P,max}$	0.04	0.2	0.0056
$\tau_{e_r,max}$	ϵ	1	ϵ
CUE	0.7	0.3	0.5
$C{:}N_M$	10	10	10
$C{:}P_M$	17	17	17

Table 6
Parameter values used for the *decomposition* submodel.

Parameter	Value
μ_{CN}	5.0
μ_{CP}	1.0
$\alpha^P_{e_r}$	0.001
β_{e_i,e_j}	0.5 (for any e_i, e_j)

Table 7
Experimentation scenarios. For each scenario, the single parameter denoted as x indicates the variable parameter represented on the x axis of each plot.

Scenario	**1**	**2**	**3**	**4**	**5**	**6**
$C_{microbes}$ (g)	1.0					
DOM	0	0	0	0	0.5	1
$C{:}N_{DOM}$					x	10
$C{:}P_{DOM}$					17	x
C_{labile} (g)	10	0.3	5	0.3	10	10
$C{:}N_{labile}$	x	x	40	40	40	40
$C{:}P_{labile}$	60	60	x	x	60	60
C_{recal} (g)	10.0					
$C{:}N_{recal}$	50					
$C{:}P_{recal}$	70					

$\tau_{e,min}$ is set to 0 for O and F strategists, so that they have a full adaption capability. Only the M strategists are subject to constitutive rates, as they have less adaptation capacity. How constitutive rates have been determined is described in Appendix B.

Experiments are performed following 6 scenarios, presented on Table 7. The Gama model used to perform experiments is available within the CAMMISOL project (Breugnot et al., 2024). Scenarios have been chosen to represent key features of the model, but it is important to consider that the model is actually applicable to cases that can be completely different from the presented scenarios. The composition of the POM and the DAM in real soils can indeed be highly variable over time, so it rarely corresponds to one of the idealistic scenario presented here. The Buzy-pop model has notably been designed to run consistently even in unexpected contexts.

Each point is obtained from the median of 100 reproductions with different random seeds, with quartiles represented as bands. Scenarios 1 to 4 illustrate how populations adapt their enzymatic activities depending on the labile C/N/P composition. Scenarios 5 and 6 illustrate how the populations adapt to the composition of available matter in the DOM.

All experiments are independently performed with each population strategy, so we do not consider the case where several populations are decomposing a common substrate.

The requested C:N and C:P ratios of each strategist is equal to the constitutive $C{:}N_M$ and $C{:}P_M$ ratios divided by the population CUE, so that populations anticipate C that will be rejected as CO_2 in the respiration process.

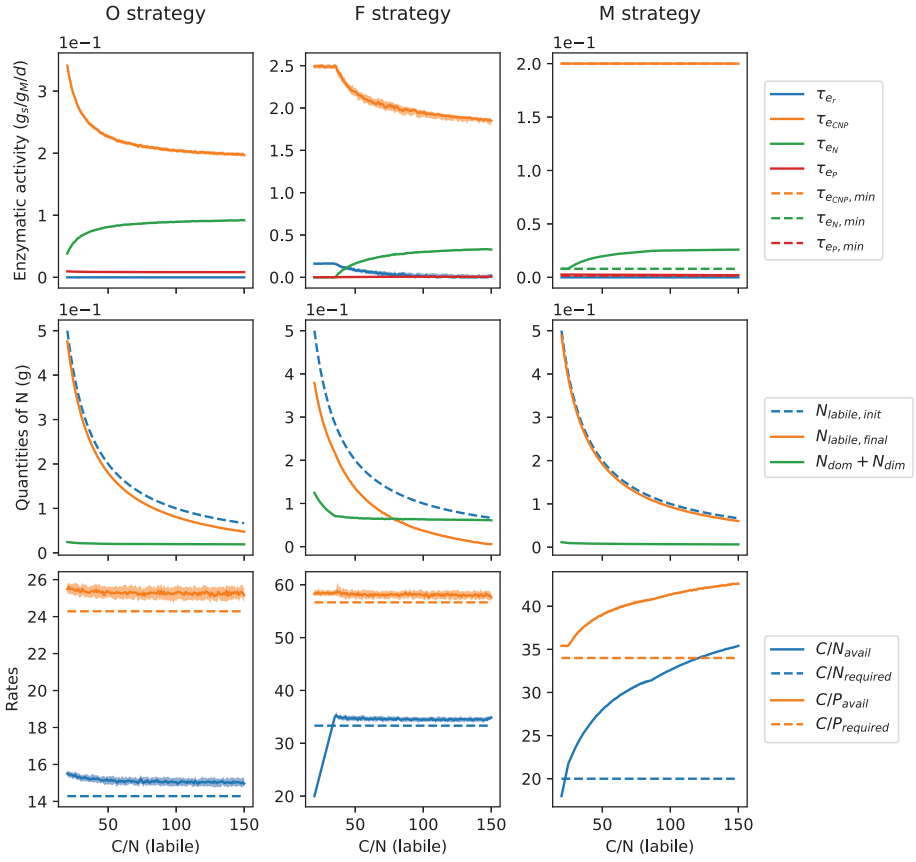


Fig. 7. Enzymatic activities and decomposition results for scenario 1, to study the response of each strategy to the variation of labile C:N while labile and recalcitrant C are in excess.

