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# SIMULATION OF VERTICAL FLOW FILTERS FOR THE TREATMENT OF DOMESTIC WASTEWATER USING SAND AND ZEOLITE AS FILTER MATERIALS

Master thesis In partial fulfilment of the requirements for the degree of Diplomingenieur

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# Table of Contents

Acki Tabl List List Abst	nowled e of Co of Tabl of Figu tract	gements ntents es res		I IV V V		
Zusa Abbi	umment reviatio	assung (in Germa	n)	VI VII		
1.	Intro	duction		1		
2.	Obie	ctives		2		
3.	Fun	damentals		3		
	3.1	General remarks				
	3.2	Subsurface f	low constructed wetlands	3		
		3.2.1 Horiz	ontal flow constructed wetlands	4		
		3.2.2 Vertic	cal flow constructed wetlands	4		
		3.2.3 Two-	stage vertical flow constructed wetlands	5		
	3.3	Modeling of (	CWs	5		
	3.4	Zeolite as a f	ilter material	6		
	••••	3.4.1 Gene	eral characteristics	6		
		3.4.2 Adso	rption processes	8		
		3.4.3 Wast	ewater treatment using zeolite	8		
4.	Mate	9				
	4.1	Pilot-scale ex	periment			
	4.2	.2 The HYDRUS Wetland module				
		4.2.1 Read	tive transport model	11		
	4.3	Simulation st	udv	13		
	_	4.3.1 Gene	eral model setup	14		
		4.3.2 Flow	simulation	14		
		4.3.3 Read	tive transport simulation	15		
		4.3.4 Analy	sis of the simulation data	17		
5.	Res	ults and disc	ussion	18		
	5.1	Pilot scale ex	cperiment	18		
		5.1.1 Gene	ral remarks			
		5.1.2 Meas	ured adsorption isotherms	18		
		5.1.3 Meas	sured effluent concentrations	19		
	5.2	Water flow simulation		20		
	5.3	Reactive trar	sport simulation	22		
		5.3.1 Stead	dy state	22		
		5.3.2 Influe	nce of influent fractionation	25		
		5.3.3 Influe	nce of nitrification rate	26		
		5.3.4 Influe	nce or neterotrophic decay rate	27		
	-	5.3.5 Final	results	27		
6.	Sum	mary and co	onclusions	30		

7.	Outlook	32
9.	References	33
10.	Appendix	37
	10.1 CW2D biokinetic model	37
	10.2 R-Code	41
	10.3 Content of the DVD	46
11.	Curriculum Vitae	47
12.	Affirmation	48

# List of Tables

Table 3-1: Hydrological classification of treatment wetlands, modified from Fonder and Headly (2013)
Table 3-2: Zeolite performance for different contaminants, literature review (Widiastuti et al, 2008)
Table 4-1: Filter material of the main layer and drainage conditions in the first stage of each system (Dal Santo, 2009)         9
Table 4-2: Influent concentrations, median values, number of samples n = 13 (Dal Santo et al.,2010)
Table 4-3: Components of CW2D (Langergraber and Šimůnek, 2005)
Table 4-4: Processes implemented in CW2D (Langergraber and Šimůnek, 2012)
Table 4-5: General setup of the model domain    14
Table 4-6: Time domain settings for water flow and reactive transport simulation
Table 4-7: Time variable boundary conditions / hydraulic loading for four consecutive times 15
Table 4-8: Literature values for soil hydraulic parameters (Langergraber, 2001)       15
Table 4-9: Mean influent concentrations (Dal Santo, 2010) including COD fractions for CW2D 16
Table 5-1: Measured influent and 1st stage effluent concentrations of the three PSCW systems, number of samples $n = 13$ (Dal Santo et al., 2010)
Table 5-2: Literature- and fitted values of the soil hydraulic parameters       20
Table 5-3: Initial and fitted influent fractions of COD    25
Table 5-4: Simulated effluent concentrations bevor and after the fitting process for the sand- impounded system       28
Table 5-5: Simulated effluent concentrations bevor and after the fitting process for the zeolite- impounded system       28
Table 5-6: Simulated effluent concentrations bevor and after the fitting process for the zeolite-free drainage system
Table 10-1: Stoichiometric coefficients for ammonium nitrogen (Langergraber and Šimůnek, 2005)
Table 10-2: Stoichiometric coefficients for ammonium nitrogen (Langergraber and Šimůnek, 2005)
Table 10-3: Stoichiometric matrix of reactions in CW2D (Langergraber and Šimůnek, 2005)38
Table 10-4: Reaction rates in CW2D (Langergraber and Šimůnek, 2005)
Table 10-5: Kinetic parameters in CW2D (Langergraber and Šimůnek, 2005)
Table 10-6: Temperature dependence, stoichiometric parameters, composition parameters and parameters describing oxygen transfer in CW2D (Langergraber and Šimůnek, 2005)

# List of Figures

Figure 3-1: Cross-section of a horizontal flow constructed wetland (Wallace and Knight, 2006).4
Figure 3-2: Cross-section of a vertical flow constructed wetland (Shresta, 1999)
Figure 3-3: Two-stage vertical flow CW system (Langergraber, 2014)
Figure 3-4: Zeolite structure (Widiastui et al., 2008)7
Figure 4-1: Schematic of the two-stage PSCW VF-system (modified after Canga, 2010)9
Figure 5-1: NH4 adsorption curve with two different concentrations (Dal Santo, 2009)
Figure 5-2: Freundlich isotherm of Zeolite at 16 hours of shaking (Dal Santo, 2009)
Figure 5-3: Comparison of the COD and NH4-N effluent concentrations in the first stage of each system (1 = sand - impounded; 2 = zeolite - impounded and 3 = zeolite - free drainage) (Dal Santo et al., 2010)
Figure 5-4: Soil water retention curve for zeolite and sand using the van Genuchten model 21
Figure 5-5: Sand - impounded observed and simulated water flow
Figure 5-6: Zeolite – free drainage observed and simulated water flow
Figure 5-7: Zeolite - impounded observed and simulated water flow
Figure 5-8: Simulated COD effluent concentration for the sand-impounded system
Figure 5-9: Simulated NH <sub>4</sub> -N effluent concentration for the sand-impounded system
Figure 5-10: Simulated NO <sub>3</sub> -N effluent concentration for the sand-impounded system23
Figure 5-11: Comparison of simulation results using standard initial conditions (black) and initial conditions at the time of 4000 hours from the prior simulation (red) of the <i>sand-impounded</i> system
Figure 5-12: Simulated growth of heterotrophic bacteria (XH) in the sand-impounded system over the filter depth
Figure 5-13: Simulated growth of <i>Nitrosomonas</i> (XANs) in the sand-impounded system over the filter depth
Figure 5-14: Simulated growth of <i>Nitrobacter</i> (XANb) in the sand-impounded system over the filter depth
Figure 5-15: Results for different COD fractionations within the last 5 days of simulation
Figure 5-16: Influence of the nitrification rate on the simulated NH <sub>4</sub> -N effluent concentration within the last 5 days of simulation
Figure 5-17: Influence of the heterotrophic lysis rate on the simulated COD effluent concentration within the last 5 days of simulation

### Abstract

For the simulation of vertical flow constructed wetlands (VFCWs), the multicomponent reactive transport module CW2D implemented in the HYDRUS software is used. This biokinetic model describes the biochemical transformation and degradation process in subsurface flow CWs, including aerobic and anoxic processes. The data used for this simulation study was measured during a pilot scale experiment at the University of Natural Resources and Life Sciences, Vienna (BOKU University), monitoring three parallel operated, not planted, two-stage VF constructed filters for the treatment of domestic wastewater. Only data from the first stage of each system were used for this simulation study. The setup of each of the first stage systems were as follows, sand-impounded drainage layer, zeolite-impounded drainage layer and zeolite-free drainage layer. The measurements addressed the hydraulic flow, influent and effluent concentrations and the Freundlich adsorption isotherms for  $NH_4$ -N and  $NO_3$ -N for both filter materials. This data is used to perform a simulation study based on these three systems to underline the conclusions made based on the measured data, (i) higher NH<sub>4</sub>-N removal within the zeolite systems based on its high adsorption capacity and (ii) higher denitrification rate within the impounded systems compared to the free drainage system. The model parameters in CW2D were calibrated within the sand - impounded system. One parameter, the maximum nitrification rate was changed in the fitting process and the COD fractions (readily, slowly and inert organic matter) were determined. These settings were used for the other two systems and the adsorption isotherm for zeolite and NH<sub>4</sub>-N was implemented, using a two-site chemical non-equilibrium model. In the last step, the lysis rate of heterotrophic bacteria had to be adjusted within the zeolite-free drainage system to fit the high measured COD effluent. An overall good fit for the three systems could be achieved using the CW2D module.

