Cellulose Biodegradation Models; An Example of Cooperative Interactions in Structured Populations

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Abstract

We introduce various models for cellulose bio-degradation by micro-organisms. Those models rely on complex chemical mechanisms, involve the structure of the cellulose chains and are allowed to depend on the phenotypical traits of the population of micro-organisms. We then use the corresponding models in the context of multiple-trait populations. This leads to classical, logistic type, reproduction rates limiting the growth of large populations but also, and more surprisingly, limiting the growth of populations which are too small in a manner similar to the effects seen in populations requiring cooperative interactions (or sexual reproduction). This study hence offers a striking example of how some mechanisms resembling *cooperation* can occur in structured biological populations, even in the absence of any actual cooperation.

1 Introduction

The goal of this article is to derive models for structured populations of micro-organisms living of cellulose degradation. Our first step is to study the mechanisms by which some micro-organisms can use cellulose. The full process is obviously complex and we have to abstract its most important features. This gives us a hierarchy of models, depending on the level of simplification that one desires.

The second step is to couple those models with the population dynamics of the corresponding micro-organisms. While the mechanism of bio-degradation that we consider is similar for each species of micro-organisms, we allow for some variability from one species to another, in the enzymes involved for instance. This leads to a population structured by a phenomenological trait that describes the exact path of bio-degradation.

As the amount of cellulose is limited, the total growth of the population is, unsurprisingly, limited as well. More interesting are the effects when the total population or the population in a given species is small. The model does not include any actual cooperation between micro-organisms but as the bio-degradation occurs in several steps, the process is non linear in the population size even if cellulose is abundant. This puts small populations at a disadvantage, introducing an effect similar to classical cooperation.

Cellulose Bio-degradation. Mechanisms and Models. Cellulose is the structural component of many plants and is therefore the most abundantly produced bio-polymer; it is a homo-polymer

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consisting of vast number of glucose units. The most important feature of cellulose as a substrate is its *insolubility*. As such, bacterial and fungal degradation of cellulose, (e.g. by fungi *Trichoderma reesei* or bacteria *Clostridium thermocellum*), occurs exocellularly. The products of cellulose hydrolysis are available as carbon and energy sources for microbes that inhabit environments in which cellulose is biodegraded [31, 32].

In this work we model cellulose bio-degradation as a multiple-step process, reflecting realistic mechanisms described in [32]. Let $\varrho(t)$ denote the mass of cellulose The biodegrading microorganism is unable to consume (degrade) the cellulose ϱ directly. Instead, the individuals produce two enzyme complexes $e_1(t)$ and $e_2(t)$ that act in a two-stage process.

During the first stage, the (endoglucanase) enzyme e_1 weakens cellulose fibers in ϱ: that is, it randomly cuts the fibers, creating the so-called reducing and non-reducing ends which serve landing sites for the (exoglucanase) enzyme e_2. During the second stage, the enzyme e_2 locates a reducing (or non-reducing) end and attaches itself to it. Once attached, it cleaves off cellobiose (a major energy source for the microorganisms) from the chain of polysaccharides. Some portion $\theta_p \in [0, 1]$ of cellobiose is consumed directly by the microorganism that produced the enzymes, and the rest is available for other individual microorganisms in the population due to diffusion. The above mechanisms can be viewed as follows:

$$\begin{gathered}\text{Growth of micro-organisms + influx of cellulose } \varrho(t)\\ \downarrow\\ \text{Production of enzyme complexes } e_1(t) \text{ and } e_2(t)\\ \downarrow\\ \text{Weakening of } \varrho(t) \text{ by } e_1(t)\\ \downarrow\\ \text{Production of cellobiose } p(t) \text{ by } e_2(t) \text{ acting on } \varrho(t).\end{gathered}$$

In the present work we develop several models of varying complexity which incorporate these mechanisms. Even in the simplest model (corresponding to $L = 1$) the aforementioned cascade of events produces a *cooperative effect* (which appears due to the fact that the cellobiose units cleaved off by the enzyme of one microorganism are available for consumption by other individuals located nearby). Mathematically, these effects are encoded in the reproduction rate $B(n)$ of the population n. In particular, for small populations, the population size $n(t)$ turns out to behave as

$$\partial_t n(\cdot, t) \sim n\big(B(n) - d\big) \quad \text{with} \quad B(n) \sim Cn^2 \quad \text{when} \quad n \ll \bar{n},$$

where $\bar{n}$ is a critical threshold.

In general, the population includes several various species of micro-organisms. In that case, the exact enzyme complexes used may change across species. We represent the different species by traits $x_j \in \{1, \dots, M\}$ and a population with trait x_j uses enzymes complexes denoted $e_{1,j}$ and $e_{2,j}$. This can be further generalized to continuous traits x with sub-populations $n(t, x)$. The case of discrete traits can be included in this framework by taking $n(t, x) = \sum_j n_j(t)\, \delta_{x_j}(x)$ with $n_j(t)$ the population of individuals with trait x_j. In this general framework, our final model is of the form

$$\partial_t n(x, t) = \Big(B[n](x, t) - d(x)\Big) n(x, t)\,, \tag{1.1}$$

where $B[n]$ is now an integral operator, see (5.2) for the precise formula.

Our model resembles systems of population dynamics, see [25] for instance. However, in contrast to many of those systems, the cellulose bio-degradation process leads to both competition

between individuals and species (for the resource) and cooperative interactions. This occurs at the interspecies level as the byproduct of the process, cellobiose, is the same independent of the enzyme complexes involved, and can benefit any individual in the population (and not only individuals using the same complexes). Cooperation also occurs specifically within each species (or between species that are close enough). This follows from the fact that an individual with similar enough enzyme complexes can use the reducing and non reducing ends created in the cellulose by the endoglucanase enzyme complex of another individual. We thus expect that the mathematical models developed in our work will produce better phenomenological results for small populations (in deterministic models) since cooperation significantly affects the dynamics, as discussed in more detail below.

Tail issue in deterministic selection dynamics. Models in population dynamics focus on selection because it is rightfully viewed as the main mechanism to explain the survival of populations and the evolution of traits. The selection mechanism in these models is often driven by competition between individuals, possibly combined with mutations to create new traits. In addition competition is well understood from the modeling point of view.

On the other hand cooperative effects are harder to model, especially at the level of micro-organisms. Several well-known cooperative effects (such as sexual reproduction for large animals) do not take place for all micro-organisms. Nevertheless, the importance of such effects has long been recognized: see for instance the works [14, 23, 24, 28] on mutualism that discuss interspecies interactions yielding reciprocal benefits.

In this paper we introduce biological mechanisms, by the example of cellulose bio-degradation, that lead to reproduction rates encoding both (intra-species) cooperative effects and competition between individuals; see Section 4. This suggests that reproduction rates that only incorporate competition may fail to describe many biochemical processes, especially at the level when $B[n]$ significantly deviates from traditional logistic terms, that is for small populations.

There are several approaches to study the phenotypical evolution driven by small mutations in replication, the main objective being to describe the dynamics of the fittest (or dominant) trait in the population. The main mechanisms affecting dynamics are usually a) the selection principle (due to competition, birth and death), and b) small mutations. These two mechanisms influence the trait dynamics on two different scales. The selection effect becomes evident on the reproduction timescale t_R, while the effect of small mutations is evident on a generation timescale $t_M \gg t_R$. The drastic difference between the two scales introduces both small and large parameters into models (mutations can be small or rare for instance, population is usually large and death rates could vary) and this causes various difficulties.

One of the best known approaches is the so-called adaptive dynamics theory, see for instance [10, 12, 3, 16, 36]. Adaptive dynamics considers evolution as a series of invasions by a small mutant population of the dominant trait population, a process which is classically modeled by a system of ODE's. Depending on the relative fitness of the mutant, this can lead to the replacement of the dominant trait or the extinction of the invading population (the cases of co-existence are usually harder to handle at this level).

Other very popular models are stochastic, or individual-centered models, see for instance [14, 5, 5] among many. Probabilistic models are natural because they take natural fluctuations of births, deaths, and mutations into account at the individual level, and are therefore considered to be the most realistic. They consist in life and death processes for each individual X_i. A typical example consists in taking Poisson processes with birth rates $b(X_i)$ and death rates increasing with the

competition between individuals, for example $d_i = d(X_i) + \sum_{j \neq i} I(X_i - X_j)$.

When a birth occurs, it simply adds another individual with the same trait, unless a mutation takes place, generally with small probability. In that case, the new individual has a different random trait, obtained through some distribution. In general of course competition could influence both the birth rate and the mortality rate. Under the right scalings, stochastic models can lead to the classical adaptive dynamics [34, 26].

When the total number of individuals is too large (it can easily reach $10^{10} - 10^{12}$ for some micro-organisms), stochastic models can become cumbersome and prohibitive to compute numerically for instance. In that case, one expects to be able to derive a deterministic model as a limit of large populations which would be simpler to use. Such a derivation was provided in [7] for example, leading to integro-differential equations such as

$$\partial_t n(x,t) = \Big(r(x) - \int I(x-y) n(t,y)\, dy\Big) n(x,t) + M[n](t,x), \tag{1.2}$$

where $r(x) = b(x) - d(x)$ and $M[\cdot]$ is the mutation kernel, a diffusion or integral operator. This is the level of modeling that we are interested in this article.

Even though deterministic models of type (1.2) are obtained from stochastic ones, simulations for these two types of models typically produce different behaviors in terms of evolutionary speeds and branching patterns. In stochastic simulations, in which a single individual represents a minimal unit necessary for survival, demographic stochasticity (the variability in population growth rates among individuals) acts drastically on small populations, leading to complete extinction of small populations with negative reproduction rates. In deterministic models however, sub-populations can never go completely extinct and can "rebound" later on if their reproduction rate becomes positive.

It is an open and difficult question of how to keep the stochastic effects for the small populations in the deterministic models. Perthame and Gauduchon [26] made an attempt in truncating the populations with less than one individual by introducing an analog of stochastic mortality for models of type (1.2), a survival threshold, which allows phenotypical traits in the small population to vanish in finite time. In [26] this is achieved by modifying (1.2) as follows

$$\partial_t n(x,t) = \Big(r(x) - I \star n\Big) n - \sqrt{\frac{n}{\bar{n}}} + M[n](t,x)\,. \tag{1.3}$$

The new term enables the population to vanish for some traits when the population density is too low in comparison with $\bar{n}$, which disallows densities corresponding to fewer than one individual.

As one wishes to see the evolution of traits generated by mutations, one needs to rescale the above equation in time. This leads to large deviation type phenomena which can be observed by defining $n_\varepsilon(t,x) = \exp(\phi_\varepsilon(t,x)/\varepsilon)$, with ε the ratio of the reproduction and mutation time scales (see [26, 13]). One now has two scales for the populations, the small population threshold $\bar{n}$ and the exponential scale $\exp \phi/\varepsilon$.

Often, the aim is to analyze the population behavior in the limit as $\varepsilon \to 0$ and therefore $\bar{n}$ should be chosen in terms of ε. Numerical simulations for the corresponding equation with initial data of monomorphic type, see [26], indicate that the evolution speeds and time of branching depend on this choice of $\bar{n}$ in terms of ε. When ε is fixed, too large a value of $\bar{n}$ leads to extinction, while too small a value of $\bar{n}$ leads to spontaneous jumps in branching, see [26, 13].