3.1. Scenario 1: variable labile C:N, labile C in excess

The results of the scenario 1 are presented on Fig. 7. In this case, the DAM is completely empty, and C_{labile} is set to a value that is significantly greater to the maximum C decomposition rate of each population (Table 5). When the C:N ratio of the labile OM is low, *O* and *F strategists* invest much energy in *CNP extraction* as it extracts matter with a low C:N ratio. Since the C:P ratio of the labile OM is higher than what is requested, energy is also invested in *P extraction* to adjust the available C:P ratio. Considering the abundance of labile C and the fact that available C is more valuable than labile C according to the definition of corresponding objectives, it might be expected that no energy should be invested by *F strategists* in *recalcitrant cleavage* to the benefit of *CNP extraction*. However, the definition of the multi-objective optimisation function (Eq. (28)) allows improvements of *MaxLabileC* to be more valuable that *MaxC* when no labile C is produced while available C is close to the possible maximum.[3] *Recalcitrant cleavage* is however quickly reduced to the benefit of *N extraction* when the labile C:N ratio increases to maintain the available C:N ratio. The overall energy invested in *recalcitant cleavage* is thus negligible compared to *CNP extraction*, what is consistent with the expected behaviour of *F strategists*.

M strategists finally cannot keep available C:N and C:P rates below requested values as their low adaptability do not allow them to reduce the budget allocated to *CNP extraction* to the benefit of *N* and *P extraction*.

[3] As explained in Section 2.4.5, such definition allows a faster convergence of the algorithm and more stable results.

3.2. Scenario 2: variable labile C:N, scarce labile C

The scenario 2 (Fig. 8) is more constrained, as labile C/N/P is limited compared to the maximum enzymatic activities (Table 7). As a consequence, the available N production ($N_{DOM}+N_{DIM}$) is globally significantly lower than for scenario 1. In addition, the model establishes strategies to deal with C/N/P scarcity.

O strategists invest in *CNP* and *N extraction* to equilibrate the available C:N ratio, until all the labile N is decomposed at $C : N_{labile} \simeq 25$. *O strategists* then invest in the negligible *recalcitrant cleavage* rate $\tau_{e_r,max} = \varepsilon$ as labile C:N increases, in order to reduce the activities of *CNP extraction*. Indeed, the total enzymatic budget is fixed, so microbe populations do not have the choice to produce less enzymes. However, in such cases of N scarcity, it can be useful to not use the complete enzymatic budget, because C extraction might dramatically increase the available C:N ratio without any possibility to increase available N, what is not in the favour of the *CapCN* objective. Setting $\tau_{e_r,max}$ to ε is an elegant way to allow populations to reduce their enzymatic activity, but other implementations might explicitly define a kind of *void* enzyme that do not decompose anything if it necessary to keep $\tau_{e,r}$ to 0. It might indeed be interesting for the population to reduce decomposition in order to maintain the C:N and C:P stoichiometries of the available matter (Achat et al., 2016).

The same tendencies are observed for *F strategists*, except that they can invest a significant part of their enzymatic budget into τ_{e_r} to feed the final N_{labile} and compensate the scarcity of labile N. Notice how *F strategists* still decompose the few available C/N/P while preserving available C:N and C:P ratios at acceptable values.

M strategists finally have a very low adaptation capability. $\tau_{e_{CNP}}$ is fixed to the constitutive rates. The resulting decomposition of labile C/N/P makes the available C:N ratio increase, as the population cannot adapt and not enough labile N is available to compensate.

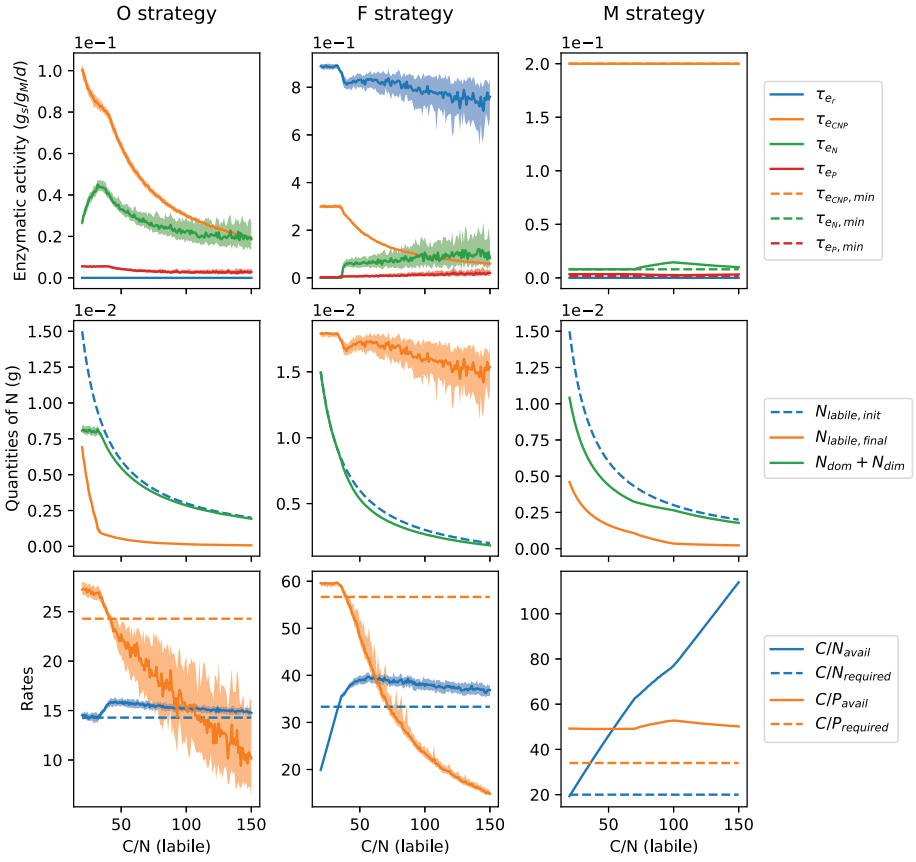


Fig. 8. Enzymatic activities and decomposition results for scenario 2, to study the response of each strategy to the variation of labile C:N while labile C is scarce and recalcitrant C is in excess.

