CWM1: a general model to describe biokinetic processes in subsurface flow constructed wetlands

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ABSTRACT

This paper presents the Constructed Wetland Model No1 (CWM1), a general model to describe biochemical transformation and degradation processes for organic matter, nitrogen and sulphur in subsurface flow constructed wetlands. The main objective of CWM1 is to predict effluent concentrations from constructed wetlands without predicting gaseous emissions. CWM1 describes aerobic, anoxic and anaerobic processes and is therefore applicable to both horizontal and vertical flow systems. 17 processes and 16 components (8 soluble and 8 particulate) are considered. CWM1 is based on the mathematical formulation as introduced by the IWA Activated Sludge Models (ASMs). It is important to note that besides the biokinetic model a number of other processes including porous media hydrodynamics, the influence of plants, the transport of particles/suspended matter to describe clogging processes, adsorption and desorption processes and physical re-aeration must be considered for the formulation of a full model for constructed wetlands

Key words | constructed wetlands, CWM1, mechanistic model, numerical simulation, subsurface flow

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INTRODUCTION

During the last few years, several models of varying complexity have been developed to describe the great variety of degradation and removal processes in subsurface flow constructed wetlands (CWs) (Langergraber 2008). These models couple hydrodynamic models for either variably saturated or saturated flow in the subsurface with reaction models. Horizontal flow (HF) systems can be simulated when only water flow saturated conditions are considered. Currently, the most advanced models using saturated water flow hydraulics are the one developed by

Rousseau (2005) and Brovelli *et al.* (2007). Both consider biokinetic models that are based on the IWA Activated Sludge Models (ASMs) (Henze *et al.* 2000). For modelling vertical flow (VF) CWs with intermittent loading, transient variably-saturated flow models are required. Due to the intermittent loading, these systems are highly dynamic, adding to the complexity of the overall system. Currently, the most advanced reaction models are implemented in CW2D (Langergraber 2001; Langergraber & Šimůnek 2005), in FITOVERT (Giraldi *et al.* 2008), both based on the

mathematical formulation of the ASMs (Henze et al. 2000); and in the model developed by Ojeda et al. (2008), that considers processes affecting solids, organic matter, nitrogen and sulphur.

Ojeda's model was developed primarily for HF CWs but, because of the underlying flow model, it is also capable of simulating VF CWs.

The aim of this paper is to present a general biokinetic model to describe biochemical transformation and degradation processes for organic matter and nitrogen in subsurface flow CWs. The Constructed Wetland Model No1 (CWM1) considers the biokinetic processes in HF and VF CWs we consider relevant with the main objective to predict effluent concentrations. In HF CWs, anaerobic processes play a major role. Therefore, the inclusion of anaerobic processes had to be considered.

Langergraber et al. (2008) reviewed and discussed the pros and cons of different model formulations for the description of anaerobic processes in CWs (Rousseau 2005; Mena 2008; Ojeda et al. 2008). Rousseau (2005) used a complex anaerobic reaction model and a simple hydraulic model consisting of a network of completely stirred tank reactors. On the contrary, Ojeda et al. (2008) used a simple anaerobic reaction model in a complex mechanistic hydraulic model. Mena (2008) presented a simplification of Rousseau's anaerobic reaction model as an extension of CW2D (Langergraber 2001). This discussion of Langergraber et al. (2008) formed the basis for the formulation of CWM1.

In terms of notation and structure of the paper, CWM1 is described in a way similar to the presentation of the ASMs (Henze et al. 2000). As with Henze's presentation of the ASMs, the objective of CWM1 is to provide a widely accepted model formulation for biochemical transformation and degradation processes in constructed wetlands that can then be implemented in various simulation tools.

CWM1: DEFINITION OF COMPONENTS IN THE MODEL

As in the ASMs concentrations of soluble components are characterized by $S_?$ and particulate components by $X_?$. All microorganisms are considered particulate components and are referred to as bacteria only. Organic nitrogen is considered as a fraction of organic matter (COD). In CWM1 16 components (8 soluble and 8 particulate components) are considered:

Definition of soluble components, $S_?$

1. S_O [M(O_2) L^{-3}]: *Dissolved oxygen*, O_2. Dissolved oxygen can be directly measured and is subject to gas exchange.

2. S_F [M(COD) L^{-3}]: *Fermentable, readily biodegradable soluble COD*. This fraction of the COD is directly available for biodegradation by heterotrophic and fermenting bacteria and is produced from hydrolysis.

3. S_A [M(COD) L^{-3}]: *Fermentation products as acetate*. For simplicity reasons all fermentation products are assumed to be acetate only. Consumption of S_A occurs by aerobic and anoxic growth of heterotrophic bacteria as well as anaerobic growths of acetotrophic bacteria.

