

Model Definition and Naming Convention

R-Package streambugs ver. 1.0
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State Variables

Names of state variables consist of three mandatory parts and one optional part separated by underline characters:

Reach_Habitat_Taxon or Reach_Habitat_Taxon_Group

where:

- Reach:** Unique, user-defined identifier for river reach.
The reaches to be modeled are extracted by the program from the names of the state variables.
- Habitat:** Unique, user-defined identifier for habitat within river reach.
Within each reach, there must be at least one habitat. Different reaches may contain different habitats. The habitats to be modeled in each reach are extracted from the names of the state variables.
- Taxon:** Unique, user-defined identifier for each taxon/substance to be modeled.
The taxa to be modeled in each habitat of each reach are extracted from the names of the state variables.
- Group:** Optional, user-defined functional group identifier that can be used to simplify the specification of joint parameters for a functional group.
The group specification does not have any influence on the food web structure; it only serves the purpose of simplifying the specification of joint parameters. It could be used to separate trophic levels in the food web or, alternatively, also groups within the same trophic level.

Only use lower or uppercase letters and numbers within each identifier. No special character and no underline ("_") character. Do not use identifiers that are the same as parameter names.

Model Parameters and Inputs

All names can be used for "parameters" (i.e. constants) or for "inputs" (i.e. time series). If there is the opportunity for several alternative names, always the value associated with the most specific name is used.

Global Parameters

<i>Syntax</i>	<i>Name</i>	<i>Unit</i>	<i>Meaning</i>	<i>Default value</i>
Par	kBoltzmann	eV/K	Boltzmann constant	8.61734e-05
	M0	g	Normalization mass	1
	ftempmax_intercept	-	critical value for ftemp if affinity score is 0, intercept with ftemp-axis	0
	ftempmax_curv	-	curvature for transformation of affinity scores for temperature, curv>0 means curved to the right, curv<0 means curved to the left, curv=0 means linear transformation	0
	fcurrent_intercept	-	see above	0
	fcurrent_curv	-		0
	fsapro_intercept	-		0
	fsapro_curv	-		0
	forgmicropollut_intercept	-		0
	forgmicropollut_curv	-		0
	fmicrohab_intercept	-		0
	fmicrohab_curv	-		0
	fsapro_intercept	-		0
	tempmaxKval_class1...n	K	mid values of temperature classes, "very cold"...	
	currentmsval_class1 ... n	m/s	mid values of current classes	
	saprowqclassval_class0 ... saprowqclassval_class4	-	mid values of water quality classes regarding saprobic conditions	
orgmicropollTUval_class1, orgmicropollTUval_class2	TU	mid values of classes of organic toxicants related to the Spear-trait		

Environmental Conditions

<i>Syntax</i>	<i>Name</i>	<i>Unit</i>	<i>Meaning</i>	<i>Default value</i>
Reach_Par Par	w	m	River width	-
	L	m	River reach length	-
Reach_Habitat_Par Habitat_Par Reach_Par Par	T	K	Temperature	-
	IO	W/m ²	Radiation at the water surface	-
	fshade		Fraction of water surface that is shaded	-
	CP	gP/m ³	Dissolved reactive phosphorus	-
	CN	gN/m ³	Inorganic dissolved nitrogen	-
	fA		Area fraction of habitat (need not be normalized)	1
	DSusPOM	gDM/m ³	Concentration of suspended organic particles	-
	tau	kg/(s ² ·m)	bottom shear force	-
	taucrit	kg/(s ² ·m)	critical bottom shear stress that induces bed-movement	-
	tempmaxK	K	maximum morning temperature in summer in Kelvin	-
	currentms	m/s	mean current velocity in m/s	-
	saprowqclass	-	water quality class regarding saprobic conditions, 1=oligo, 2=beta,3=alpha,4=pol y	
	orgmicropollTU	TU	Toxic units describing the effective concentration of organic toxicants	
	Dfish	kg/ha	Density of fish in a reach	0

Environmental conditions with a variable number of "classes" the number of which is extracted from the parameter vector by the internal function `get.inpind.parval.envcond.habitat.group()`

Reach_Habitat_Par Habitat_Par Reach_Par Par	microhabaf_type1 ...	- (m2/m2)	areal fraction of microhabitat types 1 to X, sum can be larger than 1 if the habitat surface is larger than the width*length of the river reach, sum=1 refers to the area of the river bottom (width*length)	