3.3. Scenario 3: variable labile C:P, labile C in excess

The scenario 3 (Fig. 9) is similar to scenario 1, but this time the C:P ratio of the labile matter varies while C:N is fixed, with C_{labile} set to an high value (Table 7). Results are similar to scenario 1, except that *CNP* and *N extraction* decreases to the benefit of *N extraction* to equilibrate the available C:P ratio.

3.4. Scenario 4: variable labile C:P, scarce labile C

The scenario 4 (Fig. 10) is similar to scenario 3, except that C_{labile} is set to a limited value. Explanations can be deduced from arguments similar to those presented in scenario 2, considering C:N and C:P dynamics are inverted.

3.5. Scenario 5: variable C:N in the DAM

In the scenario 5 (Fig. 11), the DAM is provided with an amount of C (Table 7). The available C:P ratio is fixed, and the C:N rate of the already available matter is variable. Labile nutrients are available in a excess.

When the C:N ratio is low, the populations mainly invest in *CNP extraction*, as the DAM composition is already satisfying. When the available C:N ratio increases, more energy is invested into *N extraction* to compensate as much as possible for the scarcity of N in the DAM compared to C. In all cases, available C:N and C:P ratios are above the required ratios in some cases, even if their increase is limited. This is due to the compromise between *MaxC* and *CapCN*/*CapCP* objectives. We might expect populations to invest more in *N extraction* to reach the required ratios, considering the weights associated to each objectives. We think that a bias might be induced by the fact that the *MaxC* objectives is optimised considering the maximum available C that might be *added* to the DAM, but does not consider the quantity of C already available. An adaptation to the *MaxC* objective could be made to limit this effect.

3.6. Scenario 6: variable C:P in the DAM

The scenario 6 (Fig. 12) is similar to the scenario 5, except that the C:P ratio of the already available matter varies while the available C:N rate is fixed. In consequence, populations invest in *P extraction* rather than *N extraction* to establish equilibrium.

4. Conclusion

Buzy-pop proposes an innovative approach based on mathematical and optimisation techniques to model the fluxes of C/N/P due to the enzymatic activity of microbes, as long as their adaptation to the environment according to the resource allocation theory. The model allows to represent both constitutive and adaptive enzymatic activities. The aggregation of enzymatic activities into a reduced set of actions allows to represent real soil systems with a limited set of parameters. This aggregation will not make it possible to test a recent hypothesis which attributes the accumulation of OM in the soil to the molecular complexity of the substrates and therefore to the variety of enzymes present in the same place and at the same time rather than to their recalcitrant bond content (Lehmann et al., 2020). However, the flexibility of this type of model leaves the possibility of thinking about future modifications to test new conceptual hypotheses, such as increasing the number of action categories and therefore the number of microbial guilds.

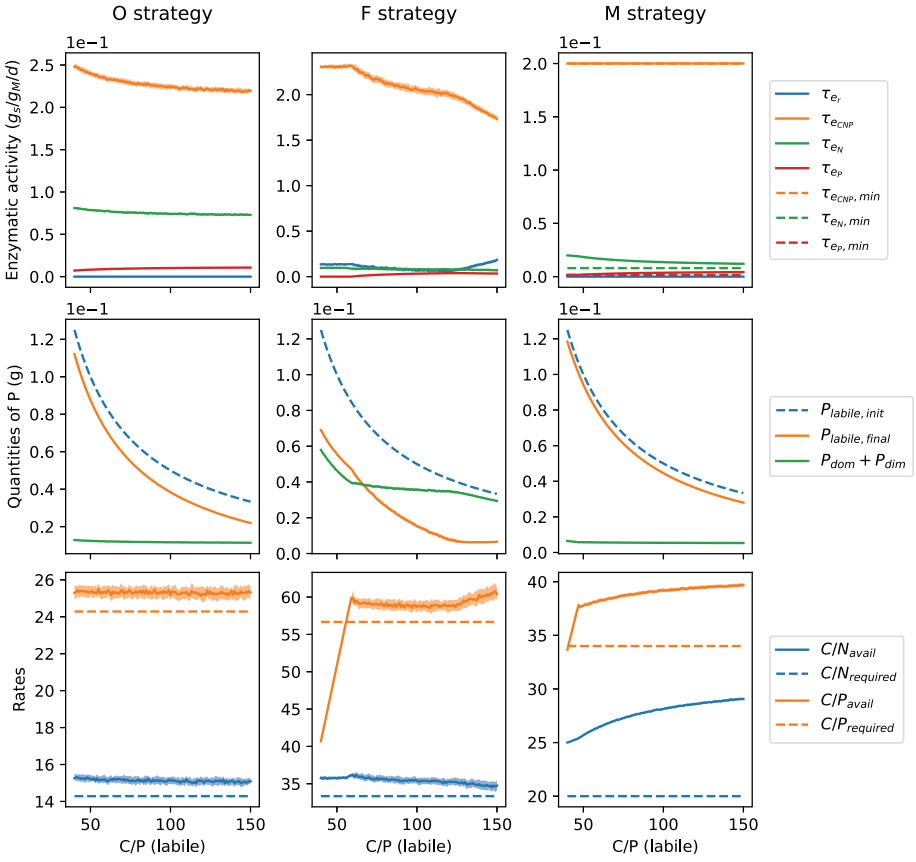


Fig. 9. Enzymatic activities and decomposition results for scenario 3, to study the response of each strategy to the variation of labile C:P while labile and recalcitrant C are in excess.