## Zusammenfassung (in German)

Für diese Simulationsstudie wurde das Mehrstoff-Transportmodell CW2D, implementiert in HYDRUS, für die Simulierung von vertikal durchflossen Bodenfiltern verwendet. Dieses biokinetische Modell beschreibt die aeroben und anoxischen Abbauprozesse in unterirdisch durchflossen Bodenfiltern. Die Daten für diese Simulationsstudie wurden im Zuge eines Laborversuchs an der Universität für Bodenkultur Wien erhoben. Dabei wurden drei 2-stufige, vertikal durchflossene Bodenfilter für die Reinigung von häuslichem Abwasser untersucht. Für die Simulierung wurden nur die ersten Stufen berücksichtigt, welche sich wie folgt zusammensetzten: Sand-eingestaut, Zeolit-eingestaut und Zeolit-freie Drainage. Bei den gemessenen Daten handelt es ich um den hydraulischen Durchfluss, Zulauf- und Ablaufkonzentrationen und die Adsorptionsisotherme für NH<sub>4</sub>-N und NO<sub>3</sub>-N für beide Filtermaterialien. Mit Hilfe dieser Daten wurde eine Simulierung der drei Systeme vorgenommen, um die Ergebnisse des Laborversuchs zu unterstreichen: erstens eine höhere NH₄-N Entfernung mittels Zeolit und zweitens eine höhere Denitrifizierungsrate in den eingestauten Systemen. Die Modellparameter in CW2D wurden für das Sand-eingestaut-System kalibriert und die Fraktionierung von CSB (schnell, langsam und nicht abbaubares organisches Material) durchgeführt. Dabei wurde einzig die maximale Nitrifizierungsrate geändert. Diese Einstellungen wurden für die beiden anderen Systeme übernommen. Die Adsorption von NH<sub>4</sub>-N durch Zeolit wurde über ein chemisches non-equilibrium Modell zugefügt. Zuletzt wurde der Lysis Faktor der heterotrophen Bakterien im System Zeolitfreie Drainage eingestellt, um den simulierten an den gemessenen CSB im Ablauf anzupassen. So konnte eine gute Übereinstimmung der mit Hilfe des CW2D Modells simulierten und der gemessen Daten erreicht werden.

# Abbreviations

ASM	Activated Sludge Model	(Henze et al., 2000)
BOD	Biological oxygen demand	
CI	Inert organic matter	
COD	Chemical Oxygen Demand	
CR	Readily biodegradable organic matter	
CS	Slowly biodegradable organic matter	
CSO	Combined sewer overflow	
CW	Constructed wetland	
CW2D	Constructed Wetland 2D	(biokinetic model)
CWM1	Constructed Wetland Model N°1	(biokinetic model)
HSSF	Horizontal subsurface flow	
N	Nitrogen	
OM	Organic matter	
Р	Phosphorus	
PE	Person Equivalent	
PSCW	Pilot scale constructed wetland	
S	Sulfur	
SSF	Subsurface flow	
VF	Vertical flow	

# 1. Introduction

In the field of wastewater treatment, constructed wetlands (CWs) are a fast growing alternative to conventional intensive technical treatment technologies - for many purposes due to their simplicity of operation and reliable treatment performance without the requirement of complex infrastructure and high investment costs. According to the USEPA (2002) a septic tank combined with a sand filter is one of the most common onsite treatment systems worldwide. The range of application starts by small systems for onsite treatment of domestic wastewater in rural areas and goes on with the treatment of storm water, combined sewer overflow (CSO), industrial wastewater and landfill leachate. Within the design of CWs sand is the most common filter material. Karlsson (2015) points out that different materials used as filter media could make filter and infiltration systems more accessible and enhance removal of pollutants. Dal Santo et al. (2010) shows the different treatment performances when comparing sand and zeolite as filter media for the treatment of pre-treated domestic wastewater, while Dalahmeh et al. (2012) found that bark or charcoal show a better performance for the treatment of greywater than sand as filter material.

When it comes to the evaluation of the treatment performance of CWs in general they are still looked at as black box systems were contaminated water enters and treated water leaves the system. This thinking also reflects in the process of the systems design, where a certain amount of surface area is requested per person equivalent (PE) (ÖNORM B 2505, 2009; DWA A-A 262, 2006) or simple first-order decay models are used (Rousseau et al. 2004). Kadlec (2000) showed that such models are not suitable to deal with the complex treatment processes occurring in CWs. With the introduction of new modelling approaches trying to describe this complex and simultaneously active physical, chemical, and biological processes that mutually influence each other, a better understanding is gained and new design tools can be developed (Kadlec and Wallace, 2009; Langergraber and Šimůnek, 2012). Nowadays the rise in available computer power and advanced numerical methods make the use of more complex and therefore more sophisticated models highly appropriate. With numerical simulation insight in the functionality and dynamics of the processes, dealing with the degradation of wastewater constituents is provided and therefore models will become a cost- and time efficient alternative for physical experiments.

The usage of numerical models is now generally accepted. In a recent review of modelling CWs Meyer et al (2015) give an overview on available models and their purpose. Three categories are presented to divide the available tools in either biokinetic models, process dedicated models, and design support models. Based on the model formulation of the Activated Sludge Models (ASMs) (Henze et al., 2000), Langergraber (2001) introduced the first biokinetic model, i.e. the CW2D model formulation, Langergraber et al. (2009b) the CWM°1.() Both biokinetic models describe transformation and degradation processes within the porous filter media. These models are included in the HYDRUS Wetland module of the HYDRUS software package (Langergraber and Šimůnek, 2011, 2012). Samsó and Garcia (2013) implemented the CWM°1 in the COMSOL Multiphysics™ platform for the BIO\_PORE model. This models have been widely applied and despite to their complexity should be improved further as for scientific purposes, where the usability is key this complexity needs to be reduced. Meyer and Dittmer (2015) developed a robust and reliable model with only few parameters for the design of CSO based on complex simulations.

# 2. Objectives

To accomplish a simulation study sophisticated data from the system the simulation is addressing, is from most importance. This thesis builds up on the measurements done by Dal Santo (2009) on three parallel operating two-stage vertical flow filters. Three objectives are addressed within this thesis:

- Setup a model to simulate vertical flow constructed filters, in particular the first stage of the pilot-scale experiments by Dal Santo (2009), using sand and zeolite respectively as filter material of the main layer
- Incorporate the adsorption capacity for NH<sub>4</sub><sup>+</sup> of the filter material zeolite within the model
- Calibrate the model to fit the effluent parameters measured in the experiment for all three systems

In chapter 3, the fundamentals are described including the basics of CW technology and simulation of CWs as well as details on why zeolite is a proper filter media. The setup of a simulation study is described within chapter 4, dealing with the methods used in this thesis. Results and discussion in chapter 5 provide the detailed outcome from the simulation as well as a comparison of the simulated and measured data.

A DVD is attached to the back cover of the printed version where the simulation files are added.

The results of this work have been presented at the 6<sup>th</sup> International Symposium on Wetland Pollutant Dynamics and Control, 13<sup>th</sup> to 18<sup>th</sup> September, 2015, York, UK.

# 3. Fundamentals

# 3.1 General remarks

The focus of this master thesis lies within the simulation of subsurface flow vertical CWs with intermitted loading. The pilot scale CW (PSCW) experiments (see chapter 4.1), providing the data for this simulation study was setup using unplanted constructed treatment filters. Per definition (Kadlec and Wallace, 2009; Fonder and Headley, 2013) these unplanted systems are not a wetland as within the definition of wetlands the presence of plants is obligatory. As for this thesis when addressing the work of Dal Santo (2009) or the discussed simulation study the system is defined as a vertical flow filter for the treatment of domestic waste water.

## 3.2 Subsurface flow constructed wetlands

Vymazal and Kropfelova (2008) define CWs as an artificially created ecosystem that would not otherwise exist without significant human intervention and are generally designed to mimic many of the conditions and/or processes that occur in natural wetlands. Such systems show an optimization of the treatment performance found in nature and therefor can be considered as a sustainable environmentally friendly solution (Langergraber and Šimůnek, 2012).