4. S_I [M(COD) L^{-3}]: *Inert soluble COD*. S_I can not be further degraded in the CW treatment process. It is assumed to be part of the influent organic matter and can be produced from hydrolysis.

5. S_{NH} [M(N) L^{-3}]: *Ammonium and ammonia nitrogen* (NH_4^+-N and NH_3-N). S_{NH} is assumed to be all NH_4^+-N. As organic nitrogen is modelled as fraction of the COD, S_{NH} is produced by degradation of organic matter. S_{NH} is transformed by nitrification and can be assimilated during biomass growth.

6. S_{NO} [M(N) L^{-3}]: *Nitrate and nitrite nitrogen* (No_3^--N and NO_2^--N). S_{NO} is assumed to include all nitrite and nitrate nitrogen since nitrite is not included as separate model component. For stoichiometric calculations, S_{NO} is considered to be NO_3^--N only. S_{NO} is produced from nitrification and consumed by denitrification and anoxic sulphide oxidation.

7. S_{SO4} [M(S) L^{-3}]: *Sulphate sulphur*. S_{SO4} is expressed as sulphur. Sulphate reducing bacteria use S_{SO4} as an

electron acceptor for oxidation of S_A. S_{SO4} is produced from aerobic and anoxic sulphide oxidation.

8. S_{H2S} [M(S) L^{-3}]: *Dihydrogensulphide sulphur*. S_{H2S} is expressed as sulphur and is subject to gas exchange. It is produced by reduction of S_{SO4} as described in component 7 and is converted back to S_{SO4} by sulphide oxidisers such as *Thiobacillus*. At higher concentrations S_{H2S} can be toxic for microorganisms.

Definition of particulate components, $X_?$

9. X_S [M(COD) L^{-3}]: *Slowly biodegradable particulate COD*. X_S represents organic substances which have to undergo cell external hydrolysis before they are available for degradation. When bacteria die, the biodegradable parts of their cells are added to the amount of X_S. X_S losses occur through hydrolysis by heterotrophic bacteria.

10. X_I [M(COD) L^{-3}]: *Inert particulate COD*. This part of the particulate organic material is not degraded in the system of interest. X_I is assumed to remain in the pore space unless higher flow rates exert enough shear stress to drag along solids.

11. X_H [M(COD) L^{-3}]: *Heterotrophic bacteria*. These are assumed to be the 'allrounder' heterotrophic organisms being responsible for hydrolysis, mineralization of organic matter (aerobic growth) and denitrification (anoxic growth).

12. X_A [M(COD) L^{-3}]: *Autotrophic nitrifying bacteria*. Nitrifying organisms are responsible for nitrification. It is assumed that S_{NH} is directly nitrified to S_{NO}. Nitrite, as an intermediate product of nitrification, is not considered.

13. X_{FB} [M(COD) L^{-3}]: *Fermenting bacteria*. Under anaerobic conditions fermenting bacteria consume fermentable, readily biodegradable soluble COD s_F and produce acetate S_A.

14. X_{AMB} [M(COD) L^{-3}]: *Acetotrophic methanogenic bacteria*. Acetotrophic methanogenic bacteria grow in anaerobic conditions, consume acetate S_A and produce methane (which is not considered as a model component).

15. X_{ASRB} [M(COD) L^{-3}]: *Acetotrophic sulphate reducing bacteria*. Sulphate reducing bacteria use S_{SO4} as an electron acceptor for oxidation of acetate S_A and produce S_{H2S}.

16. X_{SOB} [M(COD) L^{-3}]: *Sulphide oxidising bacteria*. Sulphur oxidising bacteria are chemoautotrophic organisms that use oxygen S_O or nitrate S_{NO} to oxidise sulphide S_{H2S} to sulphate S_{SO4}.

CWM1: DEFINITION OF PROCESSES IN THE MODEL

CWM1 considers the following 17 biochemical transformation and degradation processes:

1. *Hydrolysis*: Hydrolysis describes the conversion of slowly biodegradable organic matter X_S into readily biodegradable organic matter S_F, with a small fraction being converted into inert organic matter S_I. Ammonium S_{NH4} is released during this transformation process. We further assume that hydrolysis does not take place under direct dependence of the oxygen conditions. Hydrolysis is performed by heterotrophic and fermenting bacteria whereby hydrolysis by fermenting bacteria is assumed to be slower. This considered by the factor η_H.

2. *Aerobic growth of X_H on S_F*: Heterotrophic growth rates are dependent on substrate and ammonium availability as well as on electron acceptor concentrations (either oxygen or nitrate). Aerobic growth of heterotrophic bacteria X_H on readily biodegradable organic matter S_F (mineralization of organic matter) consumes oxygen S_O, while ammonium S_{NH4} is incorporated in the biomass.