Quantitative results for the presented scenarios fit particularly well with the expected behaviour of the proposed life strategies, in spite of the very limited available data that can be used to define the problem (unknown chemical composition of nutrient compartments, diversity of enzymes that cannot be simulated, unknown enzymatic activities...). Such limitations could be considered a weakness, but actually result a strength of the model, as its low requirements allow it to be easily integrated in many simulation contexts. Moreover, none of the expected behaviour has been hard coded in the model: every strategy emerges from the simple definition of objectives. This tend to validate the consistency and the robustness of the model, allowing its applicability to the infinite and continuous space of possible environmental configurations. The proposed innovative paradigm based on the multi-objective optimisation of simple and explicit functions allows a representation of the microbe population that is much closer to the real world dynamics, an essential feature for local scale simulations and the comprehension of interactions between soil processes. Even if the quality of obtained results and the proposal for a meaningful set of parameters are promising to allow the model to be applied to field or laboratory results, the model is still at the stage of initial development. More exploratory work would be required in future works, not only to validate and calibrate the model, but also to analyse the sensitivity of the output of the model (enzymatic activities and decomposition) to the variability and the uncertainty of input data (parameters of the population and environmental conditions) in order to ensure the usability of the model on real data. Possible extensions Appendix C and exploitation of Buzy-pop in more comprehensive soil models are also a motivation to pursue the development of the model.

CRediT authorship contribution statement

Paul Breugnot: Writing – review & editing, Writing – original draft, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization. **Nicolas Marilleau:** Writing – review & editing, Writing – original draft, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization. **Laetitia Bernard:** Writing – review & editing, Writing - original draft, Supervision, Validation, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal Analysis, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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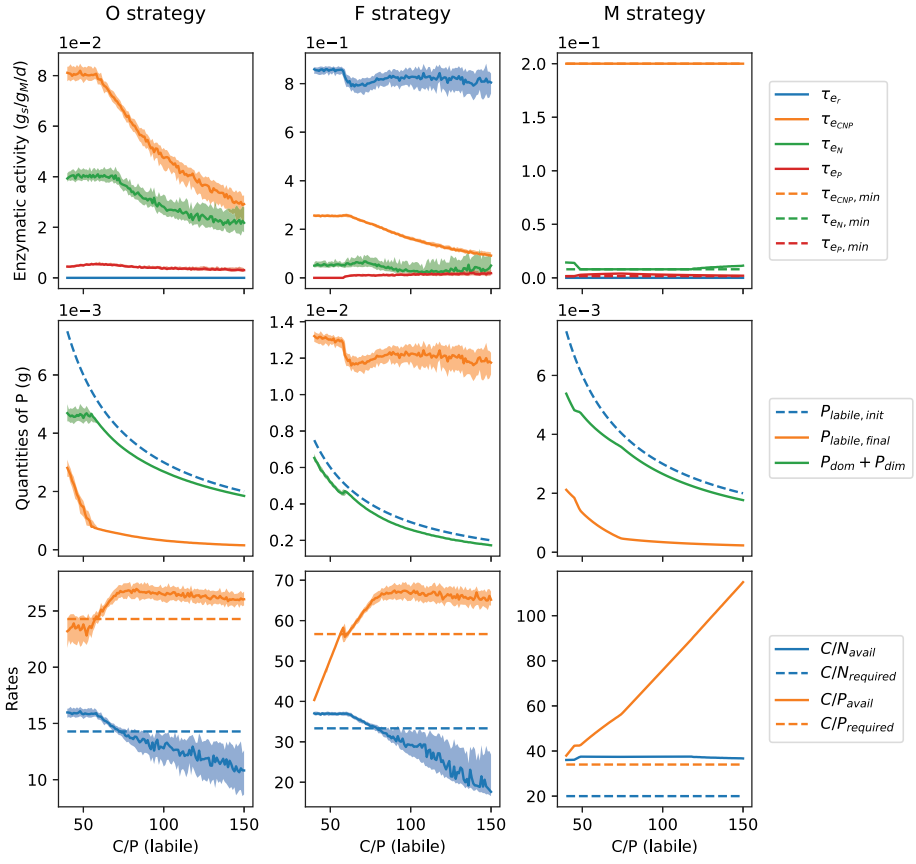


Fig. 10. Enzymatic activities and decomposition results for scenario 4, to study the response of each strategy to the variation of labile C:P while labile C is scarce and recalcitrant C is in excess.

Appendix A. Design of objectives

The purpose of this submodel is to formally define numerical values of objectives introduced in Section 2.4.5.

Be Φ_x^p the total increase of product $p \in \{C_{labile}, C_{DAM}\}$ according to the budget allocation x. Following Eqs. (20) and (23):

$$\Phi_x^{C_{labile}} = \Delta^C_{e_r,x} \tag{A.1}$$

$$\Phi_x^{C_{DAM}} = \Delta^C_{e_{CNP},x} + \Delta^C_{e_N,x} \tag{A.2}$$

Objectives maximising the quantity of each product can then be defined as follows:

$$f_p : X \to [0,1]$$
$$x \mapsto 1 - \frac{\Phi_x^p}{\Phi_{max}^p} \tag{A.3}$$

Defining $\Phi^p_{max} = \max_{x\in X} \Phi^p_x$, it can be proven that f_p is surjective. This is a desired property for the definition of objectives, since the comparison of values in the multi-objective optimisation is more robust and unbiased if each objective takes values in the full $[0,1]$ range. However, computing $\max_{x\in X} \Phi^p_x$ is harder than it looks. Analytical solutions have not been found, and it would be too costly to approximate it using optimisation methods. So we instead decided to estimate it using Eq. (A.4) below. It is assumed that, for each enzymatic activity, the maximum quantities of products are obtained investing all the enzymatic budget in a single action, so that no enzymatic activity is wasted due to competition for a requested substrate.

$$\Phi^P_{max} = \max_{e\in E}(\Phi^p_{x_e=1}) \tag{A.4}$$

Even if objectives are not perfectly bounded to $[0,1]$ using Eq. (A.4), good optimisation results have been obtained with them.

