

1 Microxanox: an R package for simulating an aquatic
2 *MICRobial* ecosystem that can occupy *OXic* or
3 *ANOXic* states.

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5 **Abstract**

Microxanox is an R package to simulate a three functional group system (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 features multiple species per functional group, where the number is only limited by computational constraints. The R 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.

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	CC BY 4.0
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 Manual
C9	Support email for questions	Rainer.Krug@uzh.ch; Rainer@krugs.de

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, 14]. They are also important for developing hypotheses that can then be
 15 tested in empirical studies. One area of ecology in which simple models have
 16 played a influential role is the area of how ecosystems respond to gradual change
 17 in an environmental driver [10]. An environmental driver is a environmental
 18 condition that affects an ecosystem, but is assumed to not be affected by the
 19 ecosystem, such as the rate of nutrient input 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 [10]. This possibility for abrupt, perhaps catastrophic
25 changes that are difficult to reverse causes considerable concern [4, 7, 13].

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. Three types of microbes occur in the model: cyanobacteria (CB)
30 dominating the oxic state, and two types of sulfur bacteria that dominate the
31 anoxic state (sulfate reducing bacteria (SB) and phototrophic sulfur bacteria
32 (PB)). This system has been investigated by Bush et al. [2] in a simulation study
33 of a mathematical model. They showed 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. Specifi-
38 cally, there was no biodiversity within each of the three types of bacteria. This
39 leaves open the question of if and how biodiversity within these types (i.e. func-
40 tional groups) of bacteria, in their model, affects the ecosystem response to
41 environmental change. This limitation is not specific to the study of Bush et al.
42 [2], there are few if any studies of the effects of biodiversity on abrupt transitions
43 between ecosystem 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 Limberger [6], and to base our work on the work and model of Bush et al.
47 [2]. It was with this goal in mind that we developed the *microxanox* package
48 [5]. 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 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](#).

63 3. Software description

64 The *microxanoz* package is for simulating a three functional group system
65 (*CB*: cyanobacteria, *PB*: phototrophic sulfur bacteria, and *SB*: sulfate-reducing
66 bacteria) with four chemical substrates (*P*: phosphorus, *O*: oxygen, *SR*: reduced
67 sulfur, *SO*: oxidized sulfur). It includes feedback between organisms and biogeo-
68 chemical processes and is based on Bush et al. [2] (See Bush et al. [2] for a detailed
69 discussion of the model). At the core of the simulations is a set of ordinary differ-
70 ential equations (specified in the function `bushplus_dynamic_model()`, though
71 this function need not be directly called). There are functions for running
72 individual simulations and for running a set of simulations across, for example,
73 a range of environmental conditions.

74 To make the simulation run with multiple species, we expressed different
75 species characteristics in the elements of vectors and matrices. We also coded
76 the ordinary differential equations to include the vectors and matrices, and to
77 use matrix mathematics. In this way, we made it possible to run simulations
78 with different numbers of species without having to change the underlying code.

79 The package functions and code have modular structure, so that new func-
80 tionality can be easily added. E.g. temporally defined events of any type could
81 be specified. Further, all parameter values required to run a simulation are
82 stored in one object. Lastly, the general structure of the code should make it
83 straightforward to adapt the model to other similar systems (described in more
84 detail in the Impact section).

85 3.1. Software architecture

86 The framework used when writing this package aimed to maximise simplicity
87 for the user, and to make it easy to reproduce results (see the supplement to
88 Limberger [6] for an example of how this is used). As such, all the parameters
89 needed to run a simulation or find a stable state (i.e. the final state of the
90 ecosystem) are contained in a single object (which can easily be created using
91 included functions). This parameter object is given to a function that runs the
92 simulations and returns the results. The returned results object is identical
93 to the parameter object but with an additional slot named `results`, which
94 contains the results of the run. Thus the returned results object contains the
95 simulation conditions (parameters) as well as the results, and can be used to
96 run the simulation again. This promotes reproducibility and makes incremental
97 changes of individual parameters and re-running the simulations straightforward.

98 In the following sections we describe how to use the package to run one
99 simulation and to find steady states across an environmental gradient.