3. *Aerobic growth of X_H on S_A*. This process is similar to the previous one and consumes oxygen S_O and acetate S_A, while ammonium S_{NH4} is incorporated in the biomass.

4. *Anoxic growth of X_H on S_F*: Anoxic growth of heterotrophs (denitrification) consumes nitrate S_{NO} and readily biodegradable organic matter S_F. Again, ammonium S_{NH4} is incorporated in the biomass.

5. *Anoxic growth of X_H on S_A*: As for aerobic growth, denitrifiers can also use acetate as substrate. This

process consumes nitrate S_{NO} and acetate S_A. Ammonium S_{NH4} is incorporated in the biomass.

6. *Lysis of X_H*: Lysis is assumed to represent the sum of all decay and sink processes for bacteria and is described similarly for all types of bacteria. Lysis of heterotrophic bacteria X_H produces organic matter (mainly slowly biodegradable particulate organic matter X_S, and small fractions of inert particulate organic matter X_I and readily biodegradable organic matter S_F) and ammonium S_{NH4}.

7. *Aerobic growth of X_A on S_{NH}*: Aerobic growth of nitrifying bacteria X_A (nitrification) consumes ammonia S_{NH4} and oxygen S_O, and produces nitrate S_{NO}. Additionally, a small portion of S_{NH4} is incorporated in the biomass.

8. *Lysis of X_A*: Lysis of X_A is described in the same way as process 6 (Lysis of X_H).

9. *Growth of X_{FB}*: Growth of fermenting bacteria X_{FB} under anaerobic conditions consumes readily biodegradable organic matter S_F and results in the production of acetate S_A. Again, ammonium S_{NH4} is incorporated in the biomass.

10. *Lysis of X_{FB}*: Lysis of X_{FB} is described in the same way as process 6.

11. *Growth of X_{AMB}*: Anaerobically growing acetotrophic, methanogenic bacteria X_{AMB} consume acetate S_A and incorporate S_{NH4} in the biomass.

12. *Lysis of X_{AMB}*: Lysis of X_{AMB} is described in the same way as process 6.

13. *Growth of X_{ASRB}*: Anaerobic growth of acetotrophic, sulphate reducing bacteria X_{ASRB} uses sulphate S_{SO4} as an electron acceptor for oxidation of acetate S_A.

This process produces sulphide S_{H2S} and, again, ammonia S_{NH4} is incorporated in the biomass.

14. *Lysis of X_{ASRB}*: Lysis of X_{ASRB} is described in the same way as process 6.

15. *Aerobic growth of X_{SOB} on S_{H2S}*: The opposite process to process 13, the oxidation of S_{H2S} to S_{SO4}, was also included in the model. This can occur either under aerobic or anoxic conditions. Aerobic growth of sulphide oxidizing bacteria X_{SOB} consumes oxygen S_O and sulphide S_{H2S} and produces sulphate S_{SO4}, whereas ammonia S_{NH4} is incorporated in the biomass.

16. *Anoxic growth of X_{SOB} on S_{H2S}*: Similar to the previous process, anoxic growth of sulphide oxidizing bacteria X_{SOB} consumes sulphide S_{H2S} and nitrate S_{NO} rather than oxygen S_O to produce sulphate S_{SO4}. As with the previous process ammonia S_{NH4} is incorporated in the biomass.

17. *Lysis of X_{SOB}*: Lysis of X_{SOB} is described in the same way as process 6.

CWM1: STOICHIOMETRY AND KINETICS

The CWM1 stoichiometric matrix is presented in Table 1 and the CWM1 process rates are defined in Table 2. The kinetic parameters used in Tables 1 and 2 are defined in Table 3, whereas the stoichiometric and composition parameters are defined in Table 4.

The presentation of the CWM1 stoichiometric matrix Table 1 is based on the IWA ASM mathematical formulation (Henze *et al.* 2000). Blank fields in the stoichiometric matrix indicate that a process does not influence the concentration of a respective component. The stoichiometric factors $v_{5,j}$ for ammonia S_{NH4} calculated from mass balances over each process are as follows:

$$v_{5,1} = i_{N,XS} - (1 - f_{HYD,SI}) \times i_{N,SF} - f_{HYD,SI} \times i_{N,SI}$$

$$v_{5,2} = v_{5,3} = i_{N,SF}/Y_H - i_{N,BM}$$

$$v_{5,4} = v_{5,5} = v_{5,11} = v_{5,13} = v_{5,15} = v_{5,16} = -i_{N,BM}$$

$$v_{5,6} = v_{5,8} = v_{5,10} = v_{5,12} = v_{5,14} = v_{5,17} = i_{N,BM} - f_{BM,SF} \times i_{N,SF} - (1 - f_{BM,SF} - f_{BM,XI}) \times i_{N,XS} - f_{BM,XI} \times i_{N,XI}$$

$$v_{5,7} = -i_{N,BM} - \frac{1}{Y_A}$$

$$v_{5,9} = i_{N,SF}/Y_{FB} - i_{N,BM}$$

(1)

