C-STABILITY an innovative modeling framework to leverage the continuous representation of organic matter (supplementary information)

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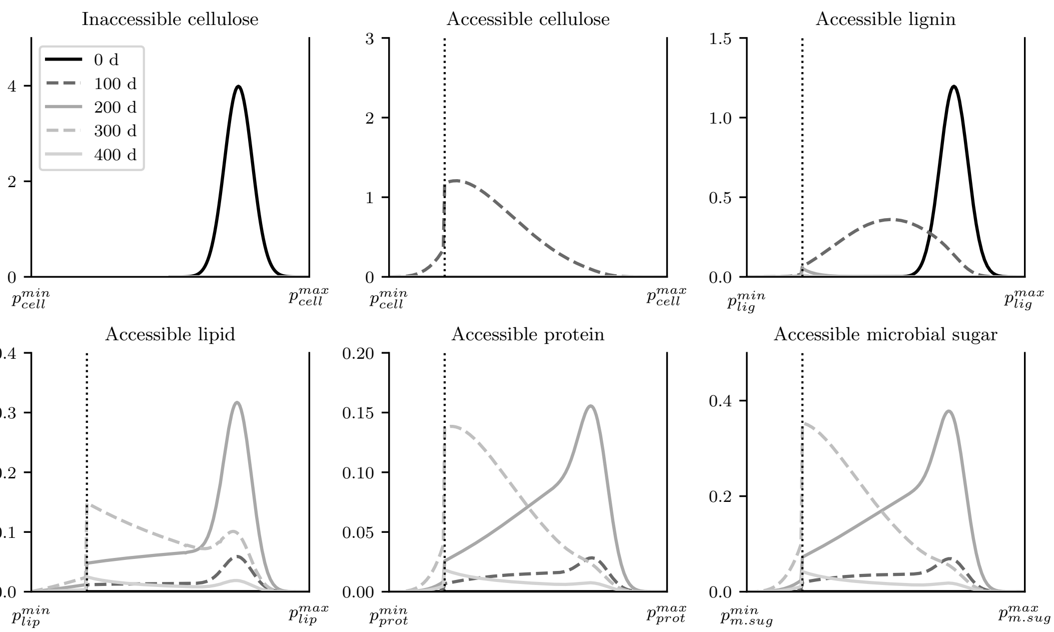
Supplementary note 1

Table 1: Studies utilized to design the scenarios.

Scenarios 1 & 2	Concurrent changes in substrate chemistry and enzymes occurence/ enzyme efficiency in laboratory litter decomposition	[1,2,3,4,5]
Scenario 3	Classification of decomposers into functional communities	[6,7,8,9]
	Successions of decomposer communities during in situ decomposition of plant litter	[10,11,12,13]
Scenario 4	Chemical characterisation of organic biomolecules present in soil organic matter	[14,15,16]