100 3.2. Running one simulation

101 A typical simulation would look as shown in 1.

102 A simulation is run using the `run_simulation()` function. In this function,
103 the ODEs are solved using the function `ode()` in the package *deSolve* package [12].
104 The `run_simulation()` function needs only one argument - an object as created
105 by the function `new_runsim_parameter()`. The parameter object returned by



Figure 1: Typical flow of a simulation. Dark Grey boxes: commands necessary for simulation; Light Grey: Saving of parameter and results; Lightest Grey: Different non specified commands.

106 `new_runsim_parameter()` contains among other things the `strain_parameter`
107 object, which can be created by the function `new_strain_parameter()`. For
108 a detailed description of the parameter objects, their meaning and how they
109 are created and have values set and changed please see the *User Guide* which
110 accompanies the package or is available at [User Guide](#).

111 After the parameter object has been defined, it can be used in the `run_simulation()`
112 function. The function returns an object which is identical to the parameter
113 object, except of an additional slot containing the results. This design produces
114 a fully reproducible object as it can be used as a parameter object to be fed
115 back into the `run_simulation()` function to run the simulation again from the
116 parameter used to generate the results before.

117 3.3. Finding Stable States

118 The general approach used to find the stable state of the system with a
119 specific parameter set is to run the simulation for a long time and record the
120 final state. When one does this across a range of environmental conditions, one
121 discovers how the steady state of the system responds to the environmental
122 conditions. The package contains functionality for finding steady states that
123 correspond to values of one environmental driver, namely the value of oxygen
124 diffusivity.

125 Two methods for finding steady states are implemented. The first runs a
126 separate simulation for each combination of starting conditions and oxygen
127 diffusivity (we term this the *Replication method*). This is the method used in
128 the Bush et al. [2] study. The second runs two simulations, with step-wise and
129 slowly temporally increasing oxygen diffusivity, and the other with step-wise
130 and slowly decreasing or decreasing oxygen diffusivity. During this temporal
131 environmental change, the state of the system was recorded just before change to
132 a new oxygen diffusivity (we term this the *Temporal method*). We implemented
133 two methods since there is no definitive best method, and in order to check if
134 results were sensitive to choice of method.

135 The replication method is implemented in the function `run_replication_ssfind()`
136 which takes a parameter object as returned by the function `new_replication_ssfind_parameter()`
137 and the number of cores for multithreading the simulation. As the multithreading
138 uses the package function `mclapply()` from the package `parallel` [8], the multi-
139 threading only works on Linux and Mac. It is planned to move to `parLapply()`
140 [8] in a future release.

141 This temporal method implemented in the function `run_temporal_ssfind()`,
142 which takes a parameter object as created by the function `new_temporal_ssfind_parameter()`.
143 It is planned for a later release, to run these two simulations in parallel.

144 For a more detailed walk-through of these two approaches and explanation
145 please see the [User Guide](#).

146 3.4. Analysing and visualising results

147 From the results returned, summary measures about how the ecosystem
148 stable states respond to environmental change can be extracted. The function

149 `get_stability_measures()` returns quantities such as the amount of environ-
150 mental change required for the system to abruptly change to a different state.

151 The function `plot_dynamics()` plots a single simulation run, as returned
152 from the `run_simulation()` function. This function is only provided as a
153 convenience function to provide a way to easily see the results of a simulation
154 run. An example plot resulting from this function is shown in 2.

155 4. Impact

156 The open source implementation and extension of the model used in Bush
157 et al. [2] provides the means of reproducing the results published while at
158 the same time provides the means of doing unique, innovative, and important
159 investigations of how ecosystems respond to environmental change, and how
160 biodiversity may modulate this response.

161 The design of the package code and functionality is with reproducibility in
162 mind: the combination of all parameters being in a single parameter object
163 as well as the return of the simulation as a result object which inherits from
164 the parameter object provides a relatively easy to use framework to implement
165 reproducible experiments.

166 Here we evidence the impact of the *microxanox* package by describing three
167 use cases and then by describing how the package can be a starting point for
168 models of other ecosystems. The first two use cases are described in detail
169 (including the code for reproducing them) in the *User Guide* and the *Partial*
170 *Reproduction* vignettes. The third is taken from REF NEEDED [9].

171 4.1. Use case 1: Regime shifts during temporal environmental change

172 The study of Bush et al. [2] includes simulations of the effect of oxygen
173 diffusivity (an environmental driver, in the sense that it affects the ecosystem but
174 is not affected by it) on the ecosystem state (oxic or anoxic). The *microxanox*
175 package contains functionality to make a specific temporal pattern of change
176 in the oxygen diffusivity. As well as allowing individual simulations during
177 which oxygen diffusivity varies, this functionality forms the basis of the temporal
178 method for finding stable states.