A complete mathematical analysis of the general equations is currently intractable. One of the few situations that is currently understood [26] is when the mortality threshold is chosen as

$\bar{n}_\varepsilon = \exp(-\frac{\bar{\varphi}}{\varepsilon})$. However, the scaling $\bar{n}_\varepsilon = \exp(-\frac{\bar{\varphi}}{\varepsilon})$ for a fixed $\bar{\varphi}$ is often much too small. Recall that the threshold $\bar{n}_\varepsilon$ should correspond to a single individual in stochastic modeling. Thus, if we come back to the starting point, which means a total population $\int n(x,t)\,dx$ of $10^{10} - 10^{12}$, then for $\varepsilon = 10^{-4}$ (a typical value for many applications) and threshold $\bar{n}_\varepsilon$ of order $\exp(-\frac{1}{\varepsilon})$, an aggregate population over any fixed interval of traits would still represent much less than one individual.

Another type of correction has been proposed by Jabin [22]. The author allows the threshold $\bar{n}_\varepsilon$ to be polynomial in ε and introduces special cooperative term D_ε in the (rescaled) model

$$\partial_t n_\varepsilon(x,t) = \Big(r(x) - \int I(x-y)n(t,y) - D_\varepsilon[n]\Big)n(x,t) + M[n](t,x). \tag{1.4}$$

This term does not handle the small populations as precisely, but the new model still corrects all the abnormal behaviors of (1.2) near the limit. The cooperative effects in [22] were, however, more intuited than derived. For example, the typical cooperative term D_ε has the form

$$-D_\varepsilon[n_\varepsilon](x,t) = -D_0 + \max\big(0,\, D_0 - K(x)\,d(x, \{n_\varepsilon \geq \bar{n}_\varepsilon\})\big) \tag{1.5}$$

where $K(x)$ is a symmetric positive kernel. In that respect, the present work puts the approach in [22] on a more solid framework by actually deriving those effects from realistic biochemical processes.

The present work aims at introducing cooperative terms, similar to those of [22], that arise naturally (directly from biological processes), rather than *ad hoc* mathematical terms. The cooperative effects in the integral operator $B[n]$ in (1.1) appear naturally in the process of model construction and give a hint of what such terms should look like.

2 Cellulose bio-degradation: structure and mechanisms

2.1 Cellulose structure and enzyme systems

Cellulose is the most abundantly produced bio-polymer. It is a homo-polymer consisting of glucose units joined by β-1, 4 bonds. The size of cellulose molecules (degree of polymerization) varies from seven thousand to fourteen thousand glucose moieties per molecule in secondary walls of plants. Cellulose molecules are strongly associated through inter- and intra-molecular hydrogen-binding and van der Waals forces that result in the formation of microfibrils, which in turn form fibrils. Cellulose molecules are oriented in parallel, with reducing ends of adjacent glucan chains located at the same end of a micro-fibril. These molecules form highly ordered crystalline domains interspersed with more disordered, amorphous regions. Although cellulose forms a distinct crystalline structure, cellulose fibers in nature are not purely crystalline. The degree of crystallinity varies from purely crystalline to purely amorphous.

To degrade plant cell material, microorganisms produce multiple enzymes known as enzyme systems [32]. For microorganisms to hydrolyze and metabolize insoluble cellulose, extra-cellular cellulases (degradation enzymes) must be produced that are either *free* or *cell associated*. Microorganisms have adapted different approaches to effectively hydrolyze cellulose, naturally occurring in insoluble particles. Cellulosic filamentous fungi (and some types of aerobic bacteria) have the ability to penetrate cellulosic substrates through hyphal extensions, thus often presenting their *free* cellulase systems in confined cavities within cellulosic particles. In contrast, anaerobic bacteria lack the ability to effectively penetrate cellulosic material and perhaps had to find alternative

mechanisms for degrading cellulose. This led to the development of *complexed* cellulase systems (called cellulosomes) which position cellulase producing cells at the site of hydrolysis, as observed for clostridia and ruminal bacteria.

Overall there are three major components of cellulase systems: (i) endoglucanases, which randomly hydrolyze β-$1,4$ bonds within cellulose molecules, thereby producing reducing and non-reducing ends; (ii) exoglucanases, which cleave cellobiose units from the non-reducing ends of cellulose polymers; and (iii) $\beta-$glucosidases which hydrolyze cellobiose yielding glucose (the major product of cellulose hydrolysis used by microorganisms as energy source).

2.2 Quantities to monitor and two basic bio-mechanisms

We first consider the case of populations with one trait. In our analysis the biomass density of the microorganism that degrades cellulose is denoted by $n = n(t)$. The total mass of exoglucanases and endoglucanases produced by the microorganism are denoted by $e_1 = e_1(t)$ and $e_2 = e_2(t)$, respectively.

We view cellulose as a crystalline conglomerate of fibers (chains of polysaccharide). According to our discussion above, during the first stage of the degradation the endoglucanase enzyme e_1 weakens fibers, which means that e_1 randomly cuts the fibers by creating reducing and non-reducing ends that serve as landing sites for exoglucanases e_2. Viewing cellulose as a three-dimensional structure one can imagine such structure with punctures and cuts after the first stage. It is still the same cellulose but with more "cuts" that serve as landing sites for the second type of enzymes e_2.

There are several types of exoglucanases e_2. Some types can land on reducing ends and some on non-reducing. For simplicity, we assume that the second type of enzymes can land only on reducing ends. Once the second enzyme e_2 lands on the reducing end it cleaves off cellobiose from the chain of polysaccharide. In our work we do not consider the third type of enzymes and treat cellobiose as the major product of degradation. We instead assume that some portion $\theta_p \in [0,1]$ of cellobiose is consumed by the microorganism that produced it, and the rest diffuses and is available for everyone. Finally, we let $p(t)$ denote the total mass of the cellobiose available to everyone.

There are two main stages in which e_2 participates to produce cellobiose $p(t)$:

(a) The enzyme locates a reducing end and attaches itself to it.

(b) It keeps cleaving off cellobiose units until it either disintegrates or detaches from the chain.

This leads to several modeling approaches.

2.2.1 Cleaving Mechanism 1

Since the time spent by an individual enzyme e_2 on the reducing end can significantly differ from the time of locating a reducing end, it is useful to distinguish two states of e_2: the *attached* and *detached* states. In the first mechanism we distinguish these two states: we let $e_{21}(t)$ represent the mass of detached e_2 (which may wander freely or on a leash, that is attached to a bacterial cell wall), and let $e_{22}(t)$ represent the mass of enzymes e_2 attached to a reducing end. Also, we let m_1, $m_2 > 0$ be the masses of individual enzymes e_1, e_2, respectively, and $S(t)$ be the number of *unoccupied* reducing ends. The quantities e_{22}, S and T are then related via the equation

$$T(t) = S(t) + \frac{e_{22}(t)}{m_2}\,. \tag{2.1}$$

We suppose that, at any moment of time, unoccupied spots $S(t)$ become occupied (or attacked) by the detached enzymes e_{21} at a certain rate to be described. Next, we assume that an individual attached enzyme e_{22} cleaves off cellobiose units from the reducing end, again with a given rate. Also, we assume that some proportion of the (attached) enzyme e_{22} detaches from a reducing end, and that a fraction $\theta_r \in [0, 1]$ of those ends (from which the enzyme e_{22} detached) become unusable.

Remark 2.1. This first mechanism is more realistic since it takes into account time spent by the enzyme on the reducing end. This mechanism can be employed for modeling systems where both non-complex and complex cellulases are present.

2.2.2 Cleaving Mechanism 2

The second mechanism is somewhat simplified. It may be used to describe complex cellulases where exoglucanases are not entirely free (they are attached to bacterial cell walls, and once bacteria leaves the spot the enzyme becomes detached from the reducing end as well). Here we suppose that at any moment of time, all existing $T(t)$ reducing ends are available for an attack by the enzyme e_2. The reducing ends $T(t)$ are attacked with a certain rate $b(T(t))$ and a certain (average) amount $q > 0$ of cellobiose units is cleaved off by each individual enzyme e_2, after which the enzyme e_2 detaches itself. We view such an attack as instantaneous. Thus, after such an (instantaneous) attack, all $T(t)$ reducing ends are unoccupied again. We will assume that after the attack a certain portion $\theta_r \in [0, 1]$ of the (attacked) reducing ends becomes *unusable*. In that scenario the two processes, finding a reducing end and cleaving off cellobiose, are lumped together (with a hidden assumption that enzymes cannot remain attached to a chain for a very long time).

Remark 2.2. In the second mechanism the reducing ends $T(t)$ serve as "prey" and e_2 as "predators", with one difference: the enzymes attack the prey, use it and leave it alone. After an attack only a certain proportion of the sites is destroyed, while the rest is still usable.

3 Cleaving Models

3.1 $\{N$-$S\}$-model

In this section we consider a model in which we monitor groups of cellulose chains consisting of $l \geq 1$ cellobiose units; in that case we say that a chain is of length l. This allows us to develop a fundamental model incorporating cleaving Mechanism 1.

Assumptions and notation. Cellulose chains may have different topological configurations: they could be linear or rectangular (when fibers are embedded in a lignin matrix) or they could have a random three-dimensional structure. Monitoring the topology increases the complexity, but it does not provide a better tool for studying the population dynamics. After all, it is the number of landing spots that matters rather then the configuration of the cellulose chains. Thus we make no assumption about the configuration and monitor only the length of its constituent pieces. Another assumption we make is that the enzyme e_1 produces a reducing end (a landing site) without physically cutting the chain. This assumption decreases complexity in the model while it does not change the dynamics. Indeed, If we allow e_1 to physically cut a chain in the model, then the chain could be split into two parts when e_1 acts. In that case, the number of landing sites would be the same as in the scenario when the landing site is created without a physical cut. Finally, we impose

the requirement that only one landing site per unit of cellobiose is allowed; this reflects the fact that cellulose chains represent discrete systems of units.

We assume that the population has only one trait, that is $n = n_1$. We say that a cellulose chain is in the (l,i)-state, or is an (l,i)-chain, if it has length l (so consists of $l \geq 1$ cellobiose units) and $i \in \{0, 1, \ldots, l\}$ landing sites (previously made by enzyme e_1). We let $N_{l,i}(t)$ denote the number of (l,i)-chains. We let e_1 denote the mass of the enzyme producing landing sites. The mass of the enzyme e_2 in the detached or free state (state 1) is denoted e_{21}, while the mass of the attached enzyme (state 2) which is attached to some landing site on a chain in the (l,i)-state is denoted by $e_{22}^{l,i}$. We also let p denote the mass of cellobiose available to everyone as energy source.