Supplementary note 2

a No-cheating



b Cheating

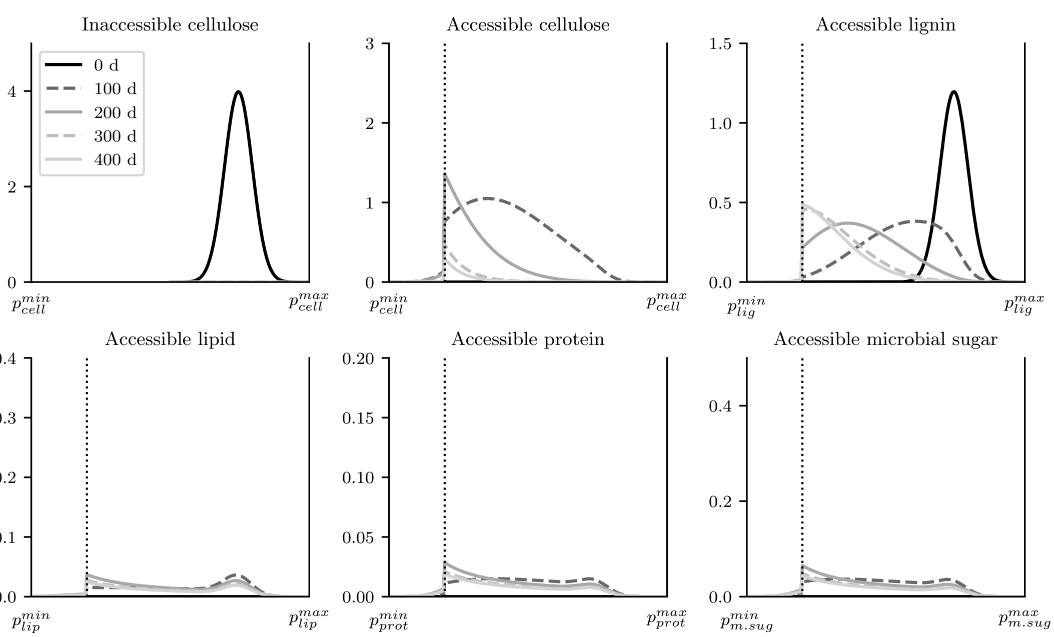


Fig. 1: **Temporal variations in polymerization distribution for each substrate pool in scenario 3**. A comparison between **a** no-cheating and **b** cheating microbial behaviour.

Supplementary note 3

Introduction We give here a proof of steady state equations for scenario 4. We recall the general equations of the system.

$$\begin{aligned}
\frac{\partial \chi_*^{ac}}{\partial t}(p,t) &= \tau_{tr,*}^{ac}\chi_*^{in}(p,t) - \tau_{tr,*}^{in}\chi_*^{ac}(p,t) \\
&\quad -\tau_{enz}^0 \sum_{\text{mic}} C_{mic}(t)\chi_*^{ac}(p,t) \\
&\quad +\tau_{enz}^0 \sum_{\text{mic}} C_{mic}(t)(\alpha_{enz}+1)(p-p_*^{min})^{\alpha_{enz}} \int_p^{p_*^{max}} \frac{\chi_*^{ac}(p',t)}{(p'-p_*^{min})^{\alpha_{enz}+1}}dp' \\
&\quad +\sum_{\text{mic}} C_{mic}(t)\left(m_{mic}^0 s_{mic,*}(p) - \mathbb{1}_{\mathcal{D}_u}(p)u_{mic,*}^0\chi_*^{ac}(p,t)\right) \\
&\quad +i_*^{ac}(p,t), \qquad \text{(S1)}\\
\frac{\partial \chi_*^{in}}{\partial t}(p,t) &= \tau_{tr,*}^{in}\chi_*^{ac}(p,t) - \tau_{tr,*}^{ac}\chi_*^{in}(p,t) + i_*^{in}(p,t). \qquad \text{(S2)}
\end{aligned}$$

where $\mathbb{1}_{\mathcal{D}_u}(p)$ equals 1 if $p \in \mathcal{D}_u$ and 0 otherwise. The dynamics of microbial C_{mic} is obtained by,

$$\frac{dC_{mic}}{dt}(t) = -m_{mic}^0 C_{mic}(t) + \sum_* u_{mic,*}^0 e_{mic,*}^0 C_{mic}(t)\int_{\mathcal{D}_u}\chi_*^{ac}(p,t)dp. \qquad \text{(S3)}$$

Specific assumptions Due to the specific design of the scenario 4, several terms of the equations can be simplified. First, we consider a single microbial community and all microbial parameters (u^0, e^0 and m^0) are considered identical for all biochemical classes. Second, we consider that all the substrate is accessible i.e. $\chi_*^{in} = 0$ and $\tau_{tr,*}^{ac} = \tau_{tr,*}^{in} = \iota_*^{in} = 0$. Then all distinction between accessible and inaccessible substrate were removed in the following. Third, we consider that input terms $\iota_*^{ac}(p,t) = \iota_*^{ac}(p)$ are constant over time. To improve readability of the proof, we note without ambiguity $\alpha_{enz} = \alpha_*$ and $\tau_{enz}^0 = \tau_*^0$ in the following. Then, for all biochemical classes $*$, we have for all $p \in [p_*^{min}, p_*^{max}]$,