179 An example of this functionality is given in the *Partial Reproduction* vignette,
180 which we briefly show here (Figure 3). The example is composed of a single
181 simulation, at the beginning of which the system is in the oxic state with high
182 abundance of cyanobacteria. Oxygen diffusivity is then slowly decreased and
183 eventually, around hour 30'000 the system switches to the anoxic state, with
184 high abundance of both sulfur bacteria types. The oxygen diffusivity is then
185 increased and at around hour 38'000 the system abruptly switches back to the
186 oxic state.

187 Also visible in the results are thick lines showing abundances of bacteria
188 when abundances are low. This is due to the implementation of a function that
189 at regular intervals, increases the abundance to a preset level. This prevents
190 abundances reducing to very small numbers. The function that implements this

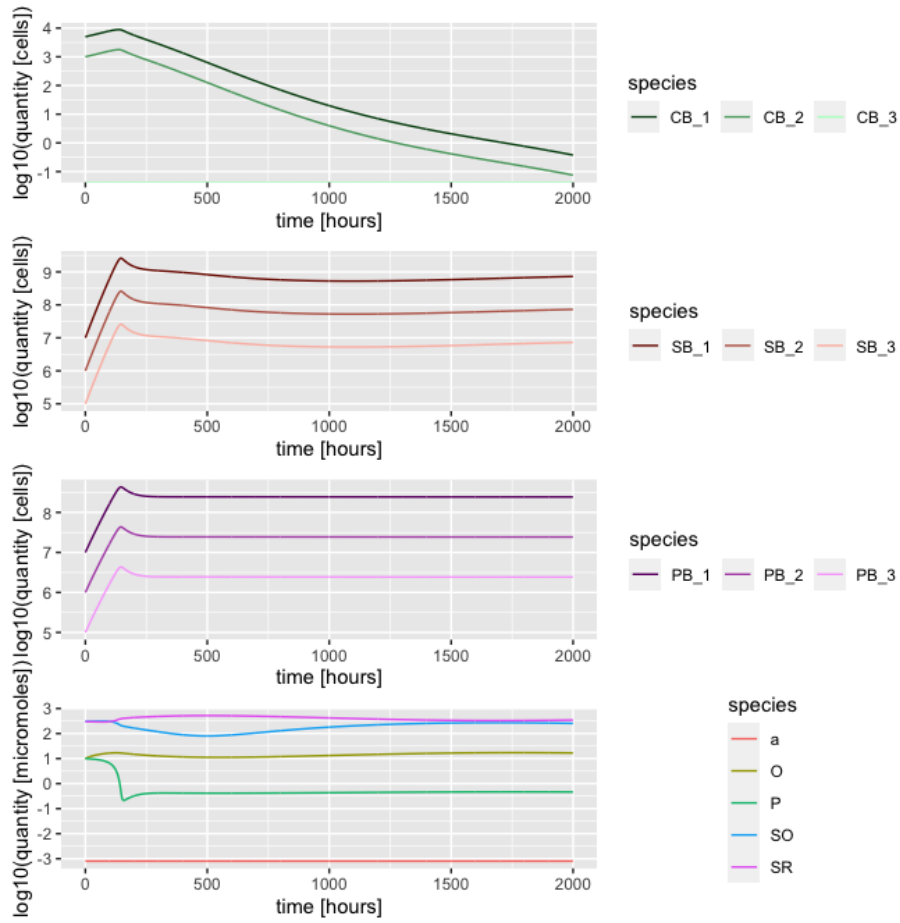


Figure 2: Results of a simulation run shown using the function `plot_dynamics()`. In this case, there were three strains per functional group, though strains within functional groups had identical properties in this example. CB extunderscore1 = cyanobacteria strain 1; SB extunderscore1 = sulfur reducing bacteria stain 1; PB = phototrophic sulfur bacteria strain 1. Here we show the figure produce by `plot_dynamics()`, which produces figures not with all features ideal for publication.

