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Response from Authors to Editor and Reviewer comments

Reviewer #1

1. Please consider reference style: Number the references (numbers in square brackets) in the list in the order in which they appear in the text.

Response:: Done

The authors in section 3.3 claim several sentences that could confuse readers. 2.1 **one discovers how the steady state of the system responds to the environmental conditions.** There are several concerns that the authors should clarify:

- a) **The steady state.** Is there a unique steady state? Is there a reported contribution concerning a formal analysis of the model in the sense of stability (stable state existence and uniqueness)? Maybe, authors should refer as **a system's stable state (if it exists).**

Response: Thank you for raising this important issue, which we had overlooked. A number of the reviewer comments below are closely related, hence we sometimes refer to this response and do so using the label "Response R1". In order to clarify about the existence and uniqueness of steady states we have added the text **When one wishes to be able to make conclusions about how the steady state of the system is affected by the environmental driver, it is very important to note that the *final state* (found by the simulation) is not guaranteed to be a *steady state*. The user must ensure that the simulation is run for sufficiently long time for any transient dynamics to disappeared, and must also check the type of long-term dynamics occurring. In the results presented here, and in the paper @Limberger2022, this was performed by visual inspection, and by checking the sensitivity of conclusions to the length of the simulation. Furthermore, the package does not include methods for a formal analysis of the stability of the system and users should take care to assess if steady states are unique.**

Response: In addition, we notice that we sometimes used the term "stable state" and sometimes "steady state". We now use only the term "steady state". Furthermore, we now use the term "final state" to refer to the state of the system at the end of a simulation.

- b) **The steady state of the system responds`.** It should be noted that the steady state does not respond to the environment. Maybe, the authors refer to the numerical result of a steady state as a function of parameter and initial condition (if a steady state is not unique).

Response: Thank you. We have edited the text so that we do not state that the steady state responds to the environment.

- 2.2 **finding steady states that correspond to values of one environmental driver.** The software does not find a steady state. Maybe the authors refer to the software running an open loop of the dynamic system under a set of initial conditions and a subset of parameter

values (oxygen diffusivity). Then, the numerical evaluation of steady states could be related to environmental conditions in real systems.

Response: We envisage and hope that Response R1 sufficiently clarifies steady state finding.

2.3 **Two methods for finding steady states are implemented.** Again, the software does not find a steady state. Maybe the authors refer to two simulations proposed to evaluate an open loop simulation of the dynamic model numerically.

Response: We envisage and hope that Response R1 sufficiently clarifies steady state finding.

2.4 **The first runs a separate simulation for each combination of starting conditions and oxygen diffusivity.** This sentence is confusing. What the authors mean with **separate simulation** and **starting conditions**. Maybe the authors refer to each initial condition and parameter set value (oxygen diffusivity) as an open loop simulation run of the dynamic system. Are these simulations results focused on obtaining a bifurcation diagram Fig. 3 and 4 from {10.1038/s41467-017-00912-x}? Please clarified this point.

Response: We have clarified what is meant by "separate simulation" by changing to "independent simulation", and change "starting conditions" to "initial conditions". We hope that this more standard terminology is clearer. Furthermore, we have added that "This is the method used in the @Bush2017 study and was used to obtain the results in figures 3 and 4 of that article."

2.5 **The second runs two simulations, one with step-wise and slowly temporally increasing oxygen diffusivity, and the other with step-wise and slowly decreasing oxygen diffusivity.** This sentence needs to be clarified. Authors refer **temporally** as several changes in the value of oxygen diffusivity during a simulation run time. Maybe the authors mean the following: to explore the parametric sensitivity of the dynamic model under oxygen diffusivity variation, subset values of this parameter are numerically evaluated. Two value vectors of oxygen diffusivity are presented step-wise, gradually increasing and decreasing.

Response: We are grateful for this different perspective on how to explain the method and have added it to the manuscript ("Put another way, to explore the sensitivity of steady states of the dynamic model under oxygen diffusivity variation, subset values of this parameter are numerically evaluated. Two value vectors of oxygen diffusivity are presented step-wise, gradually increasing and decreasing.")

2.6 **We implemented two methods since there is no definitive best method, and in order to check if results were sensitive to choice of method.** This sentence is confusing.

Response: Thank you for pointing out this source of confusion. We change the text to "Two strategies are implemented in order to allow comparison of their results." and moved it to just after we state that two strategies are provided.

a) **two methods** Maybe the authors mean the following: two numerical strategies to explore a parametric sensitivity numerical evaluation.