$$\begin{aligned}
\frac{\partial \chi_*}{\partial t}(p,t) &= -\tau_*^0 C_{mic}(t)\chi_*(p,t) \\
&\quad +\tau_*^0 C_{mic}(t)(\alpha_*+1)(p-p_*^{min})^{\alpha_*}\int_p^{p_*^{max}} \frac{\chi_*(p',t)}{(p'-p_*^{min})^{\alpha_*+1}}dp' \\
&\quad +C_{mic}(t)\left(m^0 s_*(p) - \mathbb{1}_{\mathcal{D}_u}(p)u^0\chi_*(p,t)\right) \\
&\quad +i_*(p), \qquad \text{(S4)}\\
\frac{dC_{mic}}{dt}(t) &= -m^0 C_{mic}(t) + u^0 e^0 C_{mic}(t)\sum_*\int_{\mathcal{D}_u}\chi_*(p,t)dp. \qquad \text{(S5)}
\end{aligned}$$

Integral operators We introduce $p_*^u \in [p_*^{min}, p_*^{max}]$ such that $\mathcal{D}_u = [p_*^{min}, p_*^u]$ and we define the operators A_* for a function $f :]a, p_*^{max}] \to \mathbb{R}$ with $p_*^{min} \leq a$,

$$A_* f(p) = (\alpha_*+1)(p-p_*^{min})^{\alpha_*}\int_p^{p_*^{max}} \frac{f(p')}{(p'-p_*^{min})^{\alpha_*+1}}dp', \qquad \text{(S6)}$$

and A_*^u for a function $f :]a', p_*^u] \to \mathbb{R}$ with $p_*^{min} \leq a'$,

$$A_*^u f(p) = (\alpha_*+1)(p-p_*^{min})^{\alpha_*}\int_p^{p_*^u} \frac{f(p')}{(p'-p_*^{min})^{\alpha_*+1}}dp'. \qquad \text{(S7)}$$

Steady-state equations If we set $\frac{\partial \chi_*}{\partial t}(p,t) = 0$ and $\frac{dC_{mic}}{dt}(t) = 0$, we obtain the following equations to solve to obtain $\chi_*(p)$ and C_{mic} steady state expressions for all $p \in [p_*^{min}, p_*^{max}]$,

$$\frac{\iota_*(p)}{C_{mic}} = \tau_*^0 \left(\chi_*(p) - A_*\chi_*(p)\right) + \mathbb{1}_{\mathcal{D}_u}(p) u^0 \chi_*(p) - m^0 s_*(p), \tag{S8}$$

$$\frac{m^0}{e^0} = u^0 \sum_* \int_{p_*^{min}}^{p_*^u} \chi_*(p) dp. \tag{S9}$$

Determination of C_{mic} We consider the integration over $p \in [p_*^{min}, p_*^{max}]$ of equation S8 which gives,

$$\frac{I_*}{C_{mic}} = \tau_*^0 \int_{p_*^{min}}^{p_*^{max}} \left(\chi_*(p) - A_*\chi_*(p)\right) dp + u^0 \int_{p_*^{min}}^{p_*^u} \chi_*(p) dp - m^0 S_*.$$

We can verify that $\int_{p_*^{min}}^{p_*^{max}} \left(\chi_*(p) - A_*\chi_*(p)\right) dp = 0$ and if we sum over the biochemical classes $*$,

$$\frac{I}{C_{mic}} = u^0 \sum_* \int_{p_*^{min}}^{p_*^u} \chi_*(p) dp - m^0.$$

According to equation S9,

$$C_{mic} = \frac{I e^0}{m^0(1-e^0)}. \tag{S10}$$

Determination of χ_* We define $\theta_*(p) = m^0 s_*(p) + \frac{\iota_*(p)}{C_{mic}}$ and then, we can reformulate equation S8,

$$A_*\chi_*(p) - \chi_*(p) = -\frac{\theta_*(p)}{\tau_*^0}, \qquad \text{for all } p \in]p_*^u, p_*^{max}] \tag{S11}$$

$$A_*\chi_*(p) - \frac{\tau_*^0 + u^0}{\tau_*^0}\chi_*(p) = -\frac{\theta_*(p)}{\tau_*^0}, \qquad \text{for all } p \in [p_*^{min}, p_*^u] \tag{S12}$$