Table 1 | CWM1 stoichiometric matrix

	$i \rightarrow$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
j	Process component expressed as $\rightarrow$	S_O	S_F	S_A	S_I	S_{NH}	S_{NO}	S_{SO4}	S_{H2S}	X_S	X_I	X_H	X_A	X_{FB}	X_{AMB}	X_{ASRB}	X_{SOB}
$\downarrow$		O_2	COD	COD	COD	N	N	S	S	COD	COD	COD	COD	COD	COD	COD	COD
1	Hydrolysis		$1-f_{Hyd,SI}$		$f_{Hyd,SI}$	$v_{5,1}$				-1							
2	Aerobic growth of X_H on S_F	$1-\frac{1}{Y_H}$	$-1/Y_H$			$v_{5,2}$						1					
3	Anoxic growth of X_H on S_F		$-1/Y_H$			$v_{5,3}$	$-\frac{1-Y_H}{2.86\cdot Y_H}$					1					
4	Aerobic growth of X_H on S_A	$1-\frac{1}{Y_H}$		$-1/Y_H$		$v_{5,4}$						1					
5	Anoxic growth of X_H on S_A			$-1/Y_H$		$v_{5,5}$	$-\frac{1-Y_H}{2.86\cdot Y_H}$					1					
6	Lysis of X_H		$f_{BM,SF}$			$v_{5,6}$				$v_{9,Lysis}$	$f_{BM,XI}$	-1					
7	Aerobic growth of X_A on S_{NH}	$-\frac{4.57-Y_A}{Y_A}$				$-i_{N,BM}-\frac{1}{Y_A}$	$1/Y_A$						1				
8	Lysis of X_A		$f_{BM,SF}$			$v_{5,8}$				$v_{9,Lysis}$	$f_{BM,XI}$		-1				
9	Growth of X_{FB}		$-1/Y_{FB}$	$\frac{1-Y_{FB}}{Y_{FB}}$		$v_{5,9}$								1			
10	Lysis of X_{FB}		$f_{BM,SF}$			$v_{5,10}$				$v_{9,Lysis}$	$f_{BM,XI}$			-1			
11	Growth of X_{AMB}			$-1/Y_{AMB}$		$v_{5,11}$									1		
12	Lysis of X_{AMB}		$f_{BM,SF}$			$v_{5,12}$				$v_{9,Lysis}$	$f_{BM,XI}$				-1		
13	Growth of X_{ASRB}			$-1/Y_{ASRB}$		$v_{5,13}$		$-\frac{1-Y_{ASRB}}{2\cdot Y_{ASRB}}$	$\frac{1-Y_{ASRB}}{2\cdot Y_{ASRB}}$							1	
14	Lysis of X_{ASRB}		$f_{BM,SF}$			$v_{5,14}$				$v_{9,Lysis}$	$f_{BM,XI}$					-1	
15	Aerobic growth of X_{SOB} on S_{H2S}	$-\frac{2-Y_{SOB}}{Y_{SOB}}$				$v_{5,15}$		$1/Y_{SOB}$	$-1/Y_{SOB}$								1
16	Anoxic growth of X_{SOB} on S_{H2S}					$v_{5,16}$	$-\frac{1-Y_{SOB}}{0.875\cdot Y_{SOB}}$	$1/Y_{SOB}$	$-1/Y_{SOB}$								1
17	Lysis of X_{SOB}		$f_{BM,SF}$			$v_{5,17}$				$v_{9,Lysis}$	$f_{BM,XI}$						-1