Response: Thank you for this suggestions. We have changed the text to "Two numerical strategies for finding steady states and their sensitivity to parameters are implemented."

b) **there is no definitive best method**. Under which criteria? The authors present only two numerical evaluations. Please clarified this point.

Response: We have removed this claim since it is not demonstrated to be true and is unimportant.

c) **in order to check if results were sensitive to choice of method**. This sentence needs to be clarified. There is no comparison between numerical evaluations in any sense. The numerical simulations or simulation results are not sensitive to choice or method. Indeed, the numerical solution of the dynamical model is sensitive to a set of parameters and initial conditions. Maybe the authors mean the following: to evaluate the performance of the numerical parametric sensitivity analysis of the dynamical model concerning one parametric variation (oxygen diffusivity) under two schemes.2.7 It is not clear why there are two **methods** for numerical parametric sensitivity analysis. The authors should include the arguments of this.

Response: We removed this text and now simply state that having two methods allows the comparison of their results.

2.8 Please consider rewrite the section 3.3 (see previous 2.1 - 2.7 points) in the sense of Parametric sensitivity analysis, Open loop dynamical behavior, Equilibrium points (see Khalil, H. K. (2002). Nonlinear Systems. Prentice Hall, New Jersey.)

Response: We have the opinion that the with the revisions already made and detailed above, and those below, that the terminology is now more in line with this text, and will be clearly understandable by the target audience (theoretical ecologists) even when the section is not more substantially rewritten.

3. Please consider the following suggestions:

Line 5 **types of ecosystem**

Changed to **types of ecosystems**

Line 10 **Permanent link to**

Changed to **Permanent links to**

Line 12 **role in the development of understanding about how ecosystems**

role in understanding how ecosystems Changed to **Mathematical models play a key role in the development of ecosystem models and the understanding about how ecosystems work**

Line 13: **and how they respond**

Changed to **and respond**

Line 15 **have played a influential role is 16 how ecosystems respond to gradual change**

have been influential in how ecosystems respond to a gradual change changed to **One area of ecology in which models have been influential is the understanding of their response to a gradual change in an environmental driver [Scheffer2001].**

Line 16 is a environmental

Changed to is an environmental

Line 17 affects an ecosystem, but 18 is assumed to not be

Changed to affects an ecosystem. Still, it is assumed not to be

Line 27 change of the system

Changed to change in the system

Line 28 to anaerobic

Changed to to an anaerobic

Line 34 termed the oxygen diffusitivity

Changed to termed oxygen diffusivity

Line 38 This leaves open the question of if and how biodiversity within these types (i.e. functional groups) of bacteria affects the ecosystem

Changed to This leaves the question of if and how bacteria's biodiversity within these types (i.e., functional groups) affects the ecosystem

Line 47 It was with this goal in mind that we developed the microxanox package

Changed to With this goal in mind, we developed the microxanox package

Line 58 conditions, addition

Changed to conditions, the addition

Line 60 some functions to analyse the results as well as to visualize the results to provide a starting

some functions to analyze the results and visualize them to provide a starting
changed to some functions to analyse the results and visualize these to provide a
starting point

Line 71 for running individual simulations and for running a set of simulations

Changed to for running individual simulations and a set of simulations

Line 76 the vectors and matrices, and to use matrix mathematics

Changed to the vectors and matrices and used matrix mathematics

Line 80 code have modular structure so that new functionality can be easily added. E.g. temporally

Changed to code have a modular structure so that new functionality can be easily added. E.g., temporally

Line 87 to maximise simplicity for the user, and

Changed to to maximize simplicity for the user and

Line 95 results of the run

Changed to simulation results

Line 98 parameters and re-running the simulations straightforward. In the following sections we

parameters, and reruns the simulations straightforwardly. In the following sections, we changed to This promotes reproducibility and makes incremental changes of individual parameters with a consecutive and re-running of the simulations straightforward.

Line 107 contains among other things the

Changed to contains, among other things, the

Line 109 their meaning and how they are created and have values set and changed please

Changed to their meaning, and how they are created and have values set and changed, please

Line 113 an object which is identical to the parameter

Changed to an object identical to the parameter

Line 116 to run the simulation again from

Changed to to rerun the simulation from

Line 119 The general approach used to find the stable state of the system

Changed to The general approach to finding the numerical value of a system's stable state (if it exists)

Line ...

4. Please, consider English Editing Service or Proofread Your Paper.

The paper has been proofread and edited.

The manuscript has been proofread by a native speaker with extensive experience in publishing scientific articles.

5. Please, consider include two or three references of SoftwareX Journal.

Added three references from SoftwareX.

I hope we addressed all the comments to your satisfaction.

Sincerely,

Rainer M Krug