In general, CWs are extensive solution for wastewater treatment. Their applications range from implementation for single households and municipal wastewater to treating agricultural wastewater, mining water and storm water runoff or water from CSO. For subsurface flow CWs, two main systems, namely horizontal flow (HF) and vertical flow (VF) are used.

Fonder and Headly (2013) are listing three categories describing the purpose of CWs, i.e.

- i. restored wetlands support a near-natural wetland ecosystem after natural wetlands were lost or heavily degraded,
- ii. created wetlands placed were no wetland previously existed and/or
- iii. treatment wetlands, artificially created to enhance and optimise physical and biochemical processes with the purpose of removing contaminants from polluted waters.

Along with this thesis the focus lies on the third categories, namely treatment wetlands, defined by Fonder and Headly (2013) as planted systems with water-logged or saturated conditions for at least part of the time with an inflow of contaminated waters with constituents that are to be removed. Table 3-1 gives a general overview on the classification of treatment wetlands.

Table 3-1: Hydrological classification of treatment wetlands, modified from Fonder and Headly (2013)

Specific trait	Description	Defined classes	Sub classes
Water position	Position of water surface relative to soil or substrate	Surface flow Subsurface flow	
Flow direction	Dominant direction of flow through the systems	Horizontal Vertical	Down; up; mixed
Saturation of media	Degree of saturation in media-based systems	Free drainage Intermittent Constant	
Influent loading	Position and type of influent distribution	Surface inflow Subsurface inflow Basal inflow	

#### 3.2.1 Horizontal flow constructed wetlands

In horizontal subsurface flow (HSSF) CWs (Figure 3-1) the wastewater is loaded at the inlet and flows mainly horizontally trough the filter media along to the outlet. Due to continuously loading the system is operating under permanent waterlogged conditions. The degradation of the wastewater constituents is done within a network of aerobic, anoxic, and anaerobic zones. The main process for nitrogen elimination is denitrification. Aerobic conditions are mainly restricted to the area near the surface where oxygen can enter the system via diffusion and the root zone. This limits the zones where nitrification can take place. Degradation of phosphorous is either low and mainly occurs due to ligand exchange reactions, where P displaces water or hydroxyls from the surface of iron and aluminium hydrous oxides (Kadlec and Wallace, 2009; Vymazal, 2010).





#### 3.2.2 Vertical flow constructed wetlands

In addition to the classification of the influent loading in Table 3-1, for VF CWs the wastewater loading generally is done intermittent, also known as pulse loading (Cooper et al., 1996), generating variably saturated conditions in the porous media. After one batch is irrigated onto the filter surface, the wastewater is pulled down through the porous media by gravity. After the loading oxygen is able to enter the unsaturated pore space again. Figure 3-2: Cross-section of a vertical flow constructed wetland (Shresta, 1999) ilustrates a generall setup of a VF system.



Figure 3-2: Cross-section of a vertical flow constructed wetland (Shresta, 1999)

Three processes can provide oxygen to the porous filter media, (i) dissolved oxygen from the wastewater and (ii) oxygen provided by plants, which both can be neglected, while (iii) direct transfer from the atmosphere by convective and dispersive fluxes is highly important. Estimations

of oxygen renewal is carried out with several methods such as, mass balance and stoichiometric calculations, gas transfer experiments or in-suit measurements. Also modelling provides a link between physical understanding, quantification and communication (Kadlec and Wallace, 2009; Tyroller et al., 2010; Petitjean et al., 2012).

This enables aerobic conditions in the system and therefore show high BOD and ammonium nitrogen removal. Anaerobic conditions are more or less unlikely and denitrification is inhibited. One possibility to achieve denitrification within a VF-system is to impound the drainage layer in order to create saturated hydraulic conditions in the lower part of the system (Canga et al., 2011; Reed et al., 2006; Vymazal, 2010; Haberl et al., 2003).

#### 3.2.3 Two-stage vertical flow constructed wetlands

A two-stage VF CW system with intermitted loading for the treatment of mechanically pre-treated wastewater was introduced by Langergraber et al. (2008) to obtain full nitrification and high nitrogen elimination rates. Along with this development also an optimization of the specific surface area required by the Austrian design standard (ÖNORM B2505, 2009) for vertical flow beds can be achieved. With a specific surface area of 2 m<sup>2</sup> per PE this system shows similar effluent concentrations and removal efficiencies like the single stage system using 4 m<sup>2</sup> per PE according to the Austrian design standards (ÖNORM B2505, 2009).

Figure 3-3 illustrates the schematic setup of the two-stage VF system. The beds of this system are operated in series whereby the first stage has an impounded drainage layer, while the second has a free flow drainage layer.



Figure 3-3: Two-stage vertical flow CW system (Langergraber, 2014)

Indoor and Outdoor experiments show that high nitrogen removal rates can be achieved by this system with up to 70%. In the first stage a high nitrification rate provides nitrate which is used for the denitrification in the impounded layer. Due to the coarser grain size of 1/4mm no complete mineralization of organic matter (OM) takes place, so enough OM is available for denitrification. Within the second stage a full nitrification and removal of OM is guaranteed. Due to the second stage, the system is very robust and overall stable effluent concentrations are achieved (Langergraber et al., 2008).

## 3.3 Modeling of CWs

The processes contributing to the treatment of wastewater in CW, namely physical, chemical and biological, interact heavily at the same time and influence each other. These complex systems

are therefore often looked at as 'black boxes'. For the design standards of treatment wetlands this means, that mostly empirical rules of thumb or first- order decay models are used. Based on fundamental laws governing water flow and solute transport first – order decay models can be useful to evaluate water flow and transport of inter solutes including the estimation of residence time, degree of mixing and hydrodynamic dispersive. However, Kadlec (2000) shows that first-order decay models are not suitable for modelling reactive and degradation processes. To establish a better insight in this 'black box' by addressing the governing biological and chemical degradation processes, and further on improve the existing design criteria, numerical modelling is and will be a strong tool. (Langergraber et al., 2009a; Langergraber, 2011).

Meyer et al. (2015) summarizes the need for CW models as follows:

- describing the phenomena on going in a CW system, namely water flow, adsorption, O2 transfer
- using models as a tool to compare two similar systems and their behaviour under different conditions
- predicting the performance of a given system
- answering "what if?" questions in terms of over and under loading, etc.
- performing system control

Langergraber (2011) lists three key factors influencing the treatment performance of CWs and how they link to modelling. A crucial part in the transformation and degradation process of wastewater constituents has the microbial community. The biomass characterization, quantitative and qualitative, is most important (Faulwetter et al., 2009). The next key factor is addressing the performance of the vegetation. The attributes of plants in SSF CWs address physical filtering by root-mats, provision of surface area for attached microbes growth, insulation by aerial tissue and litter during winter, uptake and storage of nutrients and other elements, release of oxygen and other substances by roots and the contribution of organic carbon to the substrate (Brix, 1997). Physical processes also play a large role within CWs and their modelling. Soil hydraulic properties such as porosity, hydraulic conductivity and grain size distribution influence the hydraulic efficiency and therefor can lead to good or poor treatment or model performance (Kadlec and Wallace, 2009).

These three factors not only present the wide range of processes to be included but also the different scientific fields where these processes are explained. Therefor the communication with specialists from different fields is from upmost importance that the right data for modelling is produced.

For the simulation study, the Wetland module of the HYDRUS 2D/3D software package was used. HYDRUS numerically solves variably saturated water flow and solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The solute transport equations consider convective-dispersive transport in the liquid phase, diffusion in the gaseous phase, as well as non-linear non-equilibrium reactions between the solid and liquid phases. Version 2 of the HYDRUS wetland module includes two biokinetic model formulations simulating reactive transport in CWs: CW2D and CWM1 (Langergraber, 2001; Langergraber et al., 2009b). The multicomponent reactive transport module CW2D describing the biochemical transformation and degradation process in subsurface flow constructed wetlands or filters is used in this work. This module is mainly developed for vertical flow systems and dealing only with aerobic and anoxic transformation and degradation processes.

### 3.4 Zeolite as a filter material

#### 3.4.1 General characteristics

Since the original discovery of zeolitic minerals in a volcanogenic sedimentary rock, zeolitic tuffs have been found in many areas of the world. In the past decades, natural zeolites have found a

variety of applications in adsorption, catalysis, building industry, agriculture and soil remediation (Bish and Ming, 2001; Tsitsishvili and Andronikashvili, 1992).