$v_{9,Lysis}=1-f_{BM,SF}-f_{BM,XI}$

Table 2 | CWM1 process rates

j	Process	Process rate ρ_j
1	Hydrolysis	$k_h \times \left[\frac{X_s/(X_H + X_{FB})}{K_X + (X_s/(X_H + X_{FB}))} \right] \times (X_H + \eta_h \times X_{FB})$
2	Aerobic growth of X_H on S_F	$\mu_H \times \left(\frac{S_F}{K_{SF} + S_F} \right) \times \left(\frac{S_F}{S_F + S_A} \right) \times \left(\frac{S_O}{K_{OH} + S_o} \right) \times \left(\frac{S_{NH}}{K_{NHH} + S_{NH}} \right) \times \left(\frac{K_{H2SH}}{K_{H2SH} + S_{H2S*}} \right) \times X_H$
3	Anoxic growth of X_H on S_F	$n_g \times \mu_H \times \left(\frac{S_F}{K_{SF} + S_F} \right) \times \left(\frac{S_F}{S_F + S_A} \right) \times \left(\frac{K_{OH}}{K_{OH} + S_o} \right) \times \left(\frac{S_{NO}}{K_{NOH} + S_{NO}} \right) \times \left(\frac{S_{NH}}{K_{NHH} + S_{NH}} \right) \times \left(\frac{K_{H2SH}}{K_{H2SH} + S_{H2S*}} \right) X_H$
4	Aerobic growth of X_H on S_A	$\mu_H \times \left(\frac{S_A}{K_{SA} + S_A} \right) \times \left(\frac{S_A}{S_F + S_A} \right) \times \left(\frac{S_O}{K_{OH} + S_o} \right) \times \left(\frac{S_{NH}}{K_{NHH} + S_{NH}} \right) \times \left(\frac{K_{H2SH}}{K_{H2SH} + S_{H2S*}} \right) \times X_H$
5	Anoxic growth of X_H on S_A	$n_g \times \mu_H \times \left(\frac{S_A}{K_{SA} + S_A} \right) \times \left(\frac{S_A}{S_F + S_A} \right) \times \left(\frac{K_{OH}}{K_{OH} + S_o} \right) \times \left(\frac{S_{NO}}{K_{NOH} + S_{NO}} \right) \times \left(\frac{S_{NH}}{K_{NHH} + S_{NH}} \right) \times \left(\frac{K_{H2SH}}{K_{H2SH} + S_{H2S*}} \right) \times X_H$
6	Lysis of X_H	$b_H \times X_H$
7	Aerobic growth of X_A on S_{NH}	$\mu_A \times \left(\frac{S_{NH}}{K_{NHA} + S_{NH}} \right) \times \left(\frac{S_O}{K_{OA} + S_o} \right) \times \left(\frac{K_{H2SA}}{K_{H2SA} + S_{H2S*}} \right) \times X_A$
8	Lysis of X_A	$b_A \times X_A$
9	Growth of X_{FB}	$\mu_{FB} \times \left(\frac{S_F}{K_{SFB} + S_F} \right) \times \left(\frac{K_{H2SFB}}{K_{H2SFB} + S_{H2S*}} \right) \times \left(\frac{K_{OFB}}{K_{OFB} + S_O} \right) \times \left(\frac{K_{NOFB}}{K_{NOFB} + S_{NO}} \right) \times \left(\frac{S_{NH}}{K_{NHFB} + S_{NH}} \right) \times X_{FB}$
10	Lysis of X_{FB}	$b_{FB} \times X_{FB}$
11	Growth of X_{AMB}	$\mu_{AMB} \times \left(\frac{S_A}{K_{SAMB} + S_A} \right) \times \left(\frac{K_{H2SAMB}}{K_{H2SAMB} + S_{H2S*}} \right) \times \left(\frac{K_{OAMB}}{K_{OAMB} + S_O} \right) \times \left(\frac{K_{NOAMB}}{K_{NOAMB} + S_{NO}} \right) \times \left(\frac{S_{NH}}{K_{NHAMB} + S_{NH}} \right) \times X_{AMB}$
12	Lysis of X_{AMB}	$b_{AMB} \times X_{AMB}$
13	Growth of X_{ASRB}	$\mu_{ASRB} \times \left(\frac{S_A}{K_{SASRB} + S_A} \right) \times \left(\frac{S_{SO4}}{K_{SOASRB} + S_{SO4}} \right) \left(\frac{K_{H2SASRB}}{K_{H2SASRB} + S_{H2S*}} \right) \times \left(\frac{K_{OASRB}}{K_{OASRB} + S_O} \right) \times \left(\frac{K_{NOASRB}}{K_{NOASRB} + S_{NO}} \right) \times \left(\frac{S_{NH}}{K_{NHASRB} + S_{NH}} \right) \times X_{ASRB}$
14	Lysis of X_{ASRB}	$b_{ASRB} \times X_{ASRB}$
15	Aerobic growth of X_{SOB} on S_{H2S}	$\mu_{SOB} \times \left(\frac{S_{H2S}}{K_{SSOB} + S_{H2S}} \right) \times \left(\frac{S_O}{K_{OSOB} + S_O} \right) \times \left(\frac{S_{NH}}{K_{NHSOB} + S_{NH}} \right) \times X_{SOB}$
16	Anoxic growth of X_{SOB} on S_{H2S}	$\mu_{SOB} \times \eta_{SOB} \times \left(\frac{S_{H2S}}{K_{SSOB} + S_{H2S}} \right) \times \left(\frac{S_{NO}}{K_{NOSOB} + S_{NO}} \right) \times \left(\frac{K_{OSOB}}{K_{OSOB} + S_O} \right) \times \left(\frac{S_{NH}}{K_{NHSOB} + S_{NH}} \right) \times X_{SOB}$
17	Lysis of X_{SOB}	$b_{SOB} \times X_{SOB}$

Such as in the IWA ASMs, the kinetic expressions of CWM1 are based on switching functions (hyperbolic of saturation terms and Monod equations, Henze *et al.* 2000). In Table 2, the CWM1 kinetic expressions for the 17 processes considered are presented. Lysis processes are modelled using first-order decay rates.