Initial Conditions and Input

<i>Syntax</i>	<i>Name</i>	<i>Unit</i>	<i>Meaning</i>	<i>Default value</i>
Taxon_Reach_Habitat_Par Group_Reach_Habitat_Par Taxon_Habitat_Par Group_Habitat_Par	Dini	gDM/m2	initial density of taxon/sub_stance in the given habitat of a reach	0
Taxon_Reach_Par Group_Reach_Par Taxon_Par Group_Par Reach_Habitat_Par Habitat_Par Reach_Par Par	Input	gDM/m2/yr	input of the taxon/substance in the given habitat of a reach	0

Taxon/Substance Property Parameters

<i>Syntax</i>	<i>Name</i>	<i>Unit</i>	<i>Meaning</i>	<i>Default value</i>
Taxon_Par Group_Par Par	M	g	typical individual biomass	-
	Ea	eV	Activation energy	-
	b		Allometric scaling exponent	0.75
	i0	J/a	Allometric parameter	-
	EC	J/gDM	Energy content	-
	fbasaltax	-	factor to modify basal metabolic rate	1
trait parameters with a flexible number of classes get.inpind.parval.taxaprop.traits()				
Taxon_Par Group_Par Par	tempmaxtolval_class1 ...	-	affinity score between normalized between 0 and 1 regarding flexible number of trait classes	-
	currenttolval_class1 ...	-	affinity score between normalized between 0 and 1 regarding flexible number of trait classes	-
	microhabtolval_type1 ...	-	affinity score between normalized between 0 and 1 regarding flexible number of trait classes	-
	saprotolval_class0...	-	affinity score between normalized between 0 and 1 regarding flexible number of trait classes	-
	orgmircopolltolval_class1...	-	affinity score between normalized between 0 and 1 regarding flexible number of trait classes	-

Process Properties

The stoichiometric parameters define the processes to be used (and for which kinetic parameters are searched in the parameter vector). The stoichiometric parameters cannot depend on reach or habitat. All kinetic parameters can depend on taxon, reach and habitat.

Processes associated to a single taxon

The syntax for stoichiometry of processes associated with a taxon is

Proc_Taxon_Taxi

where "Proc" is "Miner" (mineralization), "Resp" (respiration), "Death" (death) or "Prod" (primary production), "Taxon" is the taxon/substance to which the process is associated and "Taxi" is the taxon/substance for which the stoichiometric coefficient is defined. For each realization of the process characterized by "Proc" and "Taxon", an arbitrary number of stoichiometric coefficients for different "Taxi" is allowed. Typically the stoichiometric coefficient for "Taxi"="Taxon" will be plus (Prod) or minus unity (Miner, Resp, Death).

<i>Syntax</i>	<i>Name</i>	<i>Unit</i>	<i>Meaning</i>	<i>Default value</i>
<i>Stoichiometry:</i> Proc_Taxon_Taxi <i>Kinetic Parameters:</i> Taxon_Reach_Habitat_Par Group_Reach_Habitat_Par Taxon_Habitat_Par Group_Habitat_Par Taxon_Reach_Par Group_Reach_Par Taxon_Par Group_Par Reach_Habitat_Par Habitat_Par Reach_Par Par	Proc = Miner			
	kminer	1/a	Specific mineralization rate	-
	Proc=Drift			
	cdet	s ⁴ m ² / (kg ² a)	coef. of catastrophic loss	-
	Proc = Resp			
	fresp		Ratio of respiration rate to metabolic rate	-
	Proc = Death			
	fdeath		Ratio of death rate to metabolic rate	-
	Proc = Prod			
	fprod		Ratio of maximum primary production growth rate to metabolic rate	-
	fgrotax	-	factor to modify growth rate	1
	hdens	gDM/m ²	Self-inhibition half saturation concentration in the absence of disturbances	-
	KI	W/m ²	Half-saturation light intensity of algae growth	-
	KP	gP/m ³	Half-saturation conc. of algae growth with respect to P	-
	KN	gN/m ³	Half-saturation conc. of algae growth with respect to N	-

Food web processes

The syntax for stoichiometry of food web processes is

Proc_Taxon1_Taxon2_Taxi

where "Proc" is "Cons", "Taxon1" is the first taxon and "Taxon2" the second taxon involved in the process (typically "Taxon1" feeds on "Taxon2") and "Taxi" is the taxon/substance for which the stoichiometric coefficient is defined. For each realization of the process

characterized by "Proc", "Taxon1" and "Taxon2", an arbitrary number of stoichiometric coefficients for different "Taxi" is allowed. Typically the stoichiometric coefficient for "Taxi"="Taxon1" will be unity.

