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Generalised approach to modelling a three-tiered microbial food-web

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ABSTRACT

The complexity of the anaerobic digestion process has motivated the development of complex models, such as the widely used Anaerobic Digestion Model No. 1. However, this complexity makes it intractable to identify the stability profile coupled to the asymptotic behaviour of existing steady-states as a function of conventional chemostat operating parameters (substrate inflow concentration and dilution rate). In a previous study this model was simplified and reduced to its very backbone to describe a three-tiered chlorophenol mineralising food-web, with its stability analysed numerically using consensus values for the various biological parameters of the Monod growth functions. Steady-states where all organisms exist were always stable and non-oscillatory. Here we investigate a generalised form of this three-tiered food-web, whose kinetics do not rely on the specific kinetics of Monod form. The results are valid for a large class of growth kinetics as long as they keep the signs of their derivatives. We examine the existence and stability of the identified steady-states and find that, without a maintenance term, the stability of the system may be characterised analytically. These findings permit a better understanding of the operating region of the bifurcation diagram where all organisms exist, and its dependence on the biological parameters of the model. For the previously studied Monod kinetics, we identify four interesting cases that show this dependence of the operating diagram with respect to the biological parameters. When maintenance is included, it is necessary to perform numerical analysis. In both cases we verify the discovery of two important phenomena; i) the washout steady-state is always stable, and ii) a switch in dominance between two organisms competing for hydrogen results in the system becoming unstable and a loss in viability. We show that our approach results in the discovery of an unstable operating region in its positive steady-state, where all three organisms exist, a fact that has not been reported in a previous numerical study. This type of analysis can be used to determine critical behaviour in microbial communities in response to changing operating conditions.

1. Introduction

The mathematical modelling of engineered biological systems has entered a new era in recent years with the expansion and standardisation of existing models aimed at collating disparate components of these processes and provide scientists, engineers and practitioners with the tools to better predict, control and optimise them [23]. In engineered biological systems, mechanistic modelling reached consensus with the development of the Activated Sludge Models [9,10] for wastewater treatment processes, followed by the Anaerobic Digestion Model No. 1 (ADM1) [12] a few years later. The development of ADM1 was enabled largely due to the possibilities for better identification and characterisation of functional microbial groups responsible for the chemical transformations within anaerobic digesters. It describes a set of stoichiometric and kinetic functions representing the standard anaerobic processes, remaining the scientific benchmark to the present day. However, there has been a growing awareness that the model should take advantage of improved empirical understanding and extension of biochemical processes included in its structure, to acquire a better trade-off between model realism and complexity [13].

The full ADM1 model is highly parameterised with a large number of physical, chemical and biological processes described by numerous state variables and algebraic expressions. Whilst suitable for dynamic simulation, more rigorous mathematical analysis of the model is difficult. To the authors knowledge, only numerical investigations are available [3]. Due to the analytical intractability of the full ADM1, work has been made towards the construction of simpler models that preserve biological meaning whilst reducing

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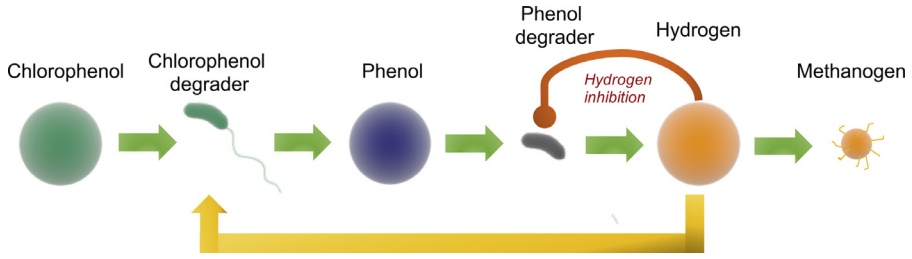

Fig. 1. Schematic of the three-tier chlorophenol mineralising food-web indicating the flow and conversion of chemical substrates and products in the system.

the computational effort required to find mathematical solutions of the model equations [7,8].