The weight of objectives have been set empirically. The main idea is that available C production must be more valuable than labile C, as the first is directly assimilable. This is modelled explicitly in the multi-objective optimisation by assigning a five times bigger weight to *MaxC* compared to *MaxLabileC*. Due to the definition of the *recalcitrant cleavage* action, maximising the production of labile C also maximises the production of labile N and P.

The population then wants to keep the C:N and C:P ratios of available matter (DAM) to values at most equal to ratios requested by the population. Maintaining those ratios at most at required values ensures that stoichiometric growth of the population is possible. Even if the assimilation of nutrients is not the purpose of this study, we assume that the total quantity of nutrients assimilated by the population is driven by the quantity of assimilated C: assimilated quantities of N and P are then fixed from the available C:N and C:P ratios. In consequence, we state that having more N and P than necessary is not considered a problem, since they do not represent a waste of assimilation capacity and N and P assimilated in excess can be rejected in the DIM.

Mathematical expressions used for all those objectives and their associated weights are summarised on Table A.8.

The weights determine the compromise between maximising nutrients acquisition and keeping acceptable C:N and C:P ratios in the DAM. The lower the weight of *CapCN* and *CapCP* objectives, the less energy will be invested in preserving C:N and C:P ratios, meaning that higher ratios than those requested by the population will be considered acceptable, and that more energy will be invested in acquisition of C rather than N and P. Weights for those objectives have currently been set empirically to twice the weight of available nutrients production. Notice that the state of the environment sometimes do not allow to preserve the available ratios below those requested. But in those "desperate" cases, it might still be useful for the population to decompose

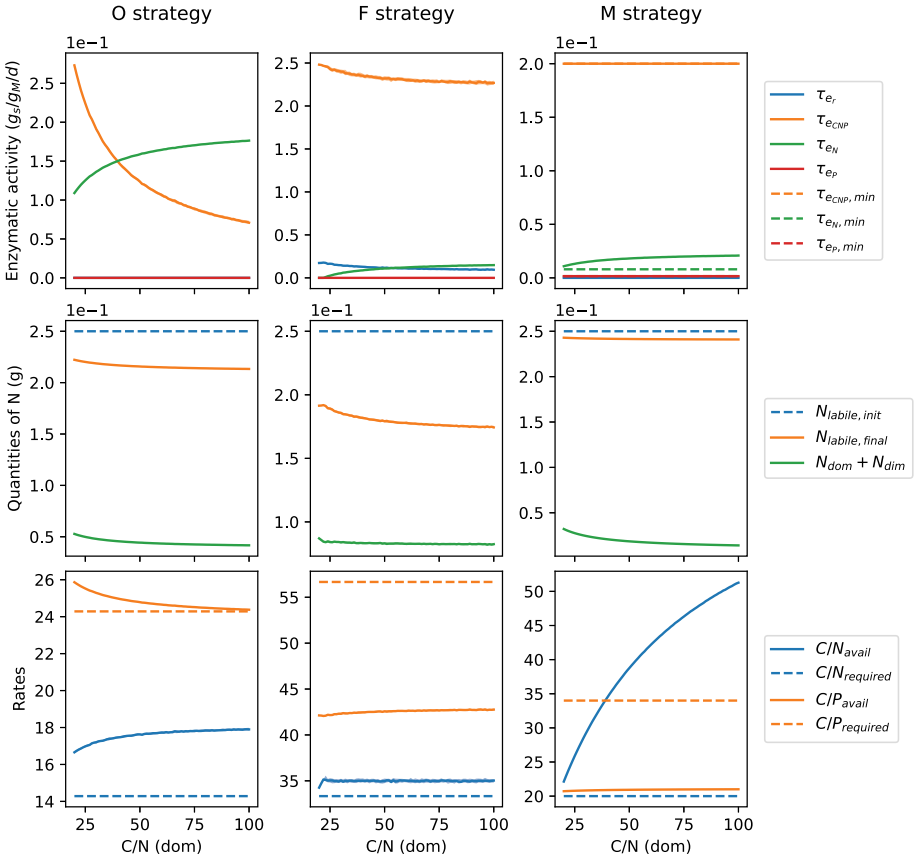


Fig. 11. Enzymatic activities and decomposition results for scenario 5, to study the response of each strategy to the variation of the C:N ratio in DOM while labile and recalcitrant C are in excess.

Table A.8
Values and weights of objectives considered in the enzymatic activity optimisation problem.

Objective	Normalised value	Weight
MaxLabileC	$1-\frac{\Phi_{x}^{C_{recal}}}{\Phi^{C_{recal}}_{x_{e_r}=1}}$	1.0
MaxC	$1-\frac{\Phi_{x}^{C_{labile}}}{\max(\Phi^{C_{labile}}_{x_{eCNP}=1},\Phi^{C_{labile}}_{x_{eN}=1})}$	5.0
CapCN	$1-\frac{C}{N}\min(\frac{N^{t+1}_{DOM}+N^{t+1}_{DIM}}{C^{t+1}_{DOM}},\frac{N}{C})$	10.0
CapCP	$1-\frac{C}{P}\min(\frac{P^{t+1}_{DOM}+P^{t+1}_{DIM}}{C^{t+1}_{DOM}},\frac{P}{C})$	10.0

poor quality nutrients at its disposal. This is properly handled by the multi-objective optimisation method, as it will push the population to maximise available C if there is no way to optimise *CapCN* and *CapCP*. In such cases, experimental results have indeed led to consistent strategies from a microbial biology point of view.