<i>Syntax</i>	<i>Name</i>	<i>Unit</i>	<i>Meaning</i>	<i>Default value</i>
<i>Stoichiometry:</i> Proc_Taxon1_Taxon2_Taxi	Proc = Cons			
	fcons		Ratio of maximum consumpti_on growth rate to metabolic rate	-
<i>Kinetic Parameters:</i> Taxon1_Taxon2_Reach_Habitat_Par Group1_Taxon2_Reach_Habitat_Par Taxon1_Group2_Reach_Habitat_Par Group1_Group2_Reach_Habitat_Par	fgrota x	-	factor to modify growth rate	1
Taxon1_Taxon2_Habitat_Par Group1_Taxon2_Habitat_Par Taxon1_Group2_Habitat_Par Group1_Group2_Habitat_Par	hdens	gDM/m2	Self-inhibition half satura_tion concentration in the absence of disturbances	-
Taxon1_Taxon2_Reach_Par Group1_Taxon2_Reach_Par Taxon1_Group2_Reach_Par Group1_Group2_Reach_Par	Kfood	gDM/m2	Half-satura_tion concentra_tion regarding food	-
Taxon1_Taxon2_Par Group1_Taxon2_Par Taxon1_Group2_Par Group1_Group2_Par	q	-	Exponent in limitation term	1
Taxon1_Reach_Habitat_Par Group1_Reach_Habitat_Par Taxon1_Habitat_Par Group1_Habitat_Par	Pref	-	relative preference factor for different food sources	1
Taxon1_Reach_Par Group1_Reach_Par Taxon1_Par Group1_Par	Proc = FishPred			
Reach_Habitat_Par Habitat_Par Reach_Par Par	cfish	gDM/kg/d	Food intake per kg fish and day	-
	Kfood	gDM/m2	Half-satura_tion concentra_tion regarding food	-
	q	-	Exponent in limitation term	1
	Pref	-	relative preference factor for different food sources	1

Overview parameter names related to traits

traitname	input file par env	par env model	par env global (e.g. midvalues of classes)	trait parameters (affinity scores)	model parameter
tempmax	Temp_max_summer tempmaxC	tempmaxK	tempmaxKval_class1 ...	tempmaxtolval_class1 ...	ftempmax
current	currentclassname/ currentms	currentms	currentmsval_class1 ...	currenttolval_class1	fcurrent
orgmicropoll	orgmicropollclassname/ orgmicropollTU	orgmicropollTU	orgmicropollTUval_class1 ...	orgmicropolltolval_class1	forgmicropoll
sapro	saprowqclassname/ saprowqclass	saprowqclass	saprowqclassval_class0 ...	saprotolval_class0	fsapro
microhab	microhabaf_type1...	microhabaf_type1...	-	microhabtolval_type1 ...	fmicrohab

History of model development

R-package streambugs ver. 1.0 includes the core functions used in Kattwinkel et al. (2016), Mondy and Schuwirth (2017), and Paillex et al. (2017).

Difference to model Streambugs 1.0 in Schuwirth & Reichert (2013):

- _ Environmental conditions and parameters can be time-dependent
- _ per reach different habitats can be modeled
- _ mineralization of organic material is introduced
- _ food limitation term has variable exponent q (default =1)
- _ Filt_scope is implemented as (still non taxon specific) parameter instead of fixed value
- _ ftemp is calculated differently from trait information

Differences in implementation:

- _ Option to run the model in C instead of R.
- _ different sites can be modeled simultaneously (allows extension with dispersal)
- _ we model now Biomass/per river length instead of Biomass per reach

Difference to Streambugs model used in Schuwirth et. al (2016):

- _ Different way to calculate factors ftempmax, fcurrent, fmicrohab, forgmicropoll, fsapro, see Mondy & Schuwirth (2017) for explanation.

References

Kattwinkel, M., P. Reichert, J. Rüegg, M. Liess, and N. Schuwirth. 2016. Modeling Macroinvertebrate Community Dynamics in Stream Mesocosms Contaminated with a Pesticide. *Environmental Science & Technology* **50**:3165-3173.

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Paillex, A., P. Reichert, A. W. Lorenz, and N. Schuwirth. 2017. Mechanistic modelling for predicting the effects of restoration, invasion and pollution on benthic macroinvertebrate communities in rivers. *Freshwater Biology* **62**:1083-1093.

Schuwirth, N., A. Dietzel, and P. Reichert. 2016. The importance of biotic interactions for the prediction of macroinvertebrate communities under multiple stressors. *Functional Ecology* **30**:974-984.

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