The most common models used to describe microbial systems are two-tiered models, which take the form of a cascade of two biological reactions where one substrate is consumed by one microorganism to produce a product that serves as the main limiting substrate for a second microorganism. When the second organism has no feedback on the first organism, the system is known as commensalistic [16,20]. The system has a cascade structure and the number of steady-states and their (mathematical) stability as a function of model inputs and parameters may be investigated [1,2,19]. When the growth of the first organism is affected by the substrate produced by the second organism the system is known as syntrophic. For instance, if the first organism is inhibited by high concentrations of the product, the extent to which the first substrate is degraded by the first organism depends on the efficiency of the removal of the product by the second organism. The mathematical analysis of such a model is more delicate than for commensalistic models, (see for instance early work by [4,14,15,27] and the more recent papers [5,11,17,18,22]). An important and interesting extension should be mentioned here: [25,26] analysed an 8-dimensional mathematical model, which includes syntrophy and inhibition, both mechanisms considered by [2] and [6].

As an example of this for anaerobic digestion, a previous study investigated the effect of maintenance on the stability of a two-tiered 'food-chain' comprising two species and two substrates [28]. Maintenance is defined as the energy consumed by an organism that is used for all biological processes other than growth. In [28] and here, it is analogous to a first-order decay rate constant, or biomass death term. Although the authors were not able to determine the general conditions under which this four dimensional syntrophic consortium was stable, further work has shown that a model with generality can be used to answer the question posed, determining that the two-tiered food-chain is always stable when maintenance is included [18].

More recently, the model described by [28] was extended by the addition of a third organism and substrate to create a three-tiered 'food-web' [24], as shown in Fig. 1. In this paper, the existence and stability of the steady-states were determined only numerically. Although the results were important in revealing emergent properties of this extended model, the motivation of this work is to give an analytical study of the model. Moreover, our analysis does not require that growth functions are of the specific form considered and are valid for a large class of growth functions. This is critical as it provides the means by which microbiologists can theoretically test the influence of the growth characteristics of organisms on the properties of the system and the interactions between multiple species.

Here, we pursue a generalised description and analysis of the model given by [24]. Chlorophenols are chemicals of importance due to their impact on the environment and to public health, their recalcitrance in food-webs and resistance to aerobic biodegradation via the oxygenase enzyme [21]. Although we consider the monochlorophenol isomer here, extension to multiple isomeric chlorophenols would be straightforward. It is important to note that, although the particular biological transformation provided is for chlorophenol mineralisation, the structure and methods employed are much more general and apply to any theoretical ecological interactions that may be hypothesised or observed in a microbial community. We therefore stress that this work can provide a good approach for analytically investigating the behaviour of microbial food-webs where numerical parameters are difficult to obtain or uncertain. Ultimately, we demonstrate here the advantage of a generalised approach for mathematical analysis of microbial ecological interactions from both a theoretical perspective and its potential if providing knowledge in applied research where these communities and processes are studied empirically.

The paper is organised as follows. In Section 2, we present a description of the model to be investigated, and its reduction in Section 3. Model assumptions and notations are provided in Section 4. In Section 5 we demonstrate the existence of the three steady-states and define four interesting cases for specific parameter values that are investigated using the solutions, whilst also indicating the regions of existence of the steady-states for the operating parameter values. We present results on the behaviour of the system whilst varying two control parameters in Section 6. In Section 7 we perform local stability analysis of the steady-states without maintenance and, in Section 8, we undertake a comprehensive numerical stability analysis of the four cases for both the model with and without maintenance. We show that our approach leads to the discovery of five operating regions in which one leads to the possibility of instability of the positive steady-state, where all three organisms exist, a fact that has not been reported by [24]. Indeed, we suggest that a stable limit-cycle can occur at the boundary with this region. Finally, in Section 9, we make comment on the role of the kinetic parameters used in the four example cases, in maintaining stability, which points to the importance of the relative aptitude of the two hydrogen consumers in sustaining a viable chlorophenol mineralising community. In the Appendix we describe the numerical method used in Section 8, give the assumptions on the growth functions we used and the proofs of the results.

2. The model

The model developed in [24] has six components, three substrate (chlorophenol, phenol and hydrogen) and three biomass (chlorophenol and phenol degraders, and a hydrogenotrophic methanogen) variables. The substrate and biomass concentrations evolve according to the six-dimensional dynamical of ODEs:

$$\frac{dX_{ch}}{dt} = -DX_{ch} + Y_{ch} f_0(S_{ch}, S_{H_2}) X_{ch} - k_{dec,ch} X_{ch} \tag{1}$$

$$\frac{dX_{ph}}{dt} = -DX_{ph} + Y_{ph} f_1\left(S_{ph}, S_{H_2}\right) X_{ph} - k_{dec,ph} X_{ph} \tag{2}$$