Appendix B. A method to define the decomposition problem

Estimating values for $\tau_{e,min}$ and $\tau_{e,max}$ is not a trivial task, especially considering the lack of data that could be used to calibrate the model. Some qualitative and common knowledge combined with further mathematical reasoning however allows us to estimate realistic parameters for each O-F-M strategy.

The method first consists in defining a *base* decomposition problem, where only $\tau_{e,max}$ should be considered, in order to reduce the set of parameters. The *complete* decomposition problem can then be deduced from an algorithmic method, depending on the fraction of the *base* enzymatic budget that should be considered constitutive.

B.1. Defining the base decomposition problem

The *base* decomposition problem consists in the definition of $\tau_{e,max}$ values, without considering constitutive rates. Those $\tau_{e,max}$ values are denoted $\tau_{e,base}$, and can be considered as the maximum enzymatic activity of each action e if no other action is available to the population, so that there is no other constitutive rate and all the budget must necessarily be invested in this action. The *complete* decomposition problem will then be deduced by splitting the *base* problem between a constitutive and an adaptable part.

Two factors should be considered when choosing $\tau_{e,base}$ values. The absolute values of each $\tau_{e,base}$ determines the overall capability of the microbe population to decompose the associated substrates. Then, the relative value of each $\tau_{e,base}$ determines the cost of e compared to other enzymes. For example, $\tau_{e_r,base} = 0.1\,\mathrm{g_{C_{recal}}}\,\mathrm{g_M^{-1}}\,\mathrm{d^{-1}}$ and $\tau_{e_{CNP},base} = 1\,\mathrm{g_{C_{labile}}}\,\mathrm{g_M^{-1}}\,\mathrm{d^{-1}}$ means that dedicating all the enzymatic budget to the *recalcitrant cleavage* activity will produce an activity of $0.1\,\mathrm{g_{C_{recal}}}\,\mathrm{g_M^{-1}}\,\mathrm{d^{-1}}$, while dedicating all the budget to *CNP extraction* will produce an activity of $1\,\mathrm{g_{C_{labile}}}\,\mathrm{g_M^{-1}}\,\mathrm{d^{-1}}$, so the cost of *recalcitrant cleavage* is 10 times bigger than the cost of *CNP extraction*.

Considering this, we can elaborate a method to estimate the *base* $\tau_{e,base}$ values for each O-F-M strategy, according to its expected behaviour.

1. The quantity of C obtained in amino acids and N-acetyl glucosamine obtained from *N extraction* is limited by the fixed composition of those chemical entities, that must be extracted individually by exocleaving enzymes. On the other hand, enzymes responsible for *CNP extraction* can use depolymerisation to quickly retrieve bigger amounts of C, by reducing the size of labile molecules using endocleaving techniques. Moreover,

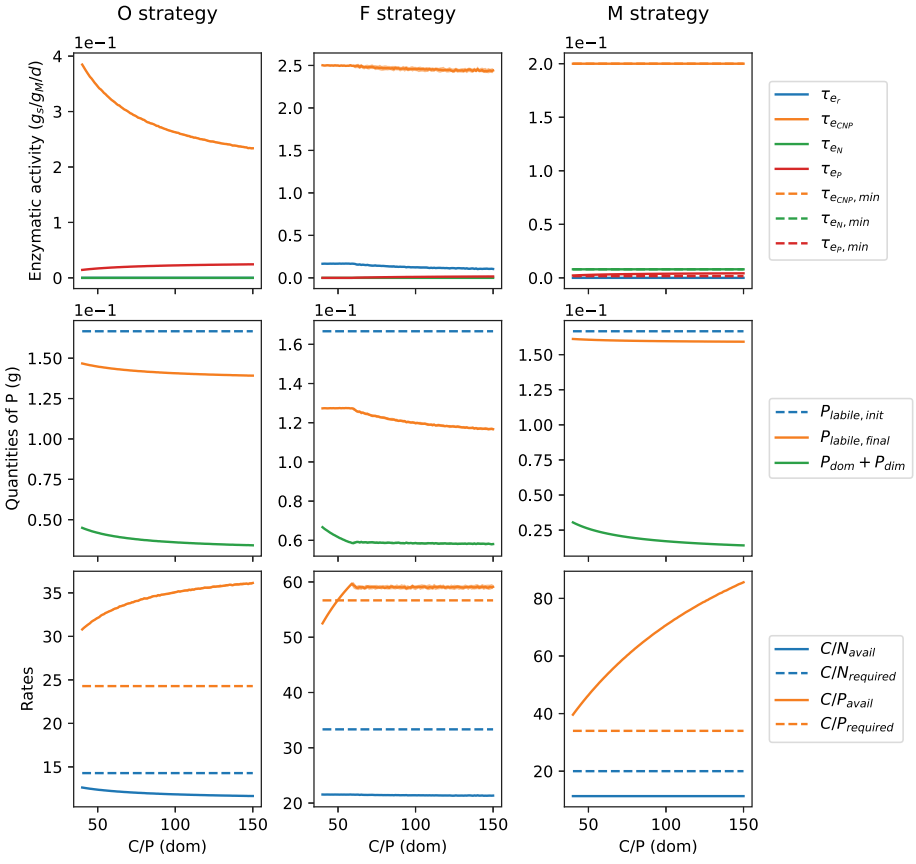


Fig. 12. Enzymatic activities and decomposition results for scenario 6, to study the response of each strategy to the variation of the C:P ratio in DOM while labile and recalcitrant C are in excess.

$\tau_{e_N,base}$ represents the ability of the population to adapt to N scarcity if *CNP extraction* does not allow stoichiometric growth. In consequence, $\tau_{e_{CNP},base}$ and $\tau_{e_N,base}$ must be chosen so that the substrate requested by *CNP extraction* is significantly bigger than for *N extraction* (see Eq. (3)).