We use indices (l,i) in the set

$$(l,i) \in I_L := \{(\tilde{l},\tilde{i}) \in \mathbb{Z} \times \mathbb{Z} : 1 \leq \tilde{l} \leq L,\, 0 \leq \tilde{i} \leq \tilde{l}\}\,, \tag{3.1}$$

with rates $r_{l,i} = 0$ for $i \neq 0$, and we also use the convention that

$$\begin{aligned} N_{l,i} &\equiv 0 \quad \text{if} \quad (l,i) \notin I_L \\ e_{22}^{l,i} &\equiv 0 \quad \text{if} \quad (l,i) \notin I_L \quad \text{or} \quad i = 0\,. \end{aligned} \tag{3.2}$$

Enzyme dynamics. We assume that the rates of production of the enzymes e_1, e_2 by the microorganism and their degradation rates are fixed. The enzymes e_1 and e_2 are catalyzers which stay in the system as long as they "live". Then e_1 satisfies

$$\partial_t e_1(t) = b_1\, n(t) - d_1 e_1(t) \quad \text{with} \quad b_1,\ d_1 > 0\,. \tag{3.3}$$

Next, the number of landing sites on (l,i)-chains is $T_{l,i} = iN_{l,i}$, so the number of unoccupied landing sites $S_{l,i}(t)$ is

$$S_{l,i}(t) = T_{l,i}(t) - \frac{e_{22}^{l,i}(t)}{m_2} = iN_{l,i}(t) - \frac{e_{22}^{l,i}(t)}{m_2}. \tag{3.4}$$

Neglecting saturation effects, we suppose that unoccupied sites $S_{l,i}$ are attacked by e_{21} with the rate $\beta_{l,i} S_{l,i}$. Also, we assume that enzyme e_2 located on a chain in (l,i)-state (randomly) detaches from the chain with rate $\sigma_{l,i} > 0$. We let $\gamma_{r,l,i} > 0$ denote the decay rate of an individual landing site (whether it is occupied or not) and assume that if an occupied reducing end degrades then the attached enzyme e_{22} disintegrates together with it. This leads to the following set of equations that monitor the dynamics of the enzyme e_2:

$$\begin{aligned} \partial_t e_{21}(t) &= b_2\, n(t) - \sum_{l,i} \beta_{l,i} S_{l,i}(t)\; e_{21}(t) + \sum_{l,i} \sigma_{l,i}\, e_{22}^{l,i}(t) - d_{21}\, e_{21}(t) \\ &= b_2\, n(t) - \sum_{l,i} \left[\beta_{l,i} \Big(iN_{l,i}(t) - \frac{e_{22}(t)}{m_2} \Big) e_{21}(t) - \sigma_{l,i}\, e_{22}^{l,i}(t) \right] - d_{21}\, e_{21}(t) \\ \partial_t e_{22}^{l,i}(t) &= \beta_{l,i} S_{l,i}(t)\; e_{21}(t) - \Big(\sigma_{l,i} + d_{22}^{l,i} + \gamma_{r,l,i} \Big)\, e_{22}^{l,i} \\ &= \beta_{l,i} \Big(iN_{l,i}(t) - \frac{e_{22}(t)}{m_2} \Big) e_{21}(t) - \Big(\sigma_{l,i} + d_{22}^{l,i} + \gamma_{r,l,i} \Big) e_{22}^{l,i} \end{aligned} \tag{3.5}$$

where $d_{21} > 0$ and $d_{22}^{l,i} > 0$ are the degradation rates of e_{21} and $e_{22}^{l,i}$, respectively, and $b_2 > 0$ is the production rate of e_2, which equals that of e_{21}.

Chain dynamics. We neglect saturation effects and assume that the rate with which enzymes e_1 produce landing sites on the chains in (l,i)-state is

$$\alpha_{l,i}(l-i)N_{l,i}(t)\frac{e_1(t)}{m_1} = \widehat{\alpha}_{l,i}N_{l,i}(t)\,e_1(t)\,, \quad \text{with} \quad \widehat{\alpha}_{l,i} = \alpha_{l,i}\frac{(l-i)}{m_1} \tag{3.6}$$

where the multiplier $(l-i)$ reflects the requirement that only one landing site per cellobiose unit is allowed, and we have scaled the mass e_1 by m_1 to get the number of enzymes. We assume that a freshly made landing site cannot be instantaneously occupied (and different cuts don't occur simultaneously), so that the rate of production of new landing sites on (l,i)-chains is the rate of production of unoccupied $(l,i+1)$-sites $S_{l,i+1}(t)$. Thus (3.6) is the rate of transition $(l,i)\to(l,i+1)$ due to the action of e_1.

Recall that $\gamma_{r,l,i} > 0$ is the decay rate of an individual landing site on a chain in (l,i)-state. Thus the rate at which any one of the i sites on an (l,i)-chain degrades must be $i\,\gamma_{r,l,i}$, so that the rate of transition $(l,i)\to(l,i-1)$ due to degradation of landing sites is

$$\widehat{\gamma}_{l,i}N_{l,i}(t), \quad \text{with} \quad \widehat{\gamma}_{l,i} = i\gamma_{r,l,i}\,. \tag{3.7}$$

Let $q_{l,i} > 0$ denote the rate of production of cellobiose by an individual enzyme on a (l,i)-chain. Then the total rate of cellobiose production by the enzymes $e_{22}^{l,i}$ is

$$q_{l,i}\frac{e_{22}^{l,i}(t)}{m_2} = \widehat{q}_{l,i}\,e_{22}^{l,i}(t)\,, \quad \text{with} \quad \widehat{q}_{l,i} = \frac{q_{l,i}}{m_2}\,, \tag{3.8}$$

where $e_{22}^{l,i}(t)/m_2$ is the total number of occupied landing sites on (l,i)-chains. Thus, the rate (3.8) is the rate of transition $(l,i)\to(l-1,i)$ due to the cleaving activity of e_2.

Let $\theta_r > 0$ denote the proportion of landing sites that become unusable after $e_{22}^{l,i}$ detaches from a chain or dies. This contributes to the transition $(l,i)\to(l,i-1)$ and the corresponding rate is

$$\widehat{\theta}_{l,i}\,e_{22}^{l,i}(t) \quad \text{with} \quad \widehat{\theta}_{l,i} = \theta_r(\sigma_{l,i} + d_{22}^{l,i})\frac{1}{m_2}\,. \tag{3.9}$$

Combining (3.6)–(3.9) we obtain the equations that monitor the dynamics of $N_{l,i}(t)$, namely

$$\begin{aligned}\partial_t N_{l,i}(t) = r_{l,i} &+ \Big(\widehat{\alpha}_{l,i-1}N_{l,i-1}(t) - \widehat{\alpha}_{l,i}N_{l,i}(t)\Big)e_1(t) + \Big(\widehat{\gamma}_{l,i+1}N_{l,i+1}(t) - \widehat{\gamma}_{l,i}N_{l,i}(t)\Big)\\ &+ \Big(\widehat{q}_{l+1,i}\,e_{22}^{l+1,i}(t) - \widehat{q}_{l,i}\,e_{22}^{l,i}(t)\Big) + \Big(\widehat{\theta}_{l,i+1}\,e_{22}^{l,i+1}(t) - \widehat{\theta}_{l,i}\,e_{22}^{l,i}(t)\Big) - \gamma_{\varrho,l,i}N_{l,i}(t),\end{aligned} \tag{3.10}$$

where $r_{l,i}$ is the unit rate of production of cellulose, and $\gamma_{\varrho,l,i}$ is the rate at which the cellulose naturally decays or becomes unavailable to the microorganism (that is, decay not directly attributable to the bacteria). We assume for simplicity that the cellulose provided by the environment has no reducing ends, so that $r_{l,i} = 0$ for $i \geq 1$, and in particular, the sum $\sum_i i\,r_{l,i} = 0$.

Population dynamics. Let $\theta_p \in [0,1]$ denote the proportion of produced cellobiose available for everyone. Then, using (3.8), the equations for the total mass $p(t)$ of cellobiose available for everyone, and the total mass of the microorganism are respectively

$$\begin{aligned}\partial_t p(t) &= \theta_p\, m_c \sum_{l,i}\widehat{q}_{l,i}\,e_{22}^{l,i}(t) - \gamma n(t)p(t) - \gamma_p p(t), \quad \text{and}\\ \partial_t n(t) &= \frac{\mu n(t)}{\bar{n}+n(t)}\Big(\gamma p(t) + (1-\theta_p)m_c\sum_{l,i}\widehat{q}_{l,i}\,e_{22}^{l,i}(t)\Big) - \gamma_n n(t),\end{aligned} \tag{3.11}$$

where m_c is the mass of one cellobiose unit, γ is the consumption rate, μ is the conversion efficiency, and γ_p, γ_n are decay rates of p and n, respectively. Here $\bar{n}$ represents a critical population threshold: if n is large, $n = O(\bar{n})$, the growth depends only on the cellobiose supply, while if n is small, $n \ll \bar{n}$, the growth is linear but with small growth rate, so the population is unlikely to survive (since $\mu/\bar{n} < \gamma_n$).

Remark 3.1. Clearly, creating a landing site or cleaving off a cellobiose unit does not happen instantaneously. The time for these processes is short and may depend on the configuration of the chain, the crystallinity of the cellulose as well as the life time of the enzymes. Thus it is possible that within a given period of time (no matter how short) more than one landing site is created or two or more cellobiose units are cleaved off from the same chain. In our model (3.10), however, we consider only transitions of the type $(l,i) \to (l,i+1)$ and $(l,i) \to (l-1,i)$ but do not take into account possible transitions $(l,i) \to (l-k,i+m)$ for more general k and m; see, for instance, the discussion of formulas (3.6) and (3.8). This approach is justified provided that the number and size of chains is very large compared to the amount of enzymes e_1, e_2, and the likelihood that two landing sites are created or more than two cellobiose units are cleaved off from the same chain simultaneously (or during a short period of time) is extremely small.

Another way to justify the above modeling assumptions is to consider a time-continuous Poisson counting process, that corresponds to the events of creating a landing site and/or cleaving off cellobiose. Any instance when a landing site is created (that is the moment it becomes available for the use by e_2) or cellobiose unit is cleaved off the chain can be counted as an event. It is well-known that the probability of two or more events happening instantaneously is zero (in other words the probability that two events take place over the time Δt is $o(\Delta t)$. Furthermore, the probability rate of transition $(l,i) \to (l,i+1)$ due to the activity of e_1 equals (3.6) while the probability rate of transition $(l,i) \to (l-1,i)$ due to cleaving is given in (3.8); for details see [33, 40].