191 increase abundance can also be made to add a certain abundance to each strain
192 at regular intervals, thus simulating immigration in to the system.

```
193 #>
194 #> Attaching package: 'dplyr'
195 #> The following objects are masked from 'package:stats':
196 #>
197 #>     filter, lag
198 #> The following objects are masked from 'package:base':
199 #>
200 #>     intersect, setdiff, setequal, union
```

201 4.2. Use case 2: The extent of hysteresis depends on community composition

202 The package contains a function to extract summary features of ecosystem
203 responses to environmental change, such as the amount of hysteresis displayed by
204 the ecosystem. Hysteresis is a key feature of ecosystem responses to environmental
205 change, because it is related to how difficult it can be to reverse the effects of
206 environmental change [10]. The amount of hysteresis is measured as the extent
207 of the environmental condition (here oxygen diffusivity) for which there were
208 two stable states. I.e. it is the extent of the environmental conditions for which
209 historical conditions play an important role in determining the current system
210 state (a definition of hysteresis).

211 Using the package to calculate the extent of hysteresis involves setting
212 ecosystem and simulation parameters, including parameters for the finding of
213 stable states across an environmental gradient, running the stable state finding
214 function, and analysing the results with the function that calculates extent of
215 hysteresis. The code for this is provided in the *User Guide* vignette.

216 The results show that the amount of hysteresis depends greatly on the
217 combinations of organisms present (Figure ??figL:uc2)). For example, with
218 only the CB (cyanobacteria) present, there was no hysteresis. In contrast, the
219 presence of both CB and SB (sulfate reducing bacteria) led to a large amount of
220 hysteresis. (These results are also given in the *Partial Reproduction* vignette.)

221 4.3. Use case 3: Effects of functional diversity on regime shifts

222 As discussed in the Introduction section, the package was motivated by the
223 question of how biodiversity influences ecosystem responses to environmental
224 change. Extensive results concerning this question are given in a separate
225 publication Limberger [6]. Here we describe one of the results, which is that
226 having biodiversity in a functional group can allow state changes to occur that
227 otherwise would not have. I.e. biodiversity can qualitatively change the state of
228 the ecosystem.

229 Biodiversity was added to the functional groups using the `new_strain_parameter()`
230 function to create a parameter set with multiple species per functional group
231 (albeit all with identical features) and then to add variability among the species



Figure 3: The temporal dynamics of the ecosystem model when an environmental condition (here parameter $*a^*$, the oxygen diffusivity) changes. Plot of the stable states of the simulation runs under different oxygen diffusivity. In this simulation there is only one strain in each functional group. CB extunderscore1 = cyanobacteria strain 1; SB extunderscore1 = sulfur reducing bacteria stain 1; PB = phototrophic sulfur bacteria strain 1. Here we show a figure adapted from the output of the `plot_dynamics()` function.

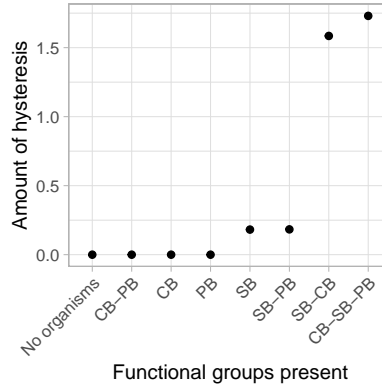


Figure 4: The amount of hysteresis depends on the combination of types of organisms present. The model is entirely deterministic, hence there are no error bars.

by calling the `add_strain_var()` function. This function takes an already existing parameter set and adds the specified amount of variation. The new parameter object is then used as before.

Figure 5 shows a simulation with two species (strains) in each of the three functional groups. The ecosystem starts in the oxic state, though with relatively high abundance of each functional group. The strain of SB that is more tolerant to oxygen (SB_1) initially decreases in abundance, but then increases, and the other (SB_2) strain then becomes abundant and SB_1 declines. Furthermore, the cyanobacteria crash in abundance, and the system switches to the anoxic state. In contrast, if there are two identical strains with tolerance half way between those in Figure 5 the ecosystem remains in the oxic state.

4.4. Adapting for other ecosystems and organisms

We anticipate that the package can be a useful starting point for investigating models of other types of ecosystem and how biodiversity in them affects responses to environmental change. The overall framework of the package, the purpose of each function, and the objects used for storing parameters and results could be retained. E.g., all such models would have parameters that differ among species and need to be described in an object, and studies will often need to run simulations and sets of simulations across environmental conditions.