To solve these equations, we study integral operators A_* and A_*^u and due to their formalism analogies, we only consider A. We verify that $A_* f$ satisfy the equation,

$$(A_* f)'(p) = \frac{\alpha_*}{p - p_*^{min}} A_* f(p) - \frac{\alpha_* + 1}{p - p_*^{min}} f(p),$$

Let be $\lambda \in \mathbb{R}$ and $F :]a, p_*^{max}] \to \mathbb{R}$, we consider the equation to solve,

$$A_* f - \lambda f = F,$$

and by assuming that F can be differentiated, we obtain,

$$\frac{\alpha_*}{p - p_*^{min}} A_* f(p) - \frac{\alpha_* + 1}{p - p_*^{min}} f(p) - \lambda f'(p) = F'(p).$$

As $A_* f = \lambda f + F$, we obtain,

$$\frac{\lambda\alpha_* - (\alpha_* + 1)}{p - p_*^{min}} f(p) - \lambda f'(p) = F'(p) + \frac{\alpha_*}{p - p_*^{min}} F(p),$$

By defining $\delta_* = \frac{\alpha_* + 1 - \lambda\alpha_*}{\lambda}$, we obtain,

$$f'(p) + \frac{\delta}{p - p_*^{min}} f(p) = -\frac{1}{\lambda} F'(p) + \frac{\alpha_*}{\lambda(p - p_*^{min})} F(p). \tag{S13}$$

The general solution of the ordinary differential equation S13 is,

$$f(p) = \frac{c}{(p - p_*^{min})^{\delta_*}} - \frac{1}{\lambda}F(p) - \frac{\alpha_* + 1}{\lambda^2 (p - p_*^{min})^{\delta_*}} \int_p^{p_*^{max}} (p' - p_*^{min})^{\delta_* - 1} F(p') dp'.$$

We remark that $c = 0$ because $A_* f(p_*^{max}) = 0$ then,

$$f(p) = -\frac{1}{\lambda}F(p) - \frac{\alpha_* + 1}{\lambda_*^2 (p - p_*^{min})^{\delta_*}} \int_p^{p_*^{max}} (p' - p^{min})^{\delta_* - 1} F(p') dp'. \tag{S14}$$

In addition, we can verify that this result remains true even if F cannot be differentiated. We easily obtain the result of equation S11 from equation S14 by setting $\lambda = 1$, which gives $\delta_* = 1$, and $F(p) = -\frac{\theta_*(p)}{\tau_*^0}$. Then, for all $p \in]p_*^u, p_*^{max}]$,

$$\chi_*(p) = \frac{\theta_*(p)}{\tau_*^0} + \frac{\alpha_* + 1}{(p - p_*^{min})} \int_p^{p_*^{max}} \frac{\theta_*(p')}{\tau_*^0} dp'. \tag{S15}$$

From now, we consider the equation S12. In particular, we have,

$$A_* \chi_*(p) = A_*^u \chi_*(p) + (\alpha_* + 1)(p - p_*^{min})^{\alpha_*} \int_{p_*^u}^{p_*^{max}} \frac{\chi_*(p')}{(p' - p_*^{min})^{\alpha_* + 1}} dp',$$

and by using the result obtained in equation S15,

$$A_* \chi_*(p) = A_*^u \chi_*(p) + \frac{(\alpha_* + 1)(p - p_*^{min})^{\alpha_*}}{(p_*^u - p_*^{min})^{\alpha_* + 1}} \int_{p_*^u}^{p_*^{max}} \frac{\theta_*(p')}{\tau_*^0} dp',$$