3.2 Reduction to S-model for Cleaving Mechanism 1

We now develop a simpler model by reducing the $\{N_i, S\}$-model, (3.3)-(3.11). Henceforth we will assume that indices l and i run through all of $\mathbb{Z}$ to avoid considering special cases. This augments the previously defined system, but by choosing appropriate initial conditions, we can ensure that $N_{l,i}$ and $e_{22}^{l,i}$ vanish for all times whenever $l \le 0$, $i \le 0$, or $i > l$. We then define the quantities

$$\begin{aligned} \varrho(t) &= m_c \sum_{l,i} l N_{l,i}(t), & e_{22}(t) &= \sum_{l,i} e_{22}^{l,i}(t), \\ T(t) &= \sum_{l,i} T_{l,i}(t) = \sum_{l,i} i N_{l,i}(t), & S(t) &= \sum_{l,i} S_{l,i}(t), \end{aligned} \tag{3.12}$$

where m_c is the mass of a cellobiose unit; these represent the total mass of cellulose, mass of attached enzyme e_2, number of landing sites and number of unoccupied sites, respectively. Note that each of these sums is finite provided we specify appropriate initial conditions. We next assume that the constants are independent of l and i, so that for each $l,\ i \in \mathbb{Z}$,

$$\beta_{l,i} = \beta\,, \quad \sigma_{l,i} = \sigma\,, \quad \gamma_{r,l,i} = \gamma_r\,, \quad d_{22}^{l,i} = d_{22}, \quad \alpha_{l,i} = \alpha, \quad q_{l,i} = q\,, \quad \gamma_{\varrho,l,i} = \gamma_\varrho\,. \tag{3.13}$$

Summing over l, i in (3.5) and using (3.4), we get

$$\begin{aligned} \partial_t e_{21}(t) &= b_2\, n(t) - \beta S(t)\, e_{21}(t) + \sigma\, e_{22}(t) - d_{21}\, e_{21}(t), \\ \partial_t e_{22}(t) &= \beta S(t)\, e_{21}(t) - \big(\sigma + d_{22} + \gamma_r\big) e_{22}(t)\,. \end{aligned} \tag{3.14}$$

To obtain equations for ϱ and T, we scale and add equations (3.10). First, we recall

$$\sum_{l,i} i\, r_{l,i} = 0 \quad \text{and define} \quad r = m_c \sum_{l,i} l\, r_{l,i} = m_c \sum_{l} l\, r_{l,0}\,, \tag{3.15}$$

so that r represents the (mass of) cellulose produced by the environment. Next, using (3.6) and making the change of variable $j = i - 1$ we obtain

$$\begin{aligned}
&\sum_{l,i} i \Big(\widehat{\alpha}_{l,i-1} N_{l,i-1}(t) - \widehat{\alpha}_{l,i} N_{l,i}(t)\Big) e_1(t) \\
&\quad = \frac{\alpha}{m_1} \sum_{l,i} \Big(i(l-(i-1))N_{l,i-1}(t) - i(l-i)N_{l,i}(t)\Big) e_1(t) \\
&\quad = \frac{\alpha}{m_1} \Big(\sum_{l,j} (j+1)(l-j) N_{l,j}(t) - \sum_{l,i} i(l-i) N_{l,i}(t)\Big) e_1(t) \\
&\quad = \frac{\alpha}{m_1} \Big(\sum_{l,j} (l-j) N_{l,j}(t)\Big) e_1(t) = \frac{\alpha}{m_1} \left(\frac{\varrho(t)}{m_c} - T(t)\right) e_1(t)
\end{aligned}$$

and similarly, with (3.7) and $j = i + 1$,

$$\begin{aligned}
&\sum_{l,i} i \Big(\widehat{\gamma}_{l,\,i+1} N_{l,i+1}(t) - \widehat{\gamma}_{l,i} N_{l,i}(t)\Big) \\
&\qquad = \gamma_r \sum_{l,i} \Big(i(i+1) N_{l,i+1}(t) - i^2 N_{l,i}(t)\Big) \\
&\qquad = \gamma_r \Big(\sum_{l,j} (j-1) j N_{l,j}(t) - \sum_{l,i} i^2 N_{l,i}(t)\Big) \\
&\qquad = -\gamma_r \sum_{l,j} j N_{l,j}(t) = -\gamma_r T(t)\,.
\end{aligned}$$

Next, using (3.8), we compute

$$\sum_{l,i} i \Big(\widehat{q}_{l+1,i}\, e_{22}^{l+1,i}(t) - \widehat{q}_{l,i}\, e_{22}^{l,i}(t)\Big) = \frac{q}{m_2} \sum_{l,i} \Big(i e_{22}^{l+1,i}(t) - i e_{22}^{l,i}(t)\Big) = 0,$$

and, using (3.9),

$$\begin{aligned}
&\sum_{l,i} i \Big(\widehat{\theta}_{l,i+1}\, e_{22}^{l,i+1}(t) - \widehat{\theta}_{l,i}\, e_{22}^{l,i}(t)\Big) \\
&\qquad = \frac{\theta_r(\sigma + d_{22})}{m_2} \sum_{l,i} \Big(i\, e_{22}^{l,i+1}(t) - i\, e_{22}^{l,i}(t)\Big) = \\
&\qquad = \frac{\theta_r(\sigma + d_{22})}{m_2} \Big(\sum_{l,j} (j-1)\, e_{22}^{l,j}(t) - \sum_{l,i} i\, e_{22}^{l,i}(t)\Big) \\
&\qquad = -\frac{\theta_r(\sigma + d_{22})}{m_2} \sum_{l,j} e_{22}^{l,j}(t) = -\theta_r(\sigma + d_{22}) \frac{e_{22}(t)}{m_2}\,.
\end{aligned}$$

Combining the above identities with (3.10) and (3.12) we conclude

$$\begin{aligned}\partial_t T(t) &= \partial_t\Big(\sum_{l,i} i N_{l,i}(t)\Big)\\ &= \frac{\alpha}{m_1}\left(\frac{\varrho(t)}{m_c} - T(t)\right)e_1(t) - \theta_r(\sigma+d_{22})\frac{e_{22}(t)}{m_2} - (\gamma_r+\gamma_\varrho)\,T(t)\,.\end{aligned} \tag{3.16}$$

Next, referring to (3.4), subtracting $\partial_t e_{22}/m_2$ from (3.16) and using (3.14), we obtain

$$\begin{aligned}\partial_t S(t) = \frac{\alpha}{m_1}\left(\frac{\varrho(t)}{m_c} - S(t) - \frac{e_{22}(t)}{m_2}\right)e_1(t) - \beta S(t)\,\frac{e_{21}(t)}{m_2}\\ + \Big((1-\theta_r)(\sigma+d_{22}) - \gamma_\varrho\Big)\frac{e_{22}(t)}{m_2} - (\gamma_r+\gamma_\varrho)\,S(t)\,.\end{aligned} \tag{3.17}$$

We now multiply each term on the right-hand side of (3.10) by l and sum to get an equation for $\varrho(t)$. First, using (3.6) and (3.7), we get

$$\begin{aligned}&\sum_{l,i} l\Big(\widehat{\alpha}_{l,i-1}N_{l,i-1}(t) - \widehat{\alpha}_{l,i}N_{l,i}(t)\Big)e_1(t)\\ &\qquad = \frac{\alpha}{m_1}\sum_l l\Big(\sum_i (l-(i-1))N_{l,i-1}(t) - \sum_i (l-i)N_{l,i}(t)\Big) = 0\,,\\ &\sum_{l,i} l\Big(\widehat{\gamma}_{l,i+1}N_{l,i+1}(t) - \widehat{\gamma}_{l,i}N_{l,i}(t)\Big)\\ &\qquad = \gamma_r\sum_l l\Big(\sum_i (i+1)N_{l,i+1}(t) - \sum_i iN_{l,i}(t)\Big) = 0\,.\end{aligned}$$

Similarly, using (3.8), we compute

$$\begin{aligned}\sum_{l,i} l\Big(\widehat{q}_{l+1,i}\,e_{22}^{l+1,i}(t) - \widehat{q}_{l,i}\,e_{22}^{l,i}(t)\Big) &= \frac{q}{m_2}\sum_{l,i}\Big[(l+1)e_{22}^{l+1,i}(t) - e_{22}^{l+1,i}(t) - le_{22}^{l,i}(t)\Big]\\ &= -\frac{q}{m_2}\sum_{l,i} e_{22}^{l+1,i}(t) = -q\,\frac{e_{22}(t)}{m_2},\end{aligned}$$

and, using (3.9),

$$\sum_{l,i} l\Big(\widehat{\theta}_{l,i+1}\,e_{22}^{l,i+1}(t) - \widehat{\theta}_{l,i}\,e_{22}^{l,i}(t)\Big) = \frac{\theta_r(\sigma+d_{22})}{m_2}\sum_l l\Big[\sum_i e_{22}^{l,i+1}(t) - \sum_i e_{22}^{l,i}(t)\Big] = 0.$$

Combining the above expressions and using (3.12),(3.13) and (3.15), we obtain

$$\partial_t\varrho(t) = m_c\partial_t\Big(\sum_{l,i} lN_{l,i}(t)\Big) = r - m_c q\frac{e_{22}(t)}{m_2} - \gamma_\varrho\,\varrho(t)\,. \tag{3.18}$$

Finally, by (3.8), (3.12) and (3.13), equations (3.11) become

$$\begin{aligned}\partial_t p(t) &= \theta_p\,m_c\,q\,\frac{e_{22}(t)}{m_2} - \gamma\,n(t)\,p(t) - \gamma_p\,p(t)\\ \partial_t n(t) &= \frac{\mu n(t)}{\bar{n}+n(t)}\Big(\gamma\,p(t) + (1-\theta_p)\,m_c\,q\,\frac{e_{22}(t)}{m_2}\Big) - \gamma_n\,n(t).\end{aligned} \tag{3.19}$$

S-system. Combining the above equations we obtain the S-system,

$$\begin{cases} \partial_t e_1(t) = b_1\, n(t) - d_1 e_1(t) \\ \partial_t e_{21}(t) = b_2\, n(t) - \beta S(t)\, e_{21}(t) + \sigma\, e_{22}(t) - d_{21}\, e_{21}(t) \\ \partial_t e_{22}(t) = \beta S(t)\, e_{21}(t) - \big(\sigma + d_{22} + \gamma_r\big) e_{22}(t) \\ \partial_t S(t) = \alpha \Big(\dfrac{\varrho(t)}{m_c} - S(t) - \dfrac{e_{22}(t)}{m_2} \Big) \dfrac{e_1(t)}{m_1} - \beta S(t) \dfrac{e_{21}(t)}{m_2} \\ \qquad\qquad + \Big((1-\theta_r)(\sigma + d_{22}) - \gamma_\varrho \Big) \dfrac{e_{22}(t)}{m_2} - (\gamma_r + \gamma_\varrho)\, S(t) \\ \partial_t \varrho(t) = r - m_c q \dfrac{e_{22}(t)}{m_2} - \gamma_\varrho\, \varrho(t) \\ \partial_t p(t) = \theta_p\, m_c q \dfrac{e_{22}(t)}{m_2} - \gamma n(t) p(t) - \gamma_p p(t) \\ \partial_t n(t) = \dfrac{\mu n(t)}{\bar{n} + n(t)} \Big(\gamma p(t) + (1-\theta_p)\, m_c q \dfrac{e_{22}(t)}{m_2} \Big) - \gamma_n n(t). \end{cases} \tag{3.20}$$

3.3 Cleaving Mechanism 2: T-model

We now modify the S-system derived for cleaving Mechanism 1 to model cleaving Mechanism 2. Here we work directly from the already reduced S-system (3.20), by making reasonable assumptions. We note that it is possible to derive this model from a more fundamental model in which we directly model the mechanism on chains of length l, similar to our derivation of the $\{N\text{-}S\}$ model above.