Using Tables 1 and 2, the reaction rate r_i for component i can be calculated as:

$$r_i = \sum_{j=1}^{R} v_{i,j} \times \rho_j \qquad (2)$$

where $i = 1, \ldots, N$, N = number of components (16), $j = 1, \ldots, R$, R = number of processes (17), $v_{i,j}$ is the stoichiometric factor for component i and process j (Table 1), and ρ_j is the reaction rate for process j as defined in Table 2.

CWM1: TYPICAL WASTEWATER CHARACTERISTICS, KINETIC AND STOICHIOMETRIC PARAMETERS

It is the responsibility of the user of CWM1 to determine the concentrations of the relevant components in the influent wastewater. In Tables 3 and 4, the kinetic and stoichiometric parameters, respectively, are listed and literature values for these parameters are given.

Kinetic parameters in Table 3 are given for 20°C and if relevant for 10°C. It is assumed that only rate constants express temperature dependencies with the exception being K_X, the saturation coefficient for hydrolysis, and K_{NHA}, the saturation/inhibition coefficient for S_{NH} for nitrification (Langergraber 2007). Temperature dependencies should be modelled as described by Henze *et al.* (2000).

The experience with CW2D (Langergraber & Šimůnek 2005) showed that a good match to measured quality data can be obtained if the hydraulic behaviour of the CW is

Table 3 | Kinetic parameters (at 20℃, values in brackets at 10℃)

Parameter	Description [unit]	Value	Reference
Hydrolysis			
K_h	Hydrolysis rate constant [1/d]	3 (2)	Henze *et al.* (2000)
K_X	Saturation/inhibition coefficient for hydrolysis [g COD_{SF}/g COD_{BM}]	0.1 (0.22)	Langergraber (2007)
η_H	Correction factor for hydrolysis by fermenting bacteria [-]	0.1	Henze *et al.* (2000)
Heterotrophic bacteria (aerobic growth and denitrification)			
μ_H	Maximum aerobic growth rate on S_F and S_A [1/d]	6 (3)	Langergraber & Šimůnek (2005)
η_g	Correction factor for denitrification by heterotrophs [-]	0.8	Henze *et al.* (2000)
b_H	Rate constant for lysis [1/d]	0.4 (0.2)	Langergraber & Šimůnek (2005)
K_{OH}	Saturation/inhibition coefficient for S_O [mg O_2/L]	0.2	Langergraber & Šimůnek (2005)
K_{SF}	Saturation/inhibition coefficient for S_F [mg COD_{SF}/L]	2	Langergraber & Šimůnek (2005)
K_{SA}	Saturation/inhibition coefficient for S_A [mg COD_{SA}/L]	4	Henze *et al.* (2000)
K_{NOH}	Saturation/inhibition coefficient for S_{NO} [mg N/L]	0.5	Henze *et al.* (2000)
K_{NHH}	Saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.05	Langergraber & Šimůnek (2005)
K_{H2SH}	Saturation/inhibition coefficient for S_{H2S} [mg S/L]	140	Rousseau (2005)
Autotrophic bacteria			
μ_A	Maximum aerobic growth rate on S_{NH} [1/d]	1 (0.35)	Henze *et al.* (2000)
b_A	Rate constant for lysis [1/d]	0.15 (0.05)	Henze *et al.* (2000)
K_{OA}	Saturation/inhibition coefficient for S_O [mg O_2/L]	1	Langergraber & Šimůnek (2005)
K_{NHA}	Saturation/inhibition coefficient for S_{NH} [mg N/L]	0.5 (5)	Langergraber (2007)
K_{H2SA}	Saturation/inhibition coefficient for S_{H2S} [mg S/L]	140	Rousseau (2005)
Fermenting bacteria			
μ_{AMB}	Maximum aerobic growth rate for X_{FB} [1/d]	3 (1.5)	Henze *et al.* (2000)
b_{AMB}	Rate constant for lysis [1/d]	0.02	Kalyuzhnyi & Fedorovich (1998)
K_{OFB}	Saturation/inhibition coefficient for S_O [mg O_2/L]	0.2	Henze *et al.* (2000)
K_{SFB}	Saturation/inhibition coefficient for S_F [mg COD_{SF}/L]	28	Kalyuzhnyi & Fedorovich (1998)
K_{NOFB}	Saturation/inhibition coefficient for S_{NO} [mg N/L]	0.5	Henze *et al.* (2000)
K_{NHFB}	Saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.01	Rousseau (2005)
K_{H2SFB}	Saturation/inhibition coefficient for S_{H2S} [mg S/L]	140	Kalyuzhnyi & Fedorovich (1998)

