Contents

1 State variables, parameters, and functions

Tables 1, 2, and 3 contain the declaration of state variables, parameters, and functions.

Table 1: Table of state variables.

Symbol	Unit	Description
c_{DO}	mg/l	Dissolved O2
c_Z	mg/l	Degradable org. matter Z
v	m3	Water volume in reactor

Table 2: Table of parameters.

Symbol	Unit	Description
q_{in}	m3/s	Inflow rate
q_{ex}	m3/s	Outflow rate
k_d	1/d	Decay rate
$s_{DO,Z}$	g/g	Stoichiometry (O2/Z)
h_{DO}	g/m3	Half-saturation O2
T	degC	Temperature
W	m/s	Wind speed
D	m	Water depth

Table 3: Table of functions.

Symbol	Unit	Description
$O2_{sat}$	mg/l	O2 saturation, f(temp)
k_a	1/d	Aeration, f(wind, depth)
$monod$	-	Monod model
$c_{Z,in}$	g/m3	Z in inflow, f(time)
$c_{DO,in}$	g/m3	O2 in inflow, f(time)

2 Simulated processes

The simulated processes are summarized in Table 4. For models with lengthy math expressions, it may be necessary to rotate this table, e. g. using `\sidewaystable` from the `rotfloat` package. Another options is to restrict the width of the table's last colum using the `width` and `align` arguments of `exportDF`.

Table 4: Table of processes.

Name	**Unit**	**Description**	**Process rate expression**
flow	m3/s	Water balance	$q_{in} - q_{ex}$
flushing	1/s	Flushing rate	q_{in}/v
decay	g/m3/s	Decay of z	$k_d \cdot c_Z \cdot monod(c_{DO}, h_{DO})$
aeration	g/m3/s	O2-exchange	$k_a(W, D) \cdot (O2_{sat}(T) - c_{DO})$

3 Stoichiometry

The link between state variables and processes is determined by the stoichiometry information. It can be presented in tabular form (Table 5), as a numeric matrix (Table 6), or as a quasi-figure (Fig. 1).

Table 5: Stoichiometry in tabular form.

Variable	**Process**	**Stoichiometry factor**
v	flow	1
c_Z	flushing	$c_{Z,in}(time) - c_Z$
c_Z	decay	-1
c_{DO}	flushing	$c_{DO,in}(time) - c_{DO}$
c_{DO}	decay	$-s_{DO,Z}$
c_{DO}	aeration	1

In order to populate the matrix with numeric data, we need to

1. assign values to parameters,
2. assign values to the state variables,
3. define any functions (in R code).

Table 6: Stoichiometry matrix for given variable values, parameters, and functions.

Process	c_{DO}	c_Z	v
flow	0	0	1
flushing	0	−1	0
decay	−2.76	−1	0
aeration	1	0	0

Process	c_{DO}	c_Z	v
flow			▲
flushing		▼	
decay	▼	▼	
aeration	▲		

Figure 1: Same information as in Tab. 6 but the sign of the stoichiometry factors is represented by triangles (▲: positive, ▼: negative). Empty cells denote missing (direct) interactions.