In Mechanism 2, we do not distinguish between attached and detached enzymes e_2. In addition, we do not distinguish occupied and unoccupied sites, preferring to count available reducing ends $T(t)$, which satisfies (2.1), namely

$$T(t) = S(t) + \frac{e_{22}(t)}{m_2}\,.$$

Our goal is to rewrite the S-system (3.20) in terms of $T(t)$ rather than $S(t)$, and to replace $e_{21}(t)$ and $e_{22}(t)$ by $e_2(t)$ in a systematic way.

First, we get an equation for $T(t)$ by adding $(3.20)_4 + (3.20)_3/m_2$. After simplifying, this gives

$$\partial_t T(t) = \alpha \Big(\frac{\varrho(t)}{m_c} - T(t) \Big) \frac{e_1(t)}{m_1} - \theta_r(\sigma + d_{22}) \frac{e_{22}(t)}{m_2} - (\gamma_r + \gamma_\varrho)\, T(t). \tag{3.21}$$

We consider the action of enzyme e_2 in Mechanism 2. In this model, there are essentially no e_{22} and the landing, cleaving off of a cellobiose unit, and detaching all occur at the same instant. Thus all of enzyme e_2 should be considered to be unattached, so should most closely resemble e_{21}. We thus take the decay rates to be $d_{22} = 0$ and $d_{21} = d_2$. Recalling that σ represents the probability of the enzyme e_{22} detaching, we set $\sigma = 1$ as the enzyme detaches immediately after the attack. To get an explicit substitution rule for e_{22}, consider $(3.20)_3$. Since decay of the cellulose won't affect enzyme e_2 as it is not attached, we drop the term $\gamma_r\, e_{22}(t)$. Since e_{21} dominates, we can also set $\partial_t e_{22}(t) = 0$. With these assumptions, $(3.20)_3$ becomes

$$0 = \beta S(t)\, e_{21}(t) - e_{22}(t) \quad \text{or} \quad e_{22}(t) = \beta\, S(t)\, e_{21}(t), \tag{3.22}$$

and since e_{22} is negligible, we can replace $S(t)$ by $T(t)$.

We now obtain a closed system by substituting

$$e_{21}(t) \to e_2(t) \quad \text{and} \quad e_{22}(t) \to \beta\, T(t)\, e_2(t),$$

and $d_{21} \to d_2$, $d_{22} = 0$ in to the remaining equations in (3.20). Doing so, we get the *T-system*:

$$\begin{cases} \partial_t e_1(t) = b_1\, n(t) - d_1 e_1(t) \\ \partial_t e_2(t) = b_2\, n(t) - d_2 e_2(t) \\ \partial_t T(t) = \alpha \left(\dfrac{\varrho(t)}{m_c} - T(t) \right) \dfrac{e_1(t)}{m_1} - \theta_r\, \beta\, T(t)\, \dfrac{e_2(t)}{m_2} - (\gamma_r + \gamma_\varrho)\, T(t) \\ \partial_t \varrho(t) = r - \dfrac{m_c\, q\, \beta}{m_2} T(t)\, e_2(t) - \gamma_\varrho\, \varrho(t) \\ \partial_t p(t) = \theta_p\, \dfrac{m_c\, q\, \beta}{m_2} T(t)\, e_2(t) - \gamma n(t) p(t) - \gamma_p p(t) \\ \partial_t n(t) = \dfrac{\mu n(t)}{\bar{n} + n(t)} \Big(\gamma p(t) + (1 - \theta_p)\, \dfrac{m_c\, q\, \beta}{m_2} T(t)\, e_2(t) \Big) - \gamma_n n(t). \end{cases} \tag{3.23}$$

Comparing this system to (3.20) modeling Mechanism 1, we make the following observations: first, the dynamics of e_2 are simpler, because we do not have to account for the different processes for e_{21} and e_{22}, which introduce an extra equation and extra nonlinearities. The cleaving rate changes as

$$m_c q\, \frac{e_{22}(t)}{m_2} \to \frac{m_c\, q\, \beta}{m_2} T(t)\, e_2(t),$$

so the (linear) term in the S-system, which represents the mass of cellobiose that is cleaved off by the attached e_{22}, is replaced by a product which represents the (unattached) e_2 finding and attacking a reducing end.

3.4 Multiple trait T-model

We now extend the T-model to a model that allows for several species of microorganisms feeding on the same cellulose. Specifically, we introduce populations n^i, with $i \in \{1, ...M\}$, equipped with different traits x^i; throughout this section, we use superscripts to distinguish traits. We assume that Mechanism 2 is used by each population to cleave off cellobiose, while the different populations have different masses and rates for the various actions.

As in the T-model, we assume that microorganism n_i produces exoglucanases enzymes e_1^i that make landing sites, and endoglucanases enzymes e_2^i that cleave off cellobiose from the cellulose chains. In analogy with $(3.23)_{1,2}$, we suppose that the enzymes e_1^i, e_2^i are produced by the microorganism n_i and degrade with fixed rates. This gives the equations

$$\begin{aligned} \partial_t e_1^i(t) &= b_1^i\, n^i(t) - d_1^i\, e_1^i(t) \\ \partial_t e_2^i(t) &= b_2^i\, n^i(t) - d_2^i\, e_2^i(t) \end{aligned} \tag{3.24}$$

where b_1^i, b_2^i and d_1^i, d_2^i are, respectively, the enzyme generation and death rates, $i \in \{1, ...M\}$.

Next, for simplicity we will not differentiate between landing sites created by the enzymes of different species. In other words, the landing sites made by e_1^i are allowed to be used by any

enzyme e_2^j for all j. Then, following Mechanism 2, and neglecting saturation effects, we assume that enzymes e_1^i make landing sites on the cellulose ϱ with the rate

$$\alpha^i \left(\frac{\varrho(t)}{m_c} - T(t) \right) \frac{e_1^i(t)}{m_1^i},$$

where α^i is the probability of an individual enzyme e_1^i finding a spot among the $\frac{\varrho(t)}{m_c} - T$ available cellobiose units (reflecting the requirement that only one landing site per cellobiose unit is allowed), and making a landing site. Next, we suppose that the landing sites T are attacked by enzymes e_2^i with the rate

$$\beta^i \, T(t) \, \frac{e_2^i(t)}{m_2^i}$$

where β^i is the probability of an individual e_2^i finding and attaching to a landing spot. Finally, as above, we let $\gamma_r > 0$ be the decay rate of an individual reducing end and suppose that the portion $\theta_r^i \in [0,1]$ of those ends is not usable after an attack by e_2^i. Then, analogous to $(3.23)_3$, we obtain the equation for T for multiple trait populations:

$$\partial_t T(t) = \sum_j \alpha^j \left(\frac{\varrho(t)}{m_c} - T(t) \right) \frac{e_1^j(t)}{m_1^j} - \sum_j \theta_r^j \, \beta^j \, T(t) \, \frac{e_2^j(t)}{m_2^j} - (\gamma_r + \gamma_\varrho) \, T(t), \tag{3.25}$$

where γ_ϱ is the degradation rate of ϱ.

Next, we let q^i be the number of cellobiose units cleaved off by e_2^i during an attack. In analogy with $(3.23)_4$, the dynamics of cellulose ϱ is then given by

$$\partial_t \varrho(t) = r - \sum_j \frac{m_c \, q^j \, \beta^j}{m_2^j} \, T(t) \, e_2^j(t) - \gamma_\varrho \, \varrho(t) \tag{3.26}$$

where as before m_c denotes the mass of a cellobiose unit.

We next let $\theta_p^i \in [0,1]$ denote the proportion of produced cellobiose produced by e_2^i that is made available to everyone. Then, similar to $(3.23)_5$, the equations for the total mass $p(t)$ of cellobiose available to everyone are

$$\partial_t p(t) = m_c \sum_j \theta_p^j \, \frac{q^j \, \beta^j}{m_2^j} \, e_2^j(t) \, T(t) - \sum_j \gamma^j n^j(t) \, p(t) - \gamma_p \, p(t) \, . \tag{3.27}$$

where γ^j is the predation rate of p by n^j, and γ_p is the decay rate of p.

Finally, we consider the dynamics of the population n^i. First, recall that cellobiose $p(t)$ is available to all species n^j, $j = 1, \ldots, M$. Since every species n^j hunts with the predation rate γ^j on the cellobiose p, the growth rate of n^i may be expressed via the logistic term

$$\mu^i \, n^i(t) \frac{\gamma^i \, p(t)}{\bar{n}^i + \frac{1}{\gamma^i} \sum_j \gamma^j \, n^j} \tag{3.28}$$

where μ^i is the conversion efficiency.

Next, comparing to (3.27), the production rate of cellobiose which is produced by e_2^j and consumed directly on the spot is given by

$$(1 - \theta_p^j) \frac{m_c \, q^j \, \beta^j}{m_2^j} \, e_2^j(t) \, T(t).$$

We assume that in view of the homogeneity and close proximity of species, the cellobiose produced by e_2^j, $j = 1, \dots, M$, can be consumed by the n^i; this manifests the cross species interaction. We express this as

$$\mu^i(1-\theta_p^j)\frac{\nu^{ij}\, n^i}{\nu^{ij}\,\bar{n}^i + \sum_s \nu^{sj} n^s}\,\frac{m_c q^j \beta^j}{m_2^j}\, e_2^j(t) T(t), \quad \text{with} \quad \sum_s \nu^{sj} = 1,$$

representing the contribution of the energy obtained from the direct consumption of cellobiose cleaved off by e_2^j to the growth rate of n^i. Combining these leads to the equation for the dynamics of the population n^i,

$$\partial_t n^i(t) = \mu^i n^i(t) \left(\frac{\gamma^i p(t)}{\bar{n}^i + \frac{1}{\gamma^i}\sum_j \gamma^j\, n^j} + \sum_j \frac{(1-\theta_p^j)\nu^{ij}}{\nu^{ij}\bar{n}_i + \sum_s \nu^{sj} n^s}\,\frac{m_c q^j \beta^j}{m_2^j}\, e_2^j(t)\, T(t) \right) - \gamma_n^i\, n^i(t) \tag{3.29}$$

where γ_n^i is the death rate of the population n^i.