Yukselen-Aksoy (2010) presents five types of natural zeolites, which are of commercial interest due to their occurrence in sufficient quantity and purity:

- Clinoptilolite
- Erionite
- Chabazite
- Mordenite
- Phillipsite

Among these zeolites, clinoptilolite is the most abundant natural zeolite and is widely used in the world. It also shows a high affinity to ammonia ions, making it highly suitable for the treatment of wastewater

Natural zeolites occur in different geological settings. Generally, they form where volcanic rocks and ash layers react with alkaline ground-, lake-, or seawater. Natural deposits occur generally at or close to the surface. Zeolites are crystalline hydrated aluminosilicates of alkali and alkaline earth elements and are accounted to the family of microporous solids known as "molecular sievs". This expression has its origin in the structure of zeolites and the size of the voids, which is smaller than two nm. The structure provides cages and tunnels that can loosely hold water molecules and are adequate for adsorbing molecules smaller than these channels/tunnels. The physiochemical properties defining zeolite are cation exchange, molecular sieve, catalysis and sorption. (Cheetham and Day, 1992; Jacobs and Förstner, 1999; Wang and Peng, 2010).

The framework of zeolite consists of symmetrically stacked alumina and silica tetrahedra creating an open and stable three dimensional honeycomb structure lined together by oxygen atoms (Figure 3-4). This linkage generates rings and cages consisting of chain- or layer-like units defined as second building units (SBUs). Variations in the composition of this structure results in different forms of zeolite, which can be classified by the 16 different ways SBUs, can be linked. Within this honeycomb structure exists a negative charge. This charge is neutralized by positive charged ions such as sodium. These cations are exchangeable with cations in solution such as heavy metals or ammonium ions. This ion-exchange behaviour of natural zeolite depends on several factors, including the framework structure, ion size and shape, charge density of the anionic framework, ionic charge and concentration of the external electrolyte solution (Curkovic et al., 1997; Barrer, 1987; Feng, 1991; Liu and Lu, 2001).

The general chemical formula of zeolite can be written as:

$$M_{x/n} \left[ A l_x S i_y O_{(x+y)} \right] \cdot p H_2 O$$

(3-1)

where M is (Na, K, Li) and/or (Ca, Mg, Ba, Sr), n is cation charge; y/x = 1-6, p/x = 1-4.





#### 3.4.2 Adsorption processes

Water in the channels of natural zeolite make up 10 to 25% of their weight. The dehydrated, void space within the zeolite molecules give an important understanding to its physical and chemical properties. In terms of adsorption the percentage of removed water due to heating up to 100°C under vacuum give a good first measure of the adsorptive capacity since the free void space is now available to take up other molecules (Kesuraoui-Ouki et al., 1994)

Two adsorption processes can be addressed when zeolite is used, physical-, and chemical adsorption respectively. The second process is ion-exchange in the in the filter media. The ion-exchange capacity is basically a function of the degree of substitutes of aluminium for silicon in the framework structure (3-1). The negative charge is created by substitution of Al<sup>3+</sup> for Si<sup>4+</sup> in the tetrahedral. Physical adsorption occurs when dissolved contaminants in the water adhere and become immobilized onto the surface of zeolite particles without disrupting the atomic structure, (Liu and Lu, 2001).

Different methods are known for regeneration when the maximum exchange capacity of zeolite is reached, which mainly results in high costs (Liu and Lu, 2001). Jung et al. (1999) showed the influence of the biofilm within a sequence batch reactor when the exchange capacity was reached. Autotrophic nitrifying bacteria oxidise the exchanged ammonium suggesting that NH<sup>4+</sup> is released back into the liquid phase for nitrification.

#### 3.4.3 Wastewater treatment using zeolite

Natural zeolites have the ability to treat wastewater due its capability of performing ion exchange and adsorption. It is possible to modify natural zeolites and so trap specific contaminants (Widiastuti et al, 2008). Table 3-2 shows a literature review on the research of zeolite performance for different contaminants (Widiastuti et al, 2008).

Liu and Lo (2001) point out several advantages when using zeolite for the treatment of wastewater such as, increase in  $NH_4^+$  uptake, a satisfying removal rate even at low temperatures, low costs compared to other highly absorbent materials and a relative small size of the system.

Contaminants	Zeolite performance
NH4+ in water and wastewater using natural zeolite from many countries	30–98% removal depending upon the type of zeolite used, contact time, initial concentration, temperature, and amount of zeolite loading and particle size
Cs+, from the discharge water of nuclear power plants in the Trans Carpathian area of Ukraine	80–100% removed in static batch processes and 40–80% in dynamic flow-through column systems
Mn2+ from drinking water	67% more reduced by K-clinoptilolite from northern Romania
Hg2	Nearly 50% Hg2+ removed using Na-clinoptilolite and heulandite
Metals such as Cd, Cr, Cu, Fe, Mn, Ni, Pb, and Zn from the composting process in Psittallia, Athens	0–100% removed using natural zeolite
P034-	90% removed using cetylpyridinium-modified-zeolite with 80 meq/100 g dosage of cethylpyridinium chloride and pH 10 at initial phosphate concentration of 10 mg/L.
Arsenate from the simulated leachate	95% removed at all concentrations tested.
Total coliforms, faecal coliform and faecal streptococci	100% removed at the tenth day for faecal coliform and seventeen days for faecal streptococci at particle size between 0.5 mm and 2.0 mm using natural phillipsite columns in a percolation reactor at a constant solution flow rate
COD and BOD	75% COD retention at the twentyfifth day and 100% BOD in the ninth day using natural phillipsite columns in a percolation reactor at a constant solution flow rate
E. coli and bacteriophage MS2	100% removed using HDTMA-modified zeolite, particularly clinoptilolite rich tuff from the St. Cloud, New Mexico.
<i>E. coli</i> from drinking water	100% removed by clinotsid, a modified clinoptilolite with amine groups-polyhexamethylene guanidine chloride (PHMG) linked with epichorohydrine, (Coli index <3) depending upon the filtration flow rate and the particle size of the organozeolite

# 4. Material and methods

### 4.1 Pilot-scale experiment

The data used for this simulation study was gained during a long-term pilot scale experiment run at the technical lab of the Institute of Sanitary Engineering at the University of Natural Resources and Life Science Vienna (BOKU University) and are described in detail in the master thesis of Dal Santo (2009). The aim of this study was to evaluate the performance of zeolite as a filter material within a two-stage vertical flow filter with intermittent loading for the treatment of domestic. Three Systems were operated at the same time using different filter materials and drainage setups. Figure 4-1 illustrates the general experimental setup of the two-stage PSCW systems.



Figure 4-1: Schematic of the two-stage PSCW VF-system (modified after Canga, 2010)

Every stage consists of a surface area of 1m<sup>2</sup>, with a main layer of 50 cm depth containing the filter material listed in Table 4-1, an intermitted sand layer 4-8 mm and a drainage layer (16-32 mm). The systems were loaded every three hours, with an amount of 15 L.m<sup>-2</sup>, using mechanical pre-treated domestic wastewater gathered from the University building and surrounding buildings. The wastewater composition is shown in Table 4-2.

Table 4-1: Filter material of the main layer and drainage conditions in the first stage of each system (Dal Santo, 2009)

	Stage 1	Stage 2	Drainage
System 1	Sand 1-4mm	Sand 0-4mm	Impounded
System 2	Zeolite 2-5mm	Sand 0-4mm	Impounded
System 3	Zeolite 2-5mm	Sand 0-4mm	Free

Table 4-2: Influent concentrations, median values, number of samples n = 13 (Dal Santo et al., 2010)

Parameter	COD	NH₄-N	NO <sub>2</sub> -N	NO <sub>3</sub> -N
Unit	[mg.L <sup>-1</sup> ]	[mg.L <sup>-1</sup> ]	[mg.L <sup>-1</sup> ]	[mg.L <sup>-1</sup> ]
Influent	394	93	0,008	0,59

During an observation period of 5-month, hydraulic measurement were carried out to determine the volumetric effluent flow rate in between two consecutive loadings. The wastewater sampling of the influent and effluent of each stage were carried out every week at the peak of the effluent flow.

The analysis was carried out in the laboratory of the Institute of Sanitary Engineering at BOKU University, according to DIN methods whereas Dr. LANGE cuvette test were used for  $NO_3$ -N (Dal Santo et al., 2010).

In the study of Dal Santo (2009) the main objective was on the determination of the COD and nitrogen parameters ( $NH_4$ -N,  $NO_3$ -N and  $NO_2$ -N) effluent concentrations for the three systems of . A second objective was to show the difference in the treatment performance for nitrification when using sand and zeolite respectively as filter material (system 1 and system 2) and for denitrification when comparing an impounded system to a system with free drainage (system 2 and system 3).