Researchers wanting to model a new ecosystem do not, therefore, have to start from scratch. This will relieve researchers from needing to making software design decisions, and rather focus on appropriately representing their ecosystem, and finding the results that interest them. Nevertheless, adaptation of the code in the package will require a person / persons that can take a conceptual model of an ecosystem and then represent that in terms of parameters and rate equations, and that is relatively proficient in R programming.

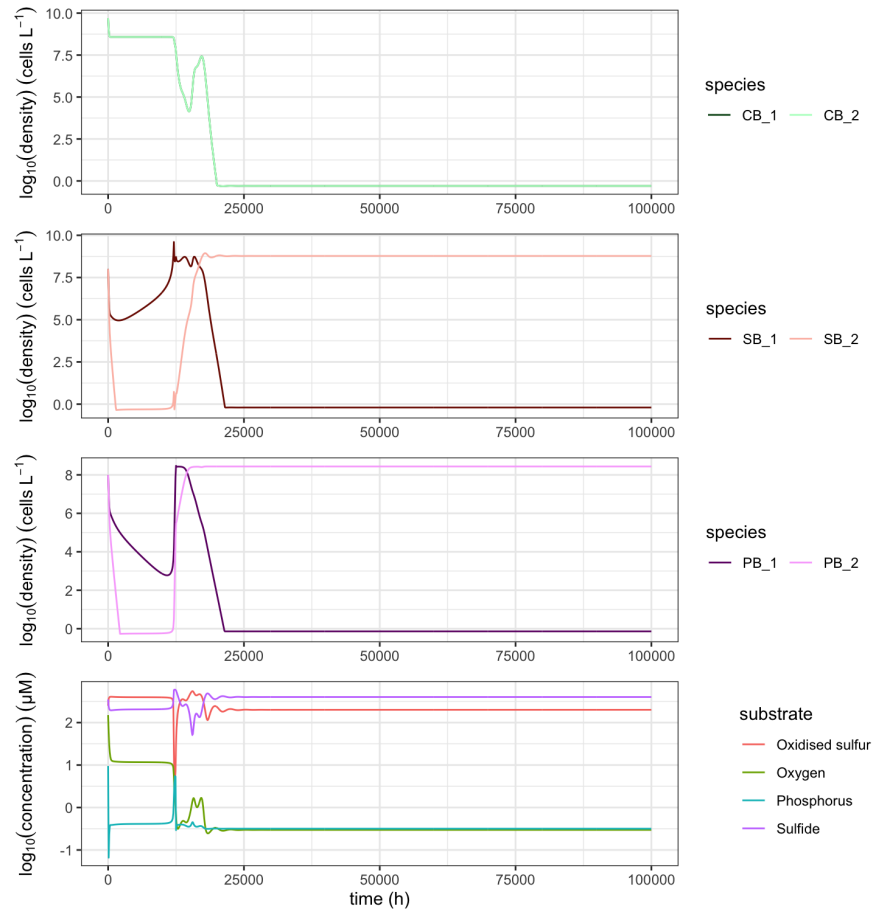


Figure 5: The dynamics of the ecosystem when there are two species in each functional group, and some variation (diversity) in species parameters.

258 5. Conclusions

259 The *microxanox* R package allows the simulation, visualisation, and analysis
260 of a model of a microbial ecosystem while allowing variation in the amount of
261 diversity containing in each of the functional groups of organisms present. It has
262 been used for the research described in another paper that describes one of the
263 first investigations of the effects of diversity on ecosystem resilience Limberger
264 [6]. In that paper, we show that diversity can have large and important effects
265 of ecosystem responses, highlighting the need for models such as ours, with
266 which one can easily manipulate the amount of biodiversity. The *microxanox*
267 package has also been used to reproduce the results of the paper that inspired
268 the package development Bush et al. [2].

269 The package greatly lowers the amount of work required in further investi-
270 gations of the specific ecosystem modelled. There has, for example, been quite
271 limited investigation of how biodiversity influences the short-term responses of
272 the modelled ecosystem to environmental change. Likewise, the package could be
273 used to power an investigation of the effects of biodiversity on the usefulness of
274 early warning signals of abrupt ecosystem change [11]. In addition this package
275 could be used as a template for the implementation for developing models of
276 other types of ecosystems and organism. By doing so, other models can profit
277 from the overall framework used, and the reproducibility aspects as well as the
278 flexibility implemented.

279 6. Conflict of Interest

280 The authors declare no known conflicting or competing interests associated
281 with this publication and there has been no significant financial support for this
282 work that could have influenced its outcome.

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