To simplify notation, we relabel the constants as

$$\widehat{\alpha}^j = \frac{\alpha^j}{m_1^j}, \quad \widehat{\beta}^j = \frac{\beta^j}{m_2^j}, \quad \widehat{q}^j = m_c \frac{q^j \beta^j}{m_2^j}, \quad \widehat{\gamma}_r = \gamma_r + \gamma_\varrho\,, \tag{3.30}$$

and we collect the above equations to obtain the *multiple trait T-system*,

$$\begin{cases} \partial_t e_1^i(t) = b_1^i n^i(t) - d_1^i e_1^i(t) \\ \partial_t e_2^i(t) = b_2^i n^i(t) - d_2^i e_2^i(t) \\ \partial_t T(t) = \Big(\dfrac{\varrho(t)}{m_c} - T(t)\Big) \displaystyle\sum_j \widehat{\alpha}^j\, e_1^j(t) - \sum_j \theta_r^j \widehat{\beta}^j\, e_2^j(t)\, T(t) - \widehat{\gamma}_r T(t) \\ \partial_t \varrho(t) = r - \displaystyle\sum_j \widehat{q}^j\, e_2^j(t)\, T(t) - \gamma_\varrho\, \varrho(t) \\ \partial_t p(t) = \displaystyle\sum_j \theta_p^j \widehat{q}^j e_2^j(t)\, T(t) - \sum_j \gamma^j n^j(t)\, p(t) - \gamma_p p(t) \\ \partial_t n^i(t) = \mu^i n^i(t) \dfrac{\gamma^i p(t)}{\bar{n}^i + \frac{1}{\gamma^i}\sum_j \gamma^j n^j} \\ \qquad\qquad + \mu^i n^i(t) \displaystyle\sum_j (1-\theta_p^j)\, \frac{\nu^{ij}}{\nu^{ij}\bar{n}^i + \sum_s \nu^{sj} n^s} \widehat{q}^j\, e_2^j(t) T(t) - \gamma_n^i n^i(t) \end{cases} \tag{3.31}$$

where $i = 1, \dots, M$.

3.4.1 Compatibility with the single trait model

We now show that the multiple trait T-model directly generalizes the single trait T-model by considering two special cases of the multiple trait model, and confirming that these reduce to the single trait model.

Our first test is to assume that all but one species (say the i-th) are absent. That is, we begin with data $n^j(0) = 0$, and similarly $e_1^j(0) = e_2^j(0) = 0$, for $j \neq i$. Then (3.31) implies that for

all $t > 0$, $j \neq i$, we have $n^j(t) = 0$. It is then evident that equations $(3.31)_{1,2,3,4,5}$ reduce to $(3.23)_{1,2,3,4,5}$ (for $n = n^i$, etc), and $(3.31)_6$ becomes

$$\partial_t n^i(t) = \mu^i\, n^i\, \frac{\gamma^i\, p}{\bar{n}^i + n^i} + \mu^i n^i\, (1 - \theta_p^i)\, \frac{\widehat{q}^i\, e_2^i\, T}{\bar{n}^i + n^i} - \gamma_n^i\, n^i,$$

which is exactly $(3.23)_6$.

Our second test is to assume that even though there are M different traits, the coefficients are independent of i, j, so there is no way to distinguish different populations in the model. In this case, we check the dynamics for the total population $n(t) = \sum_i n^i(t)$, and similarly $e_1 = \sum_i e_1^i$ and $e_2 = \sum_i e_2^i$. It is then clear that $(3.31)_{3,4,5}$ become $(3.23)_{3,4,5}$, and adding $(3.31)_{1,2}$ over i gives $(3.23)_{1,2}$. Finally, adding $(3.31)_6$ over i yields

$$\partial_t(\textstyle\sum_i n^i) = \mu \sum_i n^i\, \dfrac{\gamma\, p}{\bar{n} + \sum_j n^j} + \mu \sum_i n^i\, \dfrac{1 - \theta_p}{\bar{n} + \sum_s n^s}\, \widehat{q} \sum_j e_2^j\, T - \gamma_n \sum_i n^i,$$

which is again exactly $(3.23)_6$.

4 Cooperation

4.1 Cooperation in the T-model

In this section we consider the system (3.23) on different time scales. We assume that production of enzymes, consumption and creation of landing sites occurs at a much faster rate than changes in the population of the microorganism. In this case, over time scales on which the population changes, we can assume that equations $(3.23)_{1,2,3,4,5}$ are at equilibrium, and the dynamics is driven by the population change $(3.23)_6$. This gives the system

$$\begin{cases} 0 = b_1\, n(t) - d_1 e_1(t) \\ 0 = b_2\, n(t) - d_2 e_2(t) \\ 0 = \alpha\Big(\dfrac{\varrho(t)}{m_c} - T(t)\Big)\dfrac{e_1(t)}{m_1} - \theta_r\, \beta\, T(t)\, \dfrac{e_2(t)}{m_2} - (\gamma_r + \gamma_\varrho) T(t) \\ 0 = r - \widehat{q} T(t)\, e_2(t) - \gamma_\varrho\, \varrho(t) \\ 0 = \theta_p\, \widehat{q} T(t)\, e_2(t) - \gamma n(t) p(t) - \gamma_p p(t) \\ \partial_t n(t) = \dfrac{\mu n(t)}{\bar{n} + n(t)} \Big(\gamma p(t) + (1 - \theta_p)\, \widehat{q} T(t)\, e_2(t)\Big) - \gamma_n n(t), \end{cases} \tag{4.1}$$

where we have set $\widehat{q} = m_c\, q\, \beta / m_2$.

We use (4.1) to eliminate all the fast variables, to obtain a single equation for the population n, so that the population growth rate can be understood. The first two equations give

$$e_i = k_i n, \quad \text{with} \quad k_i := \frac{b_i}{d_i}, \quad i = 1,\ 2\,, \tag{4.2}$$

and from $(4.1)_4$, we have

$$\varrho = \frac{r}{\gamma_\varrho} - \frac{\widehat{q}}{\gamma_\varrho}\, T\, e_2 = \frac{r}{\gamma_\varrho} - \frac{\widehat{q} k_2}{\gamma_\varrho}\, T\, n.$$

Plugging these into $(4.1)_3$, we get

$$0 = \frac{\alpha\, r\, k_1}{m_c \gamma_\varrho m_1}\, n - T\,\Big(\frac{\alpha\, \widehat{q}\, k_2\, k_1}{m_c \gamma_\varrho m_1}\, n^2 + \frac{\alpha\, k_1}{m_1}\, n + \theta_r \frac{\beta\, k_2}{m_2}\, n + \gamma_r + \gamma_\varrho\Big),$$

so that

$$T = \frac{\alpha\, r\, k_1}{m_c \gamma_\varrho m_1}\, \frac{n}{P_2(n)}, \tag{4.3}$$

where $P_2(n)$ is the quadratic polynomial

$$\begin{aligned} P_2(n) &= c_2\, n^2 + c_1\, n + c_0, \\ c_2 = \frac{\alpha\, \widehat{q}\, k_2\, k_1}{m_c \gamma_\varrho m_1}, &\quad c_1 = \frac{\alpha\, k_1}{m_1} + \frac{\theta_r\, \beta\, k_2}{m_2}, \quad c_0 = \gamma_r + \gamma_\varrho. \end{aligned} \tag{4.4}$$

Next, using these in $(3.23)_5$, it follows that

$$p = \theta_p\, \widehat{q}\, k_2\, \frac{T\, n}{\gamma\, n + \gamma_p} = \theta_p\, \widehat{q}\, k_2\, \frac{\alpha\, r\, k_1}{m_c \gamma_\varrho m_1}\, \frac{n^2}{(\gamma\, n + \gamma_p)\, P_2(n)}. \tag{4.5}$$

Finally, we use (4.3), (4.5) in $(4.1)_6$ to get the scalar population equation

$$\partial_t n(t) = n(t)\Big[B(n) - \gamma_n\Big], \tag{4.6}$$

where

$$\begin{aligned} B(n) &= \frac{\mu}{\bar{n} + n}\Big(\gamma\, p + (1 - \theta_p)\, \widehat{q}\, k_2\, T\, n\Big) \\ &= \mu\, \widehat{q}\, k_2\, \frac{T\, n}{\bar{n} + n}\left(\frac{\gamma\, \theta_p}{\gamma\, n + \gamma_p} + (1 - \theta_p)\right) \\ &= K\, n^2\, \Phi(n), \end{aligned} \tag{4.7}$$

where the function $\Phi(n)$ and constant K are given by

$$\begin{aligned} \Phi(n) &= \left(\frac{\theta_p}{n + \gamma_p/\gamma} + 1 - \theta_p\right) \frac{1}{(n + \bar{n})\, P_2(n)}\,, \\ K &= \mu\, \widehat{q}\, k_2\, \frac{\alpha\, r\, k_1}{m_c \gamma_\varrho m_1} = \frac{\mu\, q\, \beta\, \alpha\, r\, b_1\, b_2}{m_1\, m_2\, \gamma_\varrho\, d_1\, d_2}\,. \end{aligned} \tag{4.8}$$

4.2 Asymptotics of $B(n)$

We are interested in the structure of $B(n)$ for small populations, $n \ll \bar{n}$. First, we note that the birth rate $B(n)$ is positive and satisfies

$$B(0) = 0 \quad \text{and} \quad \lim_{n \to \infty} B(n) = 0,$$

so that B is globally bounded.

For n small, using (4.7), (4.8) and (4.4), we have

$$\frac{B(n)}{n^2} = K\, \Phi(n) \approx K\, \Phi(0) = \frac{K}{\bar{n}\, (\gamma_\varrho + \gamma_r)}\, \Big(\theta_p \frac{\gamma}{\gamma_p} + 1 - \theta_p\Big), \tag{4.9}$$

so that $B(n) \sim n^2$ for $n \ll \bar{n}$. Thus for small populations, $B(n)$ is convex, and so superlinear. This superlinear birth rate is indicative of cooperative behavior.

More generally, $B(n)/n$ is increasing as long as $n\,\Phi(n)$ is, since

$$\frac{\partial}{\partial n}\Big(\frac{B(n)}{n}\Big) = \frac{\partial}{\partial n}\Big(K\,n\,\Phi(n)\Big) = K\,n\,\Phi(n)\,\Big(\frac{1}{n} + \frac{\partial_n \Phi}{\Phi}\Big) = K\,n\,\Phi(n)\,\Big(\frac{\partial}{\partial n}\log(n\,\Phi)\Big),$$

so the system exhibits cooperative behavior as long as

$$\frac{\partial}{\partial n}\log(n\,\Phi) = \frac{1}{n} - \frac{\theta_p}{(n+\gamma_p/\gamma)^2}\,\Big(\theta_p\,\frac{1}{n+\gamma_p/\gamma} + 1 - \theta_p\Big)^{-1} - \frac{1}{n+\bar{n}} - \frac{2c_2 n + c_1}{P_2(n)} > 0\,.$$

This condition is at least true for $n \in (0, n_*)$, where n_* is the smallest positive root of this expression; combining the fractions, it is evident that n_* is the smallest positive root of a fifth-order polynomial.

Moreover, referring to (4.9), we see that

$$\frac{\partial}{\partial \theta_p} K\,\Phi(0) = \frac{K}{\bar{n}\,(\gamma_\varrho + \gamma_r)}\,\Big(\frac{\gamma}{\gamma_p} - 1\Big),$$

which is positive if and only if $\gamma > \gamma_p$. For small population n, we expect this to persist: that is,

$$\frac{\partial}{\partial \theta_p}\Big(\frac{B(n)}{n}\Big) = \frac{\partial}{\partial \theta_p} K\,\Phi(n) > 0 \quad \text{if and only if} \quad \gamma > \gamma_p.$$

Since $\theta_p \in [0,1]$ is the proportion of produced cellulose which is shared, this last inequality suggests that for small populations *sharing food is beneficial* in terms of growth as long as the consumption rate γ is greater than the decay rate γ_p of the cleaved off cellobiose.