The third objective was to measure the adsorption properties of zeolite and sand for  $NH_4$ -N and  $NO_3$ -N. The adsorption isotherms were determined with batch test (described in detail by Dal Santo, 2009).

The results led to a Freundlich absorption isotherm (4-1)(4-1) with defined values for  $k_{1,F}$  and  $k_{2,F}$ ,

$$S_i = k_{1,F} \cdot c_i^{k_{2,F}}$$
(4-1)

where  $s_i$  = concentration of component i in the solid phase [mg<sub>i</sub>.kg<sub>s</sub><sup>-1</sup>]  $c_i$  = concentration of component I in the aqueous phase [mg<sub>i</sub>.dm<sup>-3</sup><sub>w</sub>],  $k_{1,F}$  = Freundlich coefficient and  $k_{2,F}$  = Freundlich exponent.

## 4.2 The HYDRUS Wetland module

For the simulation study HYDRUS 2D/3D is used. This software package is capable to simulate water, heat and solute movement in two- and three- dimensional variably saturated porous media. HYDRUS therefore numerically solves the Richards equation (equation 4-2) for saturated-unsaturated water flow and the convection-dispersion equation for heat and solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The heat transport equations consider stransport due to conduction and convection with flowing water. The solute transport equations consider convective-disperspersive transport in the liquid phase, as well as diffusion in the gaseous phase. The transport equations also include provisions for non-linear non equilibrium reactions between the solid and liquid phases, linear equilibrium reactions between the liquid and gaseous phases, zero-order production, and two first-order degradation reactions (Šimůnek et.at, 2012).

The governing equation for the water flow is the Richards equation (4-2), for variably saturated rigid porous media. It is valid under the assumption that the air phase plays an insignificant role in the liquid flow (Šimůnek et al., 2012):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i} \left[ K \left( K K_{ij}^A \frac{\partial h}{\partial x_j} + K_{iz}^A \right) \right] - S$$
(4-2)

where, L = length unit after preference, T = time unit after preference,  $\Theta =$  volumetric water content [L<sup>3</sup>.L<sup>-3</sup>], h = pressure head [L], S = sink term [T<sup>-1</sup>],  $x_i =$  spatial coordinates [L], t = time [T],  $K^{A_{ij}} =$  components of a dimensionless anisotropy tensor  $K^A$  to account for an anisotropic medium, K = unsaturated hydraulic conductivity function [L.T<sup>-1</sup>].

For the simulation of the water flow regime, HYDRUS offers a variety of soil hydraulic models and is able to deal with high dynamic flow conditions which occur in subsurface flow CWs with intermitted loading. A comparison of simulation results for different hydraulic models was done by Langergraber (2001). To gain a good description of water flow and further on the transport of the wastewater constituents and their degradation in the unsaturated porous media the soil hydraulic parameters are from most importance (Langergraber and Šimůnek, 2012). In HYDRUS, one can choose between several soil hydraulic models, e.g. the van Genuchten-Mualem model, the Brooks-Corey model or the Kosugi model (Šimůnek et al., 2012). For this study the van Genuchten model with no hysteresis is chosen where the volumetric water content  $\Theta(h)$  and the unsaturated hydraulic conductivity K(h) are defined as:

$$\theta(h) = \begin{cases} \theta_r + \frac{\theta_s - \theta_r}{[1 + |\alpha \cdot h|^n]^m} & h < 0 \\ \\ \theta_s & h \ge 0 \end{cases}$$

$$(4-3)$$

$$K(h) = K_{S} \cdot S_{e}^{l} \cdot \left[1 - (1 - S_{e}^{\frac{1}{m}})^{m}\right]^{2}$$
(4-4)

The parameters used are  $\Theta_r$  as the residual and  $\Theta_s$  as the saturated water content [L<sup>3</sup>.L<sup>-3</sup>],  $K_s$  defining the saturated hydraulic conductivity [L<sup>3</sup><sub>w</sub>.(L<sup>2</sup><sub>s</sub>.h)<sup>-1</sup>], the empirical parameters  $\alpha$  [L<sub>s</sub><sup>-1</sup>] and n [-] influence the shape of the functions  $\Theta(h)$  and K(h) and I [-] defined as the pore-connectivity parameter.  $S_e$  equals the effective water content as shown in equation (4-4) and m is defined as m = 1-1/n where n > 1. L = length unit after preference.

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \tag{4-5}$$

HYDRUS is capable of performing an inverse simulation to estimate the soil hydraulic parameters within the soil hydraulic model, i.e the van Genuchten model. The Marquardt-Levenberg type parameter estimation technique is used to fit the chosen soil hydraulic parameters based on the inflow of the system and the measured effluent flow, cumulative- or boundary flux respectively.

For the macroscopic transport of components in the system the following equation is used (Langergraber and Šimůnek, 2005):

$$\frac{\partial \theta c_i}{\partial t} + \frac{\partial \rho S_i}{\partial t} = \nabla(\theta \boldsymbol{D}_i \nabla c_i) - \nabla(\boldsymbol{q} \nabla c_i) + S c_{s,i} + r_i$$
(4-6)

where, M = mass unit after preference, *i* = 1,...N (N being the number of components,  $c_i$  = concentration in the aqueous phase [M.L<sup>-3</sup>],  $s_i$  = conc. In the solid phase [M.M<sup>-1</sup>],  $\Theta$  = volumetric water content [L<sup>3</sup>.L<sup>-3</sup>],  $\rho$  = soil bulk density [M.L<sup>-3</sup>],  $D_i$  = effective dispersion tensor [L<sup>2</sup>], q = volumetric flux density [L<sup>3</sup>.L<sup>-2</sup> T<sup>-1</sup>], S = source-sink term [L<sup>3</sup>.L<sup>-3</sup> T<sup>-1</sup>],  $c_{s,i}$  = conc. of source-sink [M.L<sup>-3</sup>],  $r_i$  = reaction term [M.L<sup>-3</sup>T].

#### 4.2.1 Reactive transport model

To tackle the challenge of simulating the biochemical transformation and degradation processes in subsurface flow constructed wetlands two model formulation are available within the wetland module. The Constructed wetland Model N°1 (CWM1) (Langergraber et al., 2009b) and the Constructed wetland 2D model (CW2D) (Langergraber and Šimůnek 2005).

Langergraber and Šimůnek (2012) describe the required sub-models for the simulation of a SSF CW:

- The water flow model, describing water flow in the porous media is of utmost importance.
- The transport model, describing transport of constituents, as well as adsorption and desorption processes.
- The biokinetic model, describing biochemical transformation and degradation processes.
- The plant model, describing processes such as growth, decay, decomposition, nutrient uptake, and root O2 release.
- The clogging model, describing clogging processes, i.e., transport and deposition of suspended particulate matter and bacterial and plant growth that may reduce the hydraulic capacity or conductivity of the filter medium.

A sub-model for the process of clogging is not available in HYDRUS and the wetland module. Therefore the processes of transport and deposition of suspended particulate matter and it's impact on the hydraulic conductivity would be needed, as well as a look at the growth of the biofilm and it's hydraulic impact on the porous media. In terms of wetland plants, the nutrient uptake and  $O_2$  release is well described but HYDRUS is not able to simulate the growth, decay or deposition of plants. (Langergraber and Šimůnek, 2012).

The general properties of these two biokinetic models are well described by Langergraber and Šimůnek (2012). For both models it is assumed that all components are soluble except bacteria which are also immobile and organic N and organic P are modelled as part of COD. Furthermore, no direct conversation between CW2D and CWM1 is possible.

- CW2D was mainly developed for the modelling of VF system and therefor only includes aerobic and anoxic transformation and degradation processes which are described for the main waste water constituents organic matter, N and P.
- CWM1 was developed mainly as general model to describe biochemical transformation and degradation process for organic matter, N and S in HF and VF CWs and describes all relevant aerobic, anoxic and anaerobic biokinetic processes occurring in these systems to predict effluent concentrations of organic matter, N and S.

Within this thesis, the CW2D module is chosen for the simulation of the biochemical transformation and degradation processes as it shows a good fitting for VF CW with intermitted loading where only aerobic and anoxic processes are assumed.