2. Similar arguments hold for *P extraction*. Since it is more specialised and less efficient that *CNP extraction* (as each enzyme must individually attack phosphate groups) and represents the ability of the population to adapt to P scarcity, $\tau_{e_P,base}$ is generally significantly lower that $\tau_{e_{CNP},base}$.
3. Growth and assimilation models are out of the scope of the current work, but $\tau_{e_C,base}$ have been adjusted for *F strategists* so that they can decompose enough C to at least maintain their exponential growth ($\frac{dC_M}{dt} = rC_M$) considering the provided carbon use efficiency (CUE) and a relative growth rate of $r = 1\,\mathrm{d}^{-1}$ in a context where labile nutrients are in excess. It can notably be shown that the quantity of C required by the population to maintain its exponential growth is equal to $C_M \frac{r\Delta t}{CUE}$. Assuming that this quantity can be obtained from *CNP extraction* in a context of stoichiometric growth (where C:N and C:P ratios of the labile OM are equal to those requested, so that *N* and *P extraction* are not required), Eq. (3) leads to the estimation that $\tau_{e_{CNP},base} = \frac{r}{CUE} \simeq 3\,\mathrm{g_{C_{labile}}}\,\mathrm{g_M^{-1}}\,\mathrm{d}^{-1}$. $\tau_{e_N,base}$ and $\tau_{e_P,base}$ have been set arbitrarily to 1 and 0.2, considering the previous considerations. $\tau_{e_r,base}$ has finally been set arbitrarily to $1\,\mathrm{g_{C_{recal}}}\,\mathrm{g_M^{-1}}\,\mathrm{d}^{-1}$. Notice that even if cleaving recalcitrant matter is more costly than cleaving labile matter, *recalcitrant cleavage* is expected to extract more nutrients than *CNP extraction* for the same energy invested in those actions.
4. *O strategists* spend less energy than *F strategists* in enzymatic actions, as they are focused on growth. As opportunists, they are not expected to be able to maintain their own exponential growth if there are no other populations decomposing nutrients for them. In consequence, their enzymatic rates have been set to values five times lower than *F strategists*. $\tau_{e_r,base}$ has then been set to a negligible value ϵ, since *O strategists* cannot decompose recalcitrant matter. Using a negligible value instead of zero has proven to greatly increase the stability of the model. Indeed, setting $\tau_{e_r,max}$ to ϵ allows the population to invest in it to globally reduce its enzymatic activity when there is nothing else to do (see experimental results for scenarios 2 and 4 in Section 3).
5. Finally, *M strategists* have a low nutrient assimilation rate (not represented in this model) and focus on survival in poor environments, so their decomposition capacity is lower (or slower) than for *O* and *F strategists*. Their enzymatic rates have been set to values ten times lower than *F strategists*, setting $\tau_{e_r,base}$ to ϵ.

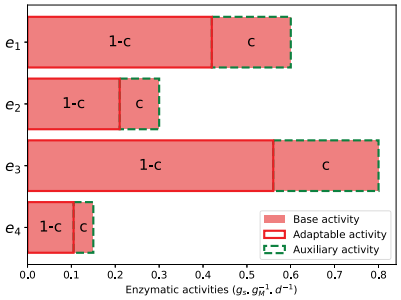
Table B.9
Base activities for O-F-M strategists.

Strategy	$\tau_{e_{CNP},max}$	$\tau_{e_N,max}$	$\tau_{e_P,max}$	$\tau_{e_r,max}$	CUE
O	0.6	0.2	0.04	ϵ	0.7
F	3	1	0.2	1	0.3
M	0.3	0.1	0.02	ϵ	0.5

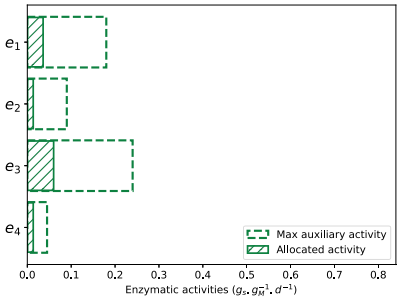
Values obtained from this procedure are summarised on Table B.9.

B.2. Deducing the complete decomposition problem

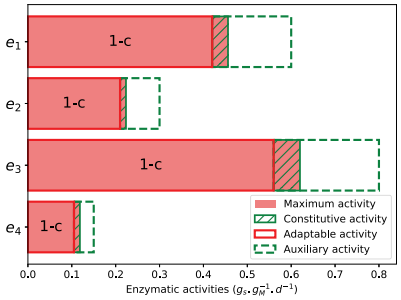
The purpose of the following method is to define a *complete* decomposition problem (values for $\tau_{e,min}$ and $\tau_{e,max}$) by splitting the previous *base* problem in a constitutive ($\tau_{e,min}$) and adaptable ($\tau_{e,max}$) part. The



(a) Base decompositon problem activities. Each base activity is decomposed into an adaptable part and an auxiliary part according to a fraction c, that will be used to compute constitutive activities.



(b) Auxiliary decomposition problem. Auxiliary activities are used as maximum activities, and enzymatic activities are allocated using a solution of this problem.



(c) Complete problem activities. The solution of the auxiliary problem is used as constitutive activities. Maximum activities are the sum of the adaptable part defined in the base problem and the computed constitutive rates. Notice how constitutive activities replaced the auxiliary part of the base problem.

Fig. B.13. Conversion from the *base* decomposition problem to the *complete* problem.

complete problem is expected to be defined so that any activities obtained from a solution x' to the *complete* problem can be obtained from a solution x to the *base* problem.