then, if we define $\gamma = \frac{\alpha_*+1}{(p_*^u - p_*^{min})^{\alpha_*+1}} \int_{p_*^u}^{p_*^{max}} \frac{\theta_*(p')}{\tau_*^0} dp'$, equation S12 becomes for all $p \in [p_*^{min}, p_*^u]$,

$$A_*^u \chi_*(p) - \frac{\tau_*^0 + u^0}{\tau_*^0} \chi_*(p) = -\frac{\theta_*(p)}{\tau_*^0} - (p - p_*^{min})^{\alpha_*} \gamma. \tag{S16}$$

To solve this equation, we use the same process as previously by considering a solution of $A_*^u f - \lambda f = F$ by setting $\lambda = \frac{\tau_*^0 + u^0}{\tau_*^0}$, which gives $\delta_* = \frac{\tau_*^0 - u^0 \alpha_*}{\tau_*^0 + u^0} = \beta_*$, and $F(p) = -\frac{\theta_*(p)}{\tau_*^0} - \gamma (p - p_*^{min})^{\alpha_*}$. We obtain for all $p \in [p_*^{min}, p_*^u]$,

$$\chi_*(p) = -\frac{\tau_*^0}{\tau_*^0 + u^0} F(p) - \frac{{\tau_*^0}^2 (\alpha_* + 1)}{(\tau_*^0 + u^0)^2 (p - p_*^{min})^{\beta_*}} \int_p^{p_*^u} (p' - p_*^{min})^{\beta_* - 1} F(p') dp'.$$

By replacing explicitly F by its formulation, we obtain,

$$\begin{aligned}
\chi_*(p) &= \frac{\theta_*(p)}{\tau_*^0 + u^0} + \frac{\tau_*^0 (\alpha_* + 1)}{(\tau_*^0 + u^0)^2 (p - p_*^{min})^{\beta_*}} \int_p^{p_*^u} (p' - p_*^{min})^{\beta_* - 1} \theta_*(p') dp' \\
&\quad + \frac{\gamma \tau_*^0}{\tau_*^0 + u^0} (p - p_*^{min})^{\alpha_*} + \frac{\gamma {\tau_*^0}^2 (\alpha_* + 1)}{(\tau_*^0 + u^0)^2 (p - p_*^{min})^{\beta_*}} \int_p^{p_*^u} (p' - p_*^{min})^{\alpha_* + \beta_* - 1} dp', \\
\chi_*(p) &= \frac{\theta_*(p)}{\tau_*^0 + u^0} + \frac{\tau_*^0 (\alpha_* + 1)}{(\tau_*^0 + u^0)^2 (p - p_*^{min})^{\beta_*}} \int_p^{p_*^u} (p' - p_*^{min})^{\beta_* - 1} \theta_*(p') dp' \\
&\quad + \frac{\gamma \tau_*^0}{\tau_*^0 + u^0} (p - p_*^{min})^{\alpha_*} + \frac{\gamma {\tau_*^0}^2 (\alpha_* + 1) \left((p_*^u - p_*^{min})^{\alpha_* + \beta_*} - (p - p_*^{min})^{\alpha_* + \beta_*} \right)}{(\tau_*^0 + u^0)^2 (\alpha_* + \beta_*)(p - p_*^{min})^{\beta_*}}.
\end{aligned}$$

We remark that $\alpha_* + \beta_* = \frac{(\alpha_*+1)\tau_*^0}{\tau_*^0+u^0}$. Then,

