

1 Microxanox: an R package for simulating an aquatic
2 *MIC*Robial ecosystem that can occupy *OX*ic or
3 *ANOX*ic states.

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5 **Abstract**

Microxanox is an R package to simulate a three functional group ecosystem (cyanobacteria, phototrophic sulfur bacteria, and sulfate-reducing bacteria) with four chemical substrates (phosphorus, oxygen, reduced sulfur, and oxidized sulfur) using a set of ordinary differential equations. Simulations can be run individually or over a parameter range, to find stable states. The model can be implemented with different numbers of species per functional group. The package is constructed in such a way that the results contain the input parameter used, so that a saved results can be loaded again and the simulation be repeated. Furthermore, the package framework and code should serve as a useful starting point for making simulation models of other types of ecosystem.

6 *Keywords:* reproducibility, regime shift, stable state, ordinary differential
7 equations

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8 1. Required Metadata

9 1.1. Current code version

10 Ancillary data table required for subversion of the codebase.

Nr.	Code metadata description	Please fill in this column
C1	Current code version	v0.9.0
C2	Permanent link to code/repository used for this code version	https://github.com/UZH-PEG/microxanox 10.5281/zenodo.6624125
C3	Code Ocean compute capsule	
C4	Legal Code License	MIT
C5	Code versioning system used	git
C6	Software code languages, tools, and services used	R
C7	Compilation requirements, operating environments	R ($\geq 4.1.0$) magrittr tibble ggplot2 patchwork grDevices stats mgcv deSolve dplyr tidyr stringr multidplyr
C8	If available Link to developer documentation/manual	User Guide
C9	Support email for questions	Rainer.Krug@uzh.ch; Owen.Petchey@ieu.uzh

11 2. Motivation and significance

12 Mathematical models play a key role in the development of understanding
 13 about how ecosystems work and how they respond to environmental changes
 14 [1, 3, 13]. They are also important for developing hypotheses to test in empirical
 15 studies. One area of ecology in which models have played a influential role is
 16 how ecosystems respond to gradual change in an environmental driver [9]. An
 17 environmental driver is a environmental condition that affects an ecosystem, but
 18 is assumed to not be affected by the ecosystem, such as the rate of nutrient input
 19 into a lake.

20 It is conceivable that an ecosystem state, such as the total biomass of a
21 particular type of bacteria, may remain unchanged when an environmental driver
22 changes. It is also possible that the ecosystem state changes gradually. It is
23 also possible that the ecosystem state changes abruptly to a new state that is
24 difficult to recover from [9]. This possibility for abrupt, perhaps catastrophic
25 changes that are difficult to reverse causes considerable concern [4, 6, 12].

26 An example where a gradual change of an environmental variable causes an
27 abrupt change of the system is the switch from an aerobic (oxygen is available
28 for metabolism) to anaerobic (oxygen generally unavailable) state in a microbial
29 ecosystem. This system has been investigated by Bush et al. [2] in a simulation
30 study of a mathematical model. Three types of microbes occur in the model:
31 cyanobacteria (CB) dominating the oxic state, and two types of sulfur bacteria
32 that dominate the anoxic state (sulfate reducing bacteria (SB) and phototrophic
33 sulfur bacteria (PB)). The model shows that gradual change in the rate at which
34 oxygen could diffuse into the ecosystem (termed the oxygen diffusivity) could
35 cause catastrophic changes in the ecosystem state that would be difficult to
36 reverse.

37 One feature of the study by Bush et al. [2] was limited biodiversity. Specifically,
38 there was no biodiversity within each of the three types of bacteria. This leaves
39 open the question of if and how biodiversity within these types (i.e. functional
40 groups) of bacteria affects the ecosystem response to environmental change. This
41 limitation is not specific to the study of Bush et al. [2]. There are few if any
42 studies of the effects of biodiversity on abrupt transitions between ecosystem
43 states.

44 We decided to fill this research gap by making a simulation study of how
45 within functional group biodiversity affects ecosystem responses to environmental
46 change [?], and to base our work on the work and model of Bush et al. [2].
47 It was with this goal in mind that we developed the *microxanox* package [5].
48 The first stage of development was to write code from scratch (as there was
49 no available code to start from) and to confirm that this new implementation
50 would reproduce the previously published results. The resulting reproduction is
51 available as one of the package vignettes: [vignette Partial reproduction of Bush](#)
52 [et al.](#)

53 The second stage was to add functionality that would be necessary to answer
54 our research question. Most importantly, we made it possible to have multiple
55 species of bacteria within each of the three functional groups, for the multiple
56 species to differ in their characteristics, and to vary the number of species and
57 amount of variability among them. We also added functionality that allowed:
58 temporally varying environmental conditions, addition of random noise to state
59 variables, and immigration. In addition to the model itself, the package includes
60 some functions to analyse the results as well as to visualize the results to provide
61 a starting point for customized visualizations based on own requirements. The
62 basic and additional functionality is described in the package [User Guide](#).