The reactive transport module CW2D includes 12 components (Table 4-3). The components include dissolved oxygen  $O_2$ , organic matter, OM, expressed as COD in three fraction as readily biodegradable CR, slowly biodegradable CS and inert organic matter CI, nitrogen including ammonium NH<sub>4</sub>-N nitrite NO<sub>2</sub>-N, nitrate NO<sub>3</sub>-N and dinitrogen N<sub>2</sub>-N, inorganic phosphor IP, heterotrophic MO XH and autotrophic MO including *Nitrosomonas* XANs and *Nitrobacter* XANb. Table 3-2 summarizes these components and points out in which phase, liquid, solid, or both, they are defined within CW2D. For components defined in both phases adsorption and desorption processes can be considered.

Nine processes describe the biochemical and transformation reactions which are modelled using Monod-type rate expressions used for ASMs introduced by Henze et al. (2000) and follow the notation of the so called Gujer matrix. In CW2D these processes are modelled based on the activities of two different groups of bacterial, namely heterotrophic and autotrophic respectively. The transformation processes of these two groups are listed in Table 4-4. The nitrification is modelled as a two step system, in the first step NH4<sup>+</sup> and O2 are consumed by *Nitrosomonas* and NO2<sup>-</sup> is produced where in the second step NO2- along with O2 is consumed by *Nitrobacter* 

and NO3<sup>-</sup> is produced. Within CW2D a constant concentration of MO in each finite element is assumed and the thickness of the biofilm is not considered (Langergraber and Šimůnek, 2005).

i	Symbole	Unit	Description	Phase
1	O2	$mg_{o2}.L^{-1}$	Dissolved oxygen	Liquid
2	CR	mg <sub>COD</sub> .L <sup>-1</sup>	Readily biodegradable OM	Both
3	CS	mg <sub>COD</sub> .L <sup>-1</sup>	Slowly biodegradable OM	Both
4	CI	mg <sub>COD</sub> .L <sup>-1</sup>	Intert OM	Both
5	XH	mg <sub>COD</sub> .L <sup>-1</sup>	Heterotrophic MO	Solid
6	XANs	mg <sub>COD</sub> .L <sup>-1</sup>	Autotrophic MO (Nitrosomonas)	Solid
7	XANb	mg <sub>COD</sub> .L <sup>-1</sup>	Autotrophic MO (Nitrobacter)	Solid
8	NH4-N	mg <sub>N</sub> .L⁻¹	Amonium nitrogen	Both
9	NO2-N	mg <sub>N</sub> .L <sup>-1</sup>	Nitrite nitrogen	Liquid
10	NO3-N	mg <sub>N</sub> .L⁻¹	Nitrate nitrogen	Liquid
11	N2-N	mg <sub>N</sub> .L⁻¹	Dinitrogen	Liquid
12	IP	mg <sub>P</sub> .L <sup>−1</sup>	Inorganic phosphorus	Both

Table 4-3: Components of CW2D (Langergraber and Šimůnek, 2005)

Table 4-4: Processes	implemented in	CW2D (Lan	dergraber and	Šimůnek.	2012)
	in promotion and		gorgrador ana	onnanon,	

Heterotro	ophic bacteria	
1	Hdrolysis	Conversion of CS into CR
2	Aerobic growth of XH on CR	Mineralization of OM
3	Anoxic growth of XH on CR	Denitrification on NO2-N
4	Anoxic growth of XH on CR	Denitrification on NO3-N
5	Lysis of XH	Production of OM
Autotrop	hic bacteria	
6	Aerobic growth of XANs on NH4+	First step of nitrification
7	Lysis of XANs	Production of OM
8	Aerobic growth of XANs on NO2-	Second step of nitrification
9	Lsis of XANs	Production of OM

## 4.3 Simulation study

The modelling process is divided into two parts, (i) simulation of the water flow in the porous media, which is done using the standard HYDRUS software package and (ii) simulation of the transformation and degradation processes of the wastewater constituents using the HYDRUS wetland module CW2D.

### 4.3.1 General model setup

For the simulation study three different models, namely *sand - impounded, zeolite - impounded* and *zeolite - free drainage*, were generated to simulate the first stage systems of the PSCWs (Dal Santo, 2009). The physical setup for the 2-D plane including domain depth, drainage properties, boundary conditions and filter material is listed in Table 4-5. The width of the domain is the same for all three systems with a value of 100 cm. For the system *zeolite - free drainage* only the 50 cm main layer is considered while the other two systems include a 25 cm drainage layer to respect the impounded characteristics. Within the water flow boundary condition, the drainage properties are incorporated in HYDRUS at the bottom of the domain. For the zeolite- free drainage systems, the boundary condition is set to 20 cm at the bottom of the drainage layer. Atmospheric boundary conditions are set to the top of each domain and no flow boundary conditions are set along the side boundaries.

	Sand impounded	Zeolite impounded	Zeolite free drainage
Main layer	50 cm	50 cm	50 cm
Filter media	Sand 1-4mm	Zeolite 2-5mm	Zeolite 2-5mm
Drainage layer	25 cm	25 cm	No drainage layer
Filter	Sand 16-32mm	Sand 16-32mm	Sand 16-32mm
Water flow bounduray condition	20 cm	20 cm	-2 cm

Table 4-5: General setup of the model domain

For the numerical solution of the water flow and the transport of the constituents within the domain, a finite element mesh is needed. Despite the two different domain setups for the impounded systems and the free drainage system respectively, the same finite element mesh parameters to generate the mesh were used. This results in the same amount of nods (341) and elements (600) within the two systems.

Table 4-6 contains the time domain settings used for the simulation of water flow and reactive transport. The initial time step is sensitive to changes, generating an overflow error within the start of the simulation when chosen greater than  $1 \times 10^{-5}$  hours.

Table 4-6: Time domain settings for water flow and reactive transport simulation

Time step	[h]
Initial	1 x 10 <sup>-5</sup>
Minimum	1 x 10 <sup>-6</sup>
Maximum	0.02

### 4.3.2 Flow simulation

The first step in this simulation study and a general first step in the workflow when using HYDRUS is the simulation of the water flow within the system. This part incorporates a soil hydraulic model, soil hydraulic properties and time variable boundary conditions, (Table 4-7) meaning the feeding of the vertical flow filter with an amount of 15 L.m<sup>-2</sup> every three hours. To fit the measured hydraulic flow curve the loading time was adjusted. Equation (4-8) explains the chosen loading rate [cm/h] according to the time of appliance at a value of 0.0055 hours. This time addresses the fast narrow

peak of the measured effluent flow (Dal Santo, 2009). The amount of a single loading sums up as  $15L.m^{-2} = 15mm = 1.5cm$ . The actual loading rate was calculated as follows:

$$loading \ rate = \frac{1.5cm}{0.0055h} = 272.72 \sim 273cm. \ h^{-1}$$
(4-8)

Table 4-7: Time variable boundary conditions / hydraulic loading for four consecutive times

	Time	Precipitation
	[h]	[cm/h]
1	0.0055	273
2	3	0
3	3.0055	273
4	6	0
5	6.0055	273
6	9	0
7	9.0055	273
8	12	0

As a first step a reference simulation of the water flow using literature values (Table 4-8) for the van Genuchten model parameter is done for each of the three systems. For zeolite, no literature values were available and thus literature values for sand were used with an increased saturated hydraulic conductivity, as the material is coarser (2-5 mm) than the used sand (1-4 mm).

Parameter	Θr	Θs	α	n	ks	Ι
Unit	[cm <sup>3</sup> .cm <sup>-3</sup> ] [cm <sup>3</sup> .cm <sup>-3</sup> ]		[cm <sup>-1</sup> ]	[-]	[cm.min <sup>-1</sup> ]	[-]
Sand (1-4mm)	0.06	0.42	0.125	3	50	0.5
Zeolite (2-5mm)	0.06	0.42	0.125	3	110	0.5
Sand (16-32mm)	0.045	0.4	0.145	2.68	60000	0.5

Table 4-8: Literature values for soil hydraulic parameters (Langergraber, 2001)

As no measured soil hydraulic parameters were available from the PSCW experiment, all soil hydraulic parameters of the main filter layer were fitted. As only water saturated flow occurred in the drainage layer, the soil hydraulic parameters of the drainage layer in the impounded systems were not fitted (Langergraber, 2001; Šimůnek et al., 2012; van Genuchten, 1980).

With the fitted parameter the simulation of the hydraulic flow is done in two steps, first using standard initial conditions for the pressure head and second using the results from the first step as initial conditions for the second simulation, which leads to pseudo-steady state, i.e. periodic behaviour.

### 4.3.3 Reactive transport simulation

After the simulation results of the volumetric effluent flow in the three systems were fitted to measured data, the biokinetic model CW2D (Langergraber and Šimůnek, 2005) was added to the simulation by the wetland module.