Table 3 | (continued)

Parameter	Description [unit]	Value	Reference
Acetotrophic methanogenic bacteria			
μ_{AMB}	Maximum aerobic growth rate on for X_{AMB} [1/d]	0.085	Kalyuzhnyi & Fedorovich (1998)
b_{AMB}	Rate constant for lysis [1/d]	0.008	Kalyuzhnyi & Fedorovich (1998)
K_{OAMB}	Saturation/inhibition coefficient for S_O [mg O_2/L]	0.0002	Rousseau (2005)
K_{SAMB}	Saturation/inhibition coefficient for S_F [mg COD_{SA}/L]	56	Kalyuzhnyi & Fedorovich (1998)
K_{NOAMB}	Saturation/inhibition coefficient for S_{NO} [mg N/L]	0.0005	Rousseau (2005)
K_{NHAMB}	Saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.01	Rousseau (2005)
K_{H2SAMB}	Saturation/inhibition coefficient for S_{H2S} [mg S/L]	140	Kalyuzhnyi & Fedorovich (1998)
Acetotrophic sulphate reducing bacteria			
μ_{ASRB}	Maximum aerobic growth rate for X_{ASRB} [1/d]	0.18	Kalyuzhnyi & Fedorovich (1998)
b_{ASRB}	Rate constant for lysis [1/d]	0.012	Kalyuzhnyi & Fedorovich (1998)
K_{OASRB}	Saturation/inhibition coefficient for S_O [mg O_2/L]	0.0002	Rousseau (2005)
K_{SASRB}	Saturation/inhibition coefficient for S_F [mg COD_{SA}/L]	24	Kalyuzhnyi & Fedorovich (1998)
K_{NOASRB}	Saturation/inhibition coefficient for S_{NO} [mg N/L]	0.0005	Rousseau (2005)
K_{NHASRB}	Saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.01	Rousseau (2005)
K_{SOASRB}	Saturation/inhibition coefficient for S_{SO4} [mg S/L]	19	Kalyuzhnyi & Fedorovich (1998)
$K_{H2SASRB}$	Saturation/inhibition coefficient for S_{H2S} [mg S/L]	140	Kalyuzhnyi & Fedorovich (1998)
Sulphide oxidising bacteria			
μ_{SOB}	Maximum aerobic growth rate for X_{SOB} [1/d]	5.28	de Wit *et al.* (1995)
b_{SOB}	Rate constant for lysis [1/d]	0.15	Rousseau (2005)
K_{OSOB}	Saturation/inhibition coefficient for S_O [mg O_2/L]	0.2	Rousseau (2005)
K_{NOSOB}	Saturation/inhibition coefficient for S_{NO} [mg N/L]	0.5	Rousseau (2005)
K_{NHSOB}	Saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.05	Rousseau (2005)
K_{SSOB}	Saturation/inhibition coefficient for S_{HsS} [mg S/L]	0.24	de Wit *et al.* (1995)

Table 4 | Stoichiometric parameters for organic matter and bacteria and composition parameters

Stoichiometric parameters			
$f_{Hyd,SI}$	Production of S_I in hydrolysis [g COD_{SI}/g COD_{XS}]	0.0	Langergraber & Šimůnek (2005)
$f_{BM,SF}$	Fraction of S_F generated in biomass lysis [g COD_{SF}/g COD_{BM}]	0.05	Langergraber & Šimůnek (2005)
$f_{BM,XI}$	Fraction of X_I generated in biomass lysis [g COD_{XI}/g COD_{BM}]	0.1	Langergraber & Šimůnek (2005)
Y_H	Yield coefficient for heterotrophic bacteria [g COD_{BM}/g COD_{SF}]	0.63	Henze *et al.* (2000)
Y_A	Yield coefficient for autotrophic bacteria [g COD_{BM}/g N]	0.24	Henze *et al.* (2000)
Y_{FB}	Yield coefficient for fermenting bacteria[g COD_{BM}/g COD_{SF}]	0.053	Kalyuzhnyi & Fedorovich (1998)
Y_{AMB}	Yield coefficient for acetotrophic methanogenic bacteria [g COD_{BM}/g COD_{SA}]	0.032	Kalyuzhnyi & Fedorovich (1998)
Y_{ASRB}	Yield coefficient for acetotrophic sulphur reducing bacteria [g COD_{BM}/g COD_{SA}]	0.05	Kalyuzhnyi & Fedorovich (1998)
Y_{SOB}	Yield coefficient for sulphide oxidizing bacteria [g COD_{BM}/g S]	0.12	de Wit *et al.* (1995)
Composition parameters			
$i_{N,SF}$	N content of S_F [g N/g COD_{SF}]	0.03	Langergraber & Šimůnek (2005)
$i_{N,SI}$	N content of S_I [g N/g COD_{SI}]	0.01	Langergraber & Šimůnek (2005)
$i_{N,XS}$	N content of X_S [g N/g COD_{XS}]	0.04	Langergraber & Šimůnek (2005)
$i_{N,XI}$	N content of X_I [g N/g COD_{XI}]	0.03	Henze *et al.* (2000)
$i_{N,BM}$	N content of biomass [g N/g COD_{BM}]	0.07	Langergraber & Šimůnek (2005)