4.3 Cooperation in multiple-trait T-model

As in Section 4.1, we consider the system (3.31) on a generational time scale. We again assume that production of enzymes, consumption and creation of landing sites happens at a much faster rate then change in the populations n^i. In other words, we assume that the equations $(3.23)_{1,2,3,4,5}$ are at equilibrium, and the dynamics of the system is driven by the population equations $(3.31)_6$. This results in the system

$$\begin{cases} 0 = b_1^i n^i(t) - d_1^i e_1^i(t), \\ 0 = b_2^i n^i(t) - d_2^i e_2^i(t), \\ 0 = \Big(\dfrac{\varrho(t)}{m_c} - T(t)\Big)\,\displaystyle\sum_j \widehat{\alpha}^j\, e_1^j(t) - \sum_j \theta_r^j \widehat{\beta}^j\, e_2^j(t)\,T(t) - \widehat{\gamma}_r T(t), \\ 0 = r - \displaystyle\sum_j \widehat{q}^j\, e_2^j(t)\,T(t) - \gamma_\varrho\,\varrho(t), \\ 0 = \displaystyle\sum_j \theta_p^j \widehat{q}^j e_2^j(t)\,T(t) - \sum_j \gamma^j n^j(t)\,p(t) - \gamma_p p(t), \\ \partial_t n^i(t) = \mu^i n^i(t) \dfrac{\gamma^i p(t)}{\bar{n}^i + \frac{1}{\gamma^i}\sum_j \gamma^j n^j}, \\ \qquad\qquad + \mu^i n^i(t)\,\displaystyle\sum_j (1-\theta_p^j)\,\frac{\nu^{ij}}{\nu^{ij}\bar{n}^i + \sum_s \nu^{sj} n^s}\widehat{q}^j\, e_2^j(t) T(t) - \gamma_n^i n^i(t). \end{cases} \tag{4.10}$$

We wish to understand the growth rate of n^i as a function of $n = (n_1, \dots, n_M) \in \mathbb{R}^M$. The first two equations of (4.10) give

$$e_1^i(t) = k_1^i n^i(t), \quad e_2^i = k_2^i n^i, \quad \text{with} \quad k^i := \frac{b^i}{d^i}, \quad i = 1, \dots, M\,. \tag{4.11}$$

We next and write n as a vector and introduce the coefficient vectors

$$\begin{aligned} A &= \Big(\widehat{\alpha}^j\, k_1^j\Big), \quad B = \Big(\theta_r^j\, \widehat{\beta}^j\, k_2^j\Big), \quad Q = \Big(\widehat{q}^j\, k_2^j\Big), \\ \Theta &= \Big(\theta_p^j\, \widehat{q}^j\, k_2^j\Big), \quad \Gamma = \Big(\gamma^j\Big), \quad N^k = \Big(\nu^{jk}\Big), \end{aligned} \tag{4.12}$$

and denote the scalar product by $\langle \cdot, \cdot \rangle$. We can then rewrite $(4.10)_{3,4,5}$ as

$$\begin{aligned} 0 &= \Big(\frac{\varrho(t)}{m_c} - T(t)\Big)\langle A, n\rangle - \langle B, n\rangle\, T(t) - \widehat{\gamma}_r T(t), \\ 0 &= r - \langle Q, n\rangle\, T(t) - \gamma_\varrho\, \varrho(t), \\ 0 &= \langle \Theta, n\rangle\, T(t) - \langle \Gamma, n\rangle\, p(t) - \gamma_p p(t). \end{aligned}$$

These immediately yield

$$\varrho(t) = \frac{1}{\gamma_\varrho}\left(r - T(t)\langle Q, n\rangle\right), \quad \text{and} \quad p(t) = \frac{\langle \Theta, n\rangle}{\langle \Gamma, n\rangle + \gamma_p}\, T(t), \tag{4.13}$$

and, plugging in, we get

$$0 = \frac{r}{\gamma_\varrho\, m_c}\, \langle A, n\rangle - \tau(n)\, T(t), \quad \text{so that} \quad T(t) = \frac{r}{\gamma_\varrho\, m_c}\, \frac{\langle A, n\rangle}{\tau(n)}, \tag{4.14}$$

where we have set

$$\tau(n) = \frac{1}{\gamma_\varrho\, m_c}\, \langle A, n\rangle\, \langle Q, n\rangle + \langle A, n\rangle + \langle B, n\rangle + \widehat{\gamma}_r\,. \tag{4.15}$$

Finally, using (4.13) and (4.14) in $(4.10)_6$, we can write our population system as

$$\partial_t n^i = n^i\left(B^i(n) - \gamma_n^i\right), \tag{4.16}$$

where the i-th population's birth rate is

$$\begin{aligned} B^i(n) &= \frac{\mu^i\, \gamma^i\, p(t)}{\bar{n}^i + \frac{1}{\gamma^i}\, \langle \Gamma, n\rangle} + \mu^i \sum_j \frac{(1 - \theta_p^j)\, \nu^{ij}\, \widehat{q}^j\, k_2^j\, n^j}{\nu^{ij}\, \bar{n}^i + \langle N^j, n\rangle}\, T(t) \\ &= \mu^i\, T(t)\left(\frac{\gamma^i\, \langle \Theta, n\rangle}{(\bar{n}^i + \frac{1}{\gamma^i}\, \langle \Gamma, n\rangle)\, (\langle \Gamma, n\rangle + \gamma_p)} + \sum_j \frac{(1 - \theta_p^j)\, \nu^{ij}\, \widehat{q}^j\, k_2^j\, n^j}{\nu^{ij}\, \bar{n}^i + \langle N^j, n\rangle}\right) \\ &= \frac{\mu^i\, r}{\gamma_\varrho\, m_c}\, \frac{\langle A, n\rangle}{\tau(n)}\left(\frac{\gamma^i\, \langle \Theta, n\rangle}{(\bar{n}^i + \frac{1}{\gamma^i}\, \langle \Gamma, n\rangle)\, (\langle \Gamma, n\rangle + \gamma_p)} + \sum_j \frac{(1 - \theta_p^j)\, \nu^{ij}\, \widehat{q}^j\, k_2^j\, n^j}{\nu^{ij}\, \bar{n}^i + \langle N^j, n\rangle}\right). \end{aligned} \tag{4.17}$$

Here the two terms in the growth rate represent intentionally shared food ($p(t)$), and food consumed as it's produced, respectively.

Asymptotic behavior of $B^i(n)$. Assuming coefficients are positive, we make the following observations about the birth rate $B^i(n)$. According to (4.15) $\tau(n)$ is quadratic in n, while all other functions in (4.16) are linear. It follows immediately that $B^i(n) \to 0$, and in fact $B^i(n) = O(\frac{1}{n})$ as $n \to \infty$.

We are more interested in the behavior for small populations, $n \sim 0$. Since $\tau(0) = \widehat{\gamma}_r$, no denominators vanish, and (4.17) yields

$$B^i(n) = O\big((\textstyle\sum n)^2\big) \quad \text{for} \quad n \sim 0.$$

More precisely, recalling that

$$\nabla_n \langle V, n\rangle = V \quad \text{and} \quad D_n^2\big(\langle V, n\rangle \langle W, n\rangle\big) = V\, W^T + W\, V^T,$$

we see that at $n = 0$, the gradient of B^i vanishes, $\nabla_n B^i(0) = 0$, and the Hessian of B^i is the symmetric matrix

$$D_n^2 B^i(0) = \frac{\mu^i\, r}{\gamma_\varrho\, m_c\, \widehat{\gamma}_r\, \bar{n}^i} \left(\frac{\gamma^i}{\gamma_p}(A\Theta^T + \Theta A^T) + A(Q-\Theta)^T + (Q-\Theta)A^T \right).$$

We cannot conclude that B^i is convex as the matrix $D_n^2 B^i(0)$ is not positive definite, but because all the entries are positive, we can conclude that the directional derivative is increasing in any direction in the positive orthant $\{n^k \geq 0\}$, which indicates cooperative behavior.

Special Case. Now, we consider the special case when $\nu^{ij} = 0$ for $i \neq j$; in this case, there is no competition for cellobiose that is not intentionally shared. In this special case, (4.17) becomes

$$\begin{aligned} B^i(n) &= \frac{\mu^i\, r}{\gamma_\varrho\, m_c} \frac{\langle A, n\rangle}{\tau(n)} \left(\frac{\gamma^i \langle \Theta, n\rangle}{(\bar{n}^i + \frac{1}{\gamma^i}\langle \Gamma, n\rangle)(\langle \Gamma, n\rangle + \gamma_p)} + \frac{(1-\theta_p^i)\, \widehat{q}^i\, k_2^i\, n^i}{\bar{n}^i + n^i} \right) \\ &=: B_1^i(n) + B_2^i(n). \end{aligned}$$

As in the single-trait case, we again see an indication that for small populations, more sharing (represented by the coefficient vector Θ) would be beneficial for the i-th population provided $\gamma^i > \gamma_p$, because it increases the derivative $\nabla_n B^i(n)$: this can be seen by differentiating with respect to the vector parameter Θ. Recall that $\gamma^i > \gamma_p$ means that cellobiose is consumed (by n^i) faster than it decays.

Lemma 4.1. *Suppose that $\nu^{ij} = 0$ for $i \neq j$. Let $i \in \{1, \dots, M\}$ be fixed and let*

$$n_0 = (n_0^1, n_0^2, \dots, n_0^{i-1}, 0, n_0^{i+1}, \dots, n_0^M) \in \mathbb{R}^M \quad \textit{with} \quad n_0^j \geq 0.$$

Then

$$\frac{\partial B_2^i}{\partial n^i}(n_0) = \frac{\mu^i\, r}{\gamma_\varrho\, m_c} \frac{\langle A, n_0\rangle}{\tau(n_0)} \frac{(1-\theta_p^i)\, \widehat{q}^i\, k_2^i}{\bar{n}^i} > 0. \tag{4.18}$$

Furthermore, suppose $\min_j \bar{\alpha}^j > 0$ and $\min_j \gamma^j > 0$. Then there exists $\varepsilon > 0$ such that for all $\max_j \theta_p^j < \varepsilon$, there holds

$$\frac{\partial B^i}{\partial n^i}(n_0) > 0 \quad \textit{for all } n_0 \neq 0\,.$$

Idea of proof. Equation (4.18) follows immediately by differentiation. When we differentiate B_1^i, we introduce negative terms each time the derivative falls on a denominator. However, each such term introduces a higher power in the denominator, so each of those terms can be represented as a product of $\langle A, n_0\rangle/\tau(n_0)$ with terms uniformly bounded in n_0. Comparing these to (4.18), it follows that by choosing $\max_j \theta_p^j < \varepsilon$ with ε small enough, the sum will be positive. □

The key conclusion in Lemma 4.18 is that the birth rate $B^i(n)$ includes some form of *cooperation*. Compare it for instance with simple logistic terms like $r - n_0^i$ which decreases with n_0^i. In contrast $B^i(n)$ actually penalizes populations which are too small (and populations which are too large of course just like a logistic term).