For the simulation of the reactive transport, the measured influent concentrations of the used wastewater are added to the variable boundary conditions. Within CW2D, 12 components (Table 4-3) are implemented and can be given a value. The measured data from the PSCW experiment

included namely, COD, ammonia, nitrite, and nitrate and the wastewater composition is the same for all three systems. The influent concentrations are listed in Table 4-9.

COD is divided into three fractions, readily-, slowly-, and inert organic matter (CR, CS, CI). Therefor also the influent concentration of COD needs to be divided into these fractions. Assuming that organic matter is almost completely degraded in a CW, CI is determined as the measured effluent concentration of COD (Langergraber, 2001). Another assumption within this study is that all three systems were working under the same laboratory conditions. Due to this generalisation, the fraction of CI is determined as 30 mg.L<sup>-1</sup> and the ratio of CR to CS with 2:1.

Table 4-9: Mean influent concentrations (Dal Santo, 2010) including COD fractions for CW2D

Parameter	CR	CS	CI	COD	NH <sub>4</sub> -N	NO <sub>2</sub> -N	NO <sub>3</sub> -N
Unit	[mg.L <sup>-1</sup> ]						
Influent concentrations	243	121	30	394	93	0.008	0.59

In a first step the simulation of the *sand* - *impounded* system is done. The standard parameter set (appendix Table 10-5) implemented in the HYDRUS wetland module (Langergraber and Šimůnek, 2005) is used. For the initial conditions the concentrations of heterotrophic- and autotrophic bacteria need to be set to a value greater than zero (set to 1), all others were set to 0. Steady state conditions were reached within a simulation time of 200 days. The simulated effluent concentration of COD was overestimated and for NH<sub>4</sub>-N when using the described initial parameter set and COD fractions.

For the adjustment of the COD effluent concentration the fractions of CR, CS and CI are changed by decreasing the value of the CI fraction and increasing the CS and CR values to achieve a good fit.

The next step addresses the parameter estimation to fit the NH<sub>4</sub>-N simulated and measured effluent concentration. The estimation is done using a try and error approach with the goal of first reaching steady state condition in the simulation and fit the median of the NH<sub>4</sub>-N effluent in a range of the 95% confidence interval according to the measurements done by Dal Santo (2009).

When looking at the description of the processes implemented in CW2D (Table 4-4) one can see that for the first step of the nitrification, the growth of *Nitrosomonas* is based on consumption of NH<sub>4</sub>-N. Equation (4-9) shows the formulation of the reaction rate growth of  $X_{ANs}$  on NH<sub>4</sub>-N and their lysis. The parameter chosen to get a better fit is the maximum aerobic growth rate  $\mu_{ANs}$ .

$$\mu_{ANS} \cdot \frac{c_{O2}}{K_{ANS,O2} + c_{O2}} \cdot \frac{c_{NH4}}{K_{ANS,NH4} + c_{NH4}} \cdot \frac{c_{IP}}{K_{ANS,IP} + c_{IP}} \cdot c_{XANS} - b_{HANS} \cdot c_{XANS}$$
(4-9)

A sensitivity analysis, done by Langergraber (2001), points out, that  $\mu_{ANs}$  shows a medium sensitivity to changes (3 on a scale of 1 to 5 where 1 suggests high and 5 low sensitivity) which is taken into account during the try and error procedure.

To address the assumption of same processes occurring due to the same laboratory settings, the adjusted parameter  $\mu_{ANs}$  is used for the simulation of the remaining two systems.

For the systems using zeolite as filter material in the main layer, namely *zeolite, impounded* and *zeolite, free drainage,* the calculated adsorption isotherm for NH<sub>4</sub>-N (Dal Santo, 2009) is added in the CW2D module as reaction term and modelled as chemical non-equilibrium two-site adsorption (equation 4-10). The time dependency of adsorption is described by the concept of two-side sorption, where one part sorption is instantaneous on one part of the exchange sides and on considered time-depended on the other side (Šimůnek et al., 2012).

$$\frac{ds_k^k}{dt} = \alpha \cdot \left[ (1-f) \cdot \frac{k_{s,k} \cdot c_k^{\beta_k}}{1 + \eta_k \cdot c_k^{\beta_k}} - s_k^k \right]$$
(4-10)

 $s_k^k$  = adsorbed concentration of sites assumed to be time dependent [mg.kgs<sup>-1</sup>], c<sub>k</sub> = concentration in the aqueous phase [mg.dmw<sup>-3</sup>],  $\alpha$  = first order exchange rate coefficient [d<sup>-1</sup>], k<sub>s,k</sub> and  $\beta_k$  are the adsorption isotherm coefficient for the Freundlich equation when  $\eta_k = 0$ . The fractions of exchange sites assumed to be in equilibrium with the solution phase is defined as *f* [-] In the wetland module it is assumed that all adsorption is time-dependent and therefor *f* = 0.

Within this process one parameter, namely the first-order rate coefficient for one-, or two-site non equilibrium adsorption  $\alpha$  [d<sup>-1</sup>] has to be determined.

In system three, namely *zeolite, free drainage*, the simulated effluent concentration of COD was underestimated compared to measurements and therefore a third parameter is adjusted within this system. In this case the process dealing mainly with the growth of heterotrophic bacteria illustrated in equation (4-11) is addressed The parameter for the maximum lysis rate  $b_h$  is chosen in order to keep the growth at the same speed, but create a faster decay of the heterotrophic MO.

$$\mu_{H} \cdot \frac{c_{O2}}{K_{Het,O2} + c_{O2}} \cdot \frac{c_{CR}}{K_{Het,CR} + c_{NH4}} \cdot f_{N,Het} \cdot c_{XH} - b_{H} \cdot c_{XH}$$
(4-11)

The definitions of the parameters used in equation (4-10) and (4-11) can be found within the Appendix.

### 4.3.4 Analysis of the simulation data

For the analysis, evaluation and statistical calculations of the simulation data, the open source software package "R statistics" is used. R is a programming language for calculation, statistical analysis, data manipulations and graphical display (Venables et al., 2015).

An R-code was created to analyse the output files from HYDRUS, namely the files "effluent.out" and "ObsNod.out", creating the effluent concentrations for each component and the concentration at each defined observation node along the domain respectively. This data is from most importance to evaluate the simulation performance. During the calculation, HYDRUS is writing this output files, line by line, so it is possible to live view the simulation process and generate a graphical output using R statistics. This is a pleasant tool along the try and error process. The generated R code is included within the DVD in the back of the printed version and in the Appendix.

# 5. Results and discussion

# 5.1 Pilot scale experiment

### 5.1.1 General remarks

The results presented here give an overview of the results gained within the work of Dal Santo (2009) which are from utmost importance for the simulation study carried out in this master thesis. A description of the pilot scale experiment can be found in chapter 4.1.

### 5.1.2 Measured adsorption isotherms

The adsorption curve (Figure 5-1) was gained within a shaking test to find out the time when adsorption process gained steady state. Two different  $NH_4$ -N concentrations were used, 50 mg.L<sup>-1</sup> and 100 mg.L<sup>-1</sup>.



Figure 5-1: NH4 adsorption curve with two different concentrations (Dal Santo, 2009)

According to Figure 5-1 the adsorption starts after three hours of shaking and the adsorption is higher when using the lower concentration. The chosen Freundlich isotherms is fitted to the data. Figure 5-2 shows the isotherm after 16 hours of shaking.

The calculated parameter values for the Freundlich isotherm are as  $k_{1,F} = 660 \text{ mL.}\mu\text{g}^{-1}$  and  $k_{2,F} = 0.76$ , (Dal Santo, 2009). These results are most important to address the adsorption behaviour of zeolite within the model. With these parameters for the Freundlich isotherm the adsorption of NH<sub>4</sub><sup>+</sup> on zeolite is implemented in the simulations for *zeolite, impounded* and *zeolite, free drainage*. No adsorption was observed for NO<sub>3</sub> on Zeolite as for NH<sub>4</sub> and NO<sub>3</sub> on sand and therefore not included in the simulation.



Figure 5-2: Freundlich isotherm of Zeolite at 16 hours of shaking (Dal Santo, 2009)

### 5.1.3 Measured effluent concentrations

Table 5-1 shows the measured influent and 1st stage effluent concentrations for all three systems at their first stage after mechanical pre-treatment. Figure 5-3 compares the measured COD and  $NH_4$ -N effluent concentrations.