correctly described. Then literature parameters for the biokinetic model can be used. It is assumed that this is also true for CWM1 and therefore the model parameters presented have been chosen from applications shown in the literature. No ranges of the parameters are given. While ranges can be easily found for model parameters describing aerobic and anoxic reactions (e.g. Reichert & Vanrolleghem 2001; Hulsbeek *et al.* 2002), there is a lack of information for model parameters describing anaerobic processes.

DISCUSSION

The CWM1 model formulation aims at using a minimum number of processes to predict the effluent concentrations based on the aerobic, anoxic and anaerobic processes occurring in subsurface flow systems. As it is not the aim to predict gaseous emissions methane and other gases (e.g. N_2) are not considered as a model components. Phosphorus is also not considered as microbial processes play a minor role for phosphorus transformation and removal in subsurface flow CWs. However, CWM1 assumes that there is no limitation of the processes due to a lack of phosphorus.

Aerobic and anoxic microbial processes affecting organic matter and nitrogen

The model formulations for aerobic degradation of organic matter as well as for nitrification and denitrification are derived from ASM2 (Henze *et al.* 2000). A Monod term for S_{H2S} is included for aerobic and anoxic processes to describe the toxicity effects at high S_{H2S} concentrations (Kalyuzhnyi *et al.* 1998).

Anaerobic microbial processes

Kinetics of anaerobic microbial processes (fermentation, methanogenesis and sulphate reduction) is based on the model presented by Kalyuzhnyi & Fedorovich (1998), which takes into account the competition between sulphate reducing and methanogenic bacteria. In order to reduce the number of overall processes, the following anaerobic processes are neglected:

1. *Processes with iron as electron acceptor*: Burgoon (1993) demonstrated that in subsurface flow CWs iron reduction contributes only a maximum of 0.1% and 0.2% of the total removed acetate in nitrate rich and sulphate rich environment, respectively. Therefore, it is

assumed that these processes play a minor role when treating domestic wastewater. However, they can be easily added if necessary e.g. for modeling the treatment of industrial and mining wastewaters.

2. *Processes with hydrogen as electron donor*: It is assumed that hydrogen occurs only as intermediate product and is rapidly consumed. Therefore, it is further assumed that processes with hydrogen as electron donor (SO_4 reduction with H_2, etc.) and H_2 volatilisation is not considered (Mena 2008).

Biological sulphide oxidation

Biological sulphide oxidation (that occurs under aerobic and anoxic conditions) has been reported to play a role in some CW systems (e.g. Gonzalias 2008) and is therefore included in the CWM1 model formulation. The model used is based on the formulation presented by de Wit *et al.* (1995) that was used by Rousseau (2005).

Hydrolysis and lysis of bacteria

The processes hydrolysis and lysis of bacteria are derived from the ASM2 formulations (Henze *et al.* 2000).

Other processes to be considered for a full model for CWs

As CWM1 describes only the biochemical transformation processes caused by microorganisms the authors want to point out that there are a number of other processes that have to be considered for the formulation of a full model for CWs. Previous experience has shown that the flow model describing water flow in the porous media is of utmost importance (see e.g. Langergraber 2008). Therefore it is suggested that finite element or finite difference models shall be used for describing water flow instead of tanks-in series models. The influence of plants on the treatment processes has to be modelled by taking into consideration plant growth, decay, decomposition, nutrient uptake, root oxygen release, etc. To model the transport of particles and suspended matter is a precondition to be able to describe and predict clogging processes. Further on, adsorption and desorption processes, as well as physical re-aeration, have to be considered.

SUMMARY

This paper introduces the Constructed Wetland Model No1 (CWM1) that describes the most relevant aerobic, anoxic and anaerobic biokinetic processes, occurring in HF and VF CWs, required to predict effluent concentrations of organic matter, nitrogen and sulphur. 17 processes and 16 components (8 soluble and 8 particulate) are considered. It is assumed that by using the CWM1 model formulation, it will be possible to model the effluent concentration of both HF and VF CWs. The authors hope that CWM1, such as the IWA ASMs, will become a widely accepted model formulation for biochemical transformation and degradation processes in subsurface flow constructed wetlands and will be implemented in many simulation platforms.

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