4.4 Cooperative interactions in $\{N$-$S\}$-model

We now consider cooperation in the $\{N$-$S\}$-model as we did for the simpler models. We are interested in the situation that the production of enzymes, consumption and creation of landing sites occurs much faster than changes in the population of the microorganism. Thus we again assume that equations (3.3), (3.5), and $(3.11)_1$ are at equilibrium, and the dynamics is driven by the population change (3.10). We also assume that the length of the cellulose chains does not exceed a given number $L > 0$. Then we obtain the system

$$
\begin{cases}
0 = b_1\, n(t) - d_1 e_1(t) \\
0 = b_2\, n(t) - \displaystyle\sum_{l,i} \Big[\beta_{l,i}\Big(iN_{l,i}(t) - \frac{e_{22}^{l,i}(t)}{m_2}\Big)e_{21}(t) - \sigma_{l,i}\, e_{22}^{l,i}(t)\Big] - d_{21}\, e_{21}(t) \\
0 = \beta_{l,i}\Big(iN_{l,i}(t) - \dfrac{e_{22}^{l,i}(t)}{m_2}\Big)e_{21}(t) - \Big(\sigma_{l,i} + d_{22}^{l,i} + \gamma_{r,l,i}\Big)e_{22}^{l,i} \\
0 = r_{l,i} + \Big(\widehat{\alpha}_{l,i-1}N_{l,i-1}(t) - \widehat{\alpha}_{l,i}N_{l,i}(t)\Big)e_1(t) + \Big(\widehat{\gamma}_{l,i+1}N_{l,i+1}(t) - \widehat{\gamma}_{l,i}N_{l,i}(t)\Big) \\
\qquad + \Big(\widehat{q}_{l+1,i}\, e_{22}^{l+1,i}(t) - \widehat{q}_{l,i}\, e_{22}^{l,i}(t)\Big) + \Big(\widehat{\theta}_{l,i+1}\, e_{22}^{l,i+1}(t) - \widehat{\theta}_{l,i}\, e_{22}^{l,i}(t)\Big) - \gamma_{\varrho,l,i}N_{l,i}(t) \\
0 = \theta_p\, m_c \displaystyle\sum_{l,i} \widehat{q}_{l,i}\, e_{22}^{l,i}(t) - \gamma n(t)p(t) - \gamma_p p(t) \\
\partial_t n(t) = \dfrac{\mu n(t)}{\bar{n} + n(t)}\Big(\gamma + \dfrac{\theta_p - 1}{\theta_p}(\gamma n(t) + \gamma_p)\Big)p(t) - \gamma_n n(t)\,,
\end{cases}
\tag{4.19}
$$

for $(l,i) \in I_L$, where (as before) the rates $r_{l,i} = 0$ when $i \neq 0$ and we use the convention (3.2); here we have used $(4.19)_5$ to simplify $(4.19)_6$.

To describe the dynamics, it is sufficient to express p in terms of n, which will in turn provide a scalar autonomous differential equation for $n(t)$. For small populations it can be shown that the equations $(4.19)_{1-5}$ can be solved uniquely in terms of n, yielding the following theorem.

Theorem 4.1. *There are $m, \bar{m} > 0$ and C^∞ functions*

$$
\widehat{e}_1(n), \quad \widehat{e}_{21}(n), \quad \widehat{e}_{22}^{l,i}(n), \quad \widehat{N}_{l,i}(n), \quad \widehat{p}(n) : (-m, \bar{m}) \to \mathbb{R} \tag{4.20}
$$

such that:

(*i*) *For each* $n \in (-m, \bar{m})$ *the equations* $(4.19)_{1-5}$ *can be solved uniquely for* e_1, e_{21}, $e_{22}^{l,i}$, N, p *in terms of* n,

$$e_1 = \widehat{e}_1(n), \quad e_{21} = \widehat{e}_{21}(n), \quad e_{22}^{l,i} = \widehat{e}_{22}^{l,i}(n), \quad N_{l,i} = \widehat{N}_{l,i}(n), \quad p = \widehat{p}(n).$$

(*ii*) *The functions from* (4.20) *are given to leading order as*

$$\widehat{N}_{l,i}(n) = \nu_{l,i}\, n^i + O(n^{i+1})\,, \tag{4.21}$$

with

$$\nu_{l,0} = \frac{r_{l,0}}{\gamma_{\varrho,l,0}} \quad \textit{and} \quad \nu_{l,i} = \nu_{l,i-1}\, \frac{\alpha_{l,i-1}}{\widehat{\gamma}_{l,i} + \gamma_{\varrho,l,i}} \frac{b_1}{d_1}\,, \quad i \geq 1\,,$$

and with

$$\begin{aligned}
&\widehat{e}_1(n) = \frac{b_1}{d_1} n, \qquad \widehat{e}_{21}(n) = \frac{b_2}{d_{21}} n + O(n^2) \\
&\widehat{e}_{22}^{l,i}(n) = i\Big(\frac{b_2\, \beta_{l,i}\, \nu_{l,i}}{d_{21}(\sigma_{l,i} + d_{22}^{l,i} + \gamma_{r,l,i})} + O(n) \Big) n^{i+1} \\
&\frac{\gamma_p}{\theta_p} \widehat{p}(n) = \bar{p}(n)\, n^2, \quad \textit{where} \quad \bar{p}(n) = \frac{b_2}{d_{21}}\, m_c \sum_l \frac{\beta_{l,1}\, \nu_{l,1}}{(\sigma_{l,1} + d_{22}^{l,1} + \gamma_{r,l,1})} + O(n)\,.
\end{aligned} \tag{4.22}$$

Sketch of proof. The quantities e_1, e_{21}, $e_{22}^{l,i}$ and p are uniquely determined in terms of n and $N_{l,i}$ by the relations $(4.19)_{1,2,3}$. Substituting these relationships into $(4.19)_4$ and employing the implicit mapping theorem allows one to conclude that $N_{l,i}$ is uniquely determined by $n \in (-m, \bar{m})$ for some $m, \bar{m} > 0$, and by induction, we discover the formulas for $\widehat{N}_{l,i}(n)$ given by (4.21). This in turn allows us to obtain the quantities e_1, e_{21}, $e_{22}^{l,i}$ and p in terms of n on the interval $(-m, \bar{m})$. □

Birth rate $B[n]$**.** By Theorem 4.1, and using $(4.19)_6$ and (4.22), we conclude that for small populations $n \in [0, \bar{m})$, the dynamics is again driven by the equation

$$\partial_t n(t) = n(t)\big(B(n) - \gamma_n\big),$$

where now the birth rate $B(n)$ is given by

$$\begin{aligned}
B(n) &= \frac{\mu}{\bar{n} + n(t)} \Big(\gamma + \frac{\theta_p - 1}{\theta_p} (\gamma n + \gamma_p) \Big) \widehat{p}(n) \\
&= \frac{\mu\, n^2}{\bar{n} + n(t)} \Big(\frac{\gamma}{\gamma_p} \theta_p + \big(1 - \theta_p\big) \big(\frac{\gamma}{\gamma_p} n + 1 \big) \Big) \bar{p}(n)\,.
\end{aligned} \tag{4.23}$$

We now divide $B(n)$ by n^2 and differentiate with respect to θ_p. Since $\bar{p}$ is independent of θ_p, we obtain

$$\frac{\partial}{\partial \theta_p} \left(\frac{B(n)}{n^2} \right) \bigg|_{n=0} = \frac{\mu}{\bar{n}} \left(\frac{\gamma}{\gamma_p} - 1 \right) \frac{b_2}{d_{21}}\, m_c \sum_l \frac{\beta_{l,1}\, \nu_{l,1}}{(\sigma_{l,1} + d_{22}^{l,1} + \gamma_{r,l,1})},$$

so that

$$\frac{\partial}{\partial \theta_p} \left(\frac{B(n)}{n^2} \right) \bigg|_{n=0} > 0 \quad \text{if and only if} \quad \gamma > \gamma_p\,.$$

Thus we arrive at a similar conclusion to that of the T-model: that is, for small populations, sharing food (within the species) is beneficial in terms of growth as long as the consumption rate γ is greater than the decay rate γ_p of the cleaved off cellobiose.

5 A Model for Continuous Traits

In this section, by analogy with our multiple trait T-model (4.16), we develop a model for a population with continuous traits. We think of the multiple-trait population as having M traits indexed by $x_1 < \cdots < x_M$, so we write

$$n^i(t) = n(x^i, t)\Delta x, \quad e_1^i(t) = e_1(x^i, t), \quad e_2^i(t) = e_2(x^i, t),$$

for some functions $n(x,t)$, $e_1(x,t)$, $e_2(x,t)$, representing the population and enzyme densities. We now simply assume that the variable x takes on a continuous range of values.

We similarly translate the coefficients (3.30) and coefficient vectors (4.12), so that these become continuous parameters: that is, we allow the parameters b_i, d_i, $\widehat{\alpha}$, $\widehat{\beta}$, $\widehat{q}$, θ_p, etc, to depend on x, and in analogy to $(4.12)_{1,2,3}$ we set

$$A(x) = \widehat{\alpha}(x)\,\frac{b_1(x)}{d_1(x)}, \quad B(x) = \theta_r(x)\,\widehat{\beta}(x)\,\frac{b_2(x)}{d_2(x)}, \quad Q(x) = \widehat{q}(x)\,\frac{b_2(x)}{d_2(x)}, \tag{5.1}$$

where these are now positive functions. In particular, we interpret $\widehat{\alpha}$, $\widehat{\beta}$ and $\widehat{q}$ as the rates of landing spot generation, occupation, and the rate of cellobiose production, per individual, respectively.

We now simply follow the development that led to (4.16), but reinterpreting the inner product, so that for each function $W(x)$,

$$\langle W, n\rangle = \int W(y)\, n(y,t)\, dy.$$

Then (4.13), (4.14) and (4.15) are unchanged. To express the population equation, we define the functional

$$\tau[n] := \frac{1}{\gamma_\varrho m_c}\langle A, n\rangle\langle Q, n\rangle + \langle A, n\rangle + \langle B, n\rangle + \gamma_p,$$

and the convolution

$$N[n](x,t) = \int \nu(s,x)\, n(s,t)\, ds,$$

which is an inner product in the first variable.

We must now model the last term in (4.17). In analogy with that term, we define

$$\Xi(z; x, t) = \frac{\nu(x,z)Q(z)}{\nu(x,z)\,\bar{n}(x,t) + N[n](z,t)}\,.$$

Now, in analogy with (4.16), (4.17), we write the population equation as

$$\partial_t n(x,t) = n(x,t)\,\Big(B[n](x,t) - \gamma_n(x)\Big),$$

where the birth rate is now the functional

$$B[n] = \frac{\mu(x)\,r}{\gamma_\varrho\, m_c}\,\frac{\langle A, n\rangle}{\tau[n]}\left(\frac{\langle \theta_p\, Q, n\rangle\gamma(x)}{\big(\bar{n}(x) + \frac{1}{\gamma(x)}\,\langle\gamma, n\rangle\big)\,\big(\langle\gamma, n\rangle + \gamma_p\big)} + \Big\langle (1-\theta_p)\,\Xi(\cdot\,; x, t)\,, n\Big\rangle\right). \tag{5.2}$$

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