Table 5-1: Measured influent and 1st stage effluent concentrations of the three PSCW systems, number of samples n = 13 (Dal Santo et al., 2010)

Parameter		COD	NH <sub>4</sub> -N	NO <sub>2</sub> -N	NO <sub>3</sub> -N
Unit		[mg.L <sup>-1</sup> ]	[mg.L <sup>-1</sup> ]	[mg.L <sup>-1</sup> ]	[mg.L <sup>-1</sup> ]
Influent conc.		394	93	0.008	0.59
Effluent conc.					
Sand impounded	Median	35	14.5	0.0026	70.8
	95% confidence interval	5	4.6	0.004	8.4
Zeolite impounded	Median	29	0.06	0.52	51.8
	95% confidence interval	6	0.05	1.1	4.6
Zeolite free drainage	Median	86	1.31	0.63	58.2
	95% confidence interval	14	0.38	0.53	5.8

For the COD effluent concentration a clear difference in the treatment performance can be seen between the impounded systems (1, 2) and the free drainage system (3). This is due to the denitrification processes occurring in the impounded layer where no oxygen is available and available carbon from the COD is used by the microorganisms responsible for this process. For the NH<sub>4</sub>-N effluent concentration a general higher treatment performance can be addressed to the systems (2, 3) using zeolite. When comparing system 1 and system 2, the hypothesis behind this behaviour addresses the performance of the filter materials. While in the coarse sand filter the influent rapidly flows through the bed and ammonia is available for nitrification.



Figure 5-3: Comparison of the COD and NH4-N effluent concentrations in the first stage of each system (1 = sand - impounded; 2 = zeolite - impounded and 3 = zeolite - free drainage) (Dal Santo et al., 2010)

Within the zeolite filter the infiltration process is mainly the same, but in addition to nitrification, adsorption of  $NH_{4^+}$  takes palace. When looking at a whole feeding period it is assumed, that adsorption takes place during the feeding procedure, while in the resting period of three hours,  $NH_{4^+}$  is oxidised by the nitrifying bacteria (Canga, 2010).

## 5.2 Water flow simulation

In order to fit the model of the water flow in each system to the measured data an inverse solution using measured data and the soil hydraulic model by van Genuchten (1980) used. This calibration step starts with literature values for the soil hydraulic parameters and fits, in this case, all the parameters in order to get a good overall fit. Table 5-2 presents literature values and fitted values for the *sand - impounded* and *zeolite - free drainage* system. For *the zeolite - impounded* system the values form *zeolite - free* drainage are used, as this values give the best fit also for this system.

Parameter	Θr	Θs	α	n	ks	Ι	Iteration	R²
Unit	[cm³.cm <sup>-3</sup> ]	[cm³.cm <sup>-</sup> 3]	[cm <sup>-1</sup> ]	[-]	[cm.min <sup>-1</sup> ]	[-]	steps	[-]
Sand (1-4mm)	0,06	0,42	0,125	3	50	0,5	-	-
Sand (fitted)	0,063	0,37	0,124	3,2	55	0,49	4	0,98
Zeolite (2-5mm)	0,06	0,42	0,125	3	110	0,5	-	-
Zeolite (fitted)	0,076	0,40	0,185	3,03	85	0,373	6	0,96

Table 5-2: Literature- and fitted values of the soil hydraulic parameters

The goodness of fit between the observed- and simulated cumulative flow data with respect to the van Genuchten model is evaluated by using the coefficient of determination (R<sup>2</sup>) (Table 5-2). A good fit fort he water flow can be achieved.

The different soil water retention curves, generated by the van Genuchten model (van Genuchten, 1980), using literature-, and fitted soil hydraulic parameters for sand and zeolite respectively, are illustrated in Figure 5-4.



Figure 5-4: Soil water retention curve for zeolite and sand using the van Genuchten model

Figure 5-5, and Figure 5-6, illustrate the simulated and observed cumulative and boundary flux flow, for the *sand - impounded* and *zeolite - free drainage* systems using the initial and fitted soil hydraulic parameters for sand and zeolite respectively. Figure 5-7 compares the observed and simulated fluxes for the *zeolite, impounded* system.



Figure 5-5: Sand - impounded observed and simulated water flow



Figure 5-6: Zeolite - free drainage observed and simulated water flow



Figure 5-7: Zeolite - impounded observed and simulated water flow

The cumulative flux reaches 150 cm<sup>2</sup> for the 2D plane of the model domain. This satisfies the input of one loading with the amount of 15  $L.m^{-2}$  by using the following euqation:

$$15 L. m^{-2} = 15 mm = 15 \times \frac{1000 cm^3}{100 cm} = 150 cm^2$$
(5-2)

### 5.3 Reactive transport simulation

#### 5.3.1 Steady state

According to the simulation results of the most interesting effluent concentrations, COD,  $NH_4$ -N and  $NO_3$ -N respectively, steady state conditions were reached within a simulation time of 200 days. Figure 5-8, Figure 5-9 and Figure 5-10 illustrate the final simulation results for the named

effluent concentrations within the *sand-impounded* system. The rapid change of the simulated concentrations at the time of 4090 hours was from further interest. Therefor a simulation, using the simulated values at 4000 hours as initial conditions trying to generate the same simulated behaviour, was performed (Figure 5-11).



Figure 5-8: Simulated COD effluent concentration for the sand-impounded system



Figure 5-9: Simulated NH<sub>4</sub>-N effluent concentration for the sand-impounded system







Figure 5-11: Comparison of simulation results using standard initial conditions (black) and initial conditions at the time of 4000 hours from the prior simulation (red) of the *sand-impounded* system

As can be seen in Figure 5-11, it was not possible to generate the same behaviour with a simulation using initial conditions just bevor the observed peaks. This is most interesting for a further evaluation of the numerical calculations, which was not performed within this thesis.

For the bacterial concentrations of XH, XANs and XANb no steady state could be achieved as continuously growth of all three can be observed along the simulation time. In addition, a significant change of the bacteria concentration, as seen bevor at the time of 4090 hours, can be observed.



Figure 5-12: Simulated growth of heterotrophic bacteria (XH) in the sand-impounded system over the filter depth



Figure 5-13: Simulated growth of *Nitrosomonas* (XANs) in the sand-impounded system over the filter depth



Figure 5-14: Simulated growth of *Nitrobacter* (XANb) in the sand-impounded system over the filter depth

### 5.3.2 Influence of influent fractionation

The chosen initial fractionation of COD, namely CR, CS and CI, and the adjustment of the same to fit the measured effluent concentration of COD are illustrated in Figure 5-15. The fitting was performed within the *sand – impounded* system and applied on the other two systems. The initial and fitted fractions of CR, CS and CI are listed in Table 5-3. The value of the median measured effluent concentration of COD used for the fitting is 35 mg.L<sup>-1</sup>. The adjustment of the nitrification rate to fit the NH<sub>4</sub>-N effluent concentration (chapter 5.3.3) results in a slight increase in the simulated COD effluent concentration.

Parameter	CR	CS	CI
Unit	[mg.L <sup>-1</sup> ] [mg.L <sup>-1</sup> ]		[mg.L <sup>-1</sup> ]
Initial fractions	243	121	30
Fitted fractions	274	100	20

Table 5-3: Initial and fitted influent fractions of COD



Figure 5-15: Results for different COD fractionations within the last 5 days of simulation

### 5.3.3 Influence of nitrification rate

In order to fit the simulated and measured NH<sub>4</sub>-N effluent concentration, adjustments to the maximal aerobic growth rate  $\mu_{ANs}$  of *Nitrosomonas* were performed. The influence of different values for  $\mu_{ANs}$  are illustrated within

Figure 5-16. The reduction of  $\mu_{ANs}$  from 0.9 to 0.6 [d<sup>-1</sup>] shows a significant impact on the effluent concentration of NH<sub>4</sub>-N. Also a small change, from 0.9 to 0.85 [d<sup>-1</sup>] shows to be significant, increasing the median effluent concentration by 7 mg.L<sup>-1</sup>. Decreasing  $\mu_{ANs}$  further to 0.8 [d<sup>-1</sup>] shows no significant change. This behaviour can be explained by the medium sensitivity of this parameter according to a sensitivity analysis done by Langergraber (2001)





#### 5.3.4 Influence of heterotrophic decay rate

For the *zeolite* – *free drainage* system, the simulated and measured COD effluent concentration do not show a satisfying fit. To gain a better fit within this system the lysis rate  $b_h$  of heterotrophic bacteria is addresses. Figure