$$\begin{aligned}
\chi_*(p) &= \frac{\theta_*(p)}{\tau_*^0+u^0} + \frac{\tau_*^0(\alpha_*+1)}{(\tau_*^0+u^0)^2(p-p_*^{min})^{\beta_*}}\int_p^{p_*^u}(p'-p_*^{min})^{\beta_*-1}\theta_*(p')dp' \\
&\quad + \frac{\gamma\tau_*^0}{\tau_*^0+u^0}(p-p_*^{min})^{\alpha_*} + \frac{\gamma\tau_*^0\left((p_*^u-p_*^{min})^{\alpha_*+\beta_*}-(p-p_*^{min})^{\alpha_*+\beta_*}\right)}{(\tau_*^0+u^0)(p-p_*^{min})^{\beta_*}}, \\
\chi_*(p) &= \frac{\theta_*(p)}{\tau_*^0+u^0} + \frac{\tau_*^0(\alpha_*+1)}{(\tau_*^0+u^0)^2(p-p_*^{min})^{\beta_*}}\int_p^{p_*^u}(p'-p_*^{min})^{\beta_*-1}\theta_*(p')dp' \\
&\quad + \frac{\tau_*^0}{\tau_*^0+u^0}(p-p_*^{min})^{\alpha_*}\left(1+\frac{(p_*^u-p_*^{min})^{\alpha_*+\beta_*}-(p-p_*^{min})^{\alpha_*+\beta_*}}{(p-p_*^{min})^{\alpha_*+\beta_*}}\right)\gamma, \\
\chi_*(p) &= \frac{\theta_*(p)}{\tau_*^0+u^0} + \frac{\tau_*^0(\alpha_*+1)}{(\tau_*^0+u^0)^2(p-p_*^{min})^{\beta_*}}\int_p^{p_*^u}(p'-p_*^{min})^{\beta_*-1}\theta_*(p')dp' \\
&\quad + \frac{\tau_*^0}{\tau_*^0+u^0}\frac{(p_*^u-p_*^{min})^{\alpha_*+\beta_*}}{(p-p_*^{min})^{\beta_*}}\gamma.
\end{aligned}$$

Finally, by replacing explicitly γ by its formulation, we obtain for all $p \in [p_*^{min}, p_*^u]$,

$$\begin{aligned}
\chi_*(p) = &\frac{\theta_*(p)}{\tau_*^0+u^0} + \frac{\tau_*^0(\alpha_*+1)}{(\tau_*^0+u^0)(p-p_*^{min})^{\beta_*}}\int_p^{p_*^u}(p'-p_*^{min})^{\beta_*-1}\frac{\theta_*(p')}{\tau_*^0+u^0}dp' \\
&+(\alpha_*+1)\frac{(p_*^u-p_*^{min})^{\beta_*-1}}{(p-p_*^{min})^{\beta_*}}\int_{p_*^u}^{p_*^{max}}\frac{\theta_*(p')}{\tau_*^0+u^0}dp'.
\end{aligned} \tag{S17}$$

Carbon stocks Based on equations S15 and S17, we can compute the amounts of C per pool and domain. The amount of carbon inaccessible to carbon uptake $C_{*,\bar{\mathcal{D}}_u}$ is,

$$\begin{aligned}
C_{*,\bar{\mathcal{D}}_u} &= \int_{p_*^u}^{p_*^{max}}\chi_*(p)dp \\
&= \frac{m^0}{\tau_*^0}\int_{p_*^u}^{p_*^{max}}\left(1+(\alpha_*+1)ln\left(\frac{p-p_*^{min}}{p_*^u-p_*^{min}}\right)\right)s_*(p)dp \\
&\quad + \frac{m^0(1-e^0)}{\tau_*^0e^0I}\int_{p_*^u}^{p_*^{max}}\left(1+(\alpha_*+1)ln\left(\frac{p-p_*^{min}}{p_*^u-p_*^{min}}\right)\right)i_*(p)dp,
\end{aligned} \tag{S18}$$

and the amount of carbon accessible to carbon uptake $C_{*,\mathcal{D}_u}$ is,

$$\begin{aligned}
C_{*,\mathcal{D}_u} &= \int_{p_*^{min}}^{p_*^u}\chi_*(p)dp \\
&= \frac{m^0}{u^0}\int_{p_*^{min}}^{p_*^{max}}s_*(p)dp + \frac{m^0(1-e^0)}{u^0e^0I}\int_{p_*^{min}}^{p_*^{max}}i_*(p)dp.
\end{aligned} \tag{S19}$$

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