This constraint implies that we cannot have $\tau_{e,max} = \tau_{e,base}$ for all e if at least one of $\tau_{e,min}$ is not null, since $\tau_{e,min}$ represents the absolute enzymatic activity that is added to the global decomposition capacity of the population, without being concerned by budget allocation. So, if $\tau_{e,min} \neq 0$ for some e, having $\tau_{e,max} = \tau_{e,base}$ for all e would imply that the budget required to obtain $\tau_e = \tau'_{e,min}$ in the base problem could be used to invest in other enzymes at the same cost in the complete problem, increasing the global decomposition capacity of the population. In consequence, setting $\tau_{e,min}$ to a non null value requires to define $\tau_{e,max}$ values less than $\tau_{e,base}$ in the *complete* problem to ensures it stays compatible with the *base* problem.

The first step of the procedure consists in choosing a fraction $c \in [0, 1]$ of the *base* enzymatic capacity that will be considered constitutive. This fraction is then removed from each value of $\tau_{e,base}$, and used to define an *auxiliary* decomposition problem with values of $c \cdot \tau_{e,base}$ as maximum activities (Fig. B.13(a)). A solution of the auxiliary problem is then picked and used to define the constitutive activities of the complete problem (Fig. B.13(b)). Remember that a *solution* to the decomposition problem is any $x \in X$ as defined in Eq. (1). In consequence, the solution picked can be arbitrary (e.g. $[0.25, 0.25, 0.25, 0.25]$) or obtained from the optimisation of the auxiliary problem in a defined context. For example, in the case of *M strategists*, the solution of the auxiliary problem, i.e. constitutive rates, might be optimised for a poor quality environment. The complete problem is then defined so that maximum activities are equal to the constitutive rates added to each value of $(1 - c)\tau_{e,base}$ (Fig. B.13(c)). As expected, a fraction $1 - c$ of the *base* problem is now subject to the enzymatic budget allocation, and it can be shown that activities obtained from any solution of the *complete* problem can be obtained from a solution of the *base* problem. For consistency, $\tau_{e,max}$ is automatically set to ε if $\tau_{e,base} = \varepsilon$.

Notice that with $c = 0$, the proposed procedure ensures that $\forall e, \tau_{e,max} = \tau_{e,base}$ and $\tau_{e,min} = 0$. Moreover, defining $c = 1$ can be useful to define a *static* version of the model to save computation time by neglecting budget optimisation. Since such static model could still be defined from the optimisation of the auxiliary problem on a specific case, it would not completely neglect the resource allocation principle.

A constitutive rate of $c = 0$ is applied to *O* and *F strategists*, and $c = 0.8$ (80 % of constitutive activity) to M strategists, from the base problem defined on Table B.9. The auxiliary budget is arbitrarily set to $[0, 0.8, 0.1, 0.1]$, to obtain values used for experiments presented on Table 5.

Appendix C. Possible extensions

A few interesting extensions that could be studied in future works are worst mentioning.

C.1. Interactions and collectives

No direct interaction between several *Microbe populations* are currently considered. However, two duplicate and independent instances of the model might be integrated with a common substrate as input. In this case, each microbe population would establish its own strategy, ignoring the presence of others. The activities of the other population would then result in external inputs and outputs in the local POM and DAM, what can be considered as a mediated interaction. Even if such possibilities have not been experimentally studied yet, similar use cases are planned to be integrated to CAMMISOL, a comprehensive multi-agent soil model, where three *Microbe populations* (one for each O-F-M

strategy) cohabit in the solution of pore particles to decompose organic particles around them.

Following this idea, collective dynamics could be considered in the model, with explicit or implicit competition and collaboration between populations. The elaboration of such collective strategies might be studied explicitly using game theory. Other solutions consist in including the enzymatic rates of other populations to the perception of each population, to observe the emergence of complex collective strategies.

C.2. Enzyme kinetics

The decomposition rates τ_e used by the model are idealistic. Indeed, the definition and usage of Eq. (3) imply that the substrate can always be decomposed at a rate of $C_M\,\tau_e$, independently of time and concentration of the substrate. This is obviously not true in reality, as the action of enzymes is not ideal: the lower the concentration, the lower the efficiency of enzymes. Even if the current study is limited to the ideal hypothesis, it seems worst noticing how enzyme kinetics could be easily integrated in the model. The $C_M\tau_e$ factor could indeed be considered as the **limiting reaction rate** v_{max} of the Michaelis–Menten kinetics model that states that:

$$v = \frac{\mathrm{d}p}{\mathrm{d}t} = \frac{V_{max}\,a}{K_m + a} \tag{C.1}$$

where v is the reaction rate of the formation of the product with concentration p, a is the concentration of the substrate and K_m is the Michaelis constant, defined as the concentration of substrate at which the reaction rate is half of V.

Many models of microbial enzymatic activity (Traving et al., 2015; Kaiser et al., 2014; Allison, 2012) already include this kinetic model, what validates how relevant is the possibility to include it in Buzy-pop.

Our Eq. (3) could then be replaced by

$$\delta_e^s = \min(v\,dt\,V, S) = \min(\frac{C_M\,\tau_e\,dt\,\frac{S}{V}}{K_e + \frac{S}{V}}, S) \tag{C.2}$$

where V is the considered volume and K_e is the kinetic constant associated to the enzymatic action e and dt is assumed sufficiently small (contrary to the former Δt). The rest of the model can be left unchanged, using the same *requested* substrates formulas δ_e^s to include kinetics. For $K_e = 0$, what literally means that the maximum reaction rate is reached for any concentration, Eq. (C.2) falls back to the previous Eq. (3) that corresponds to the ideal case, proving the consistency of the model.

Data availability

The source code of the model is open and permanently available from the specified SWHID thanks to the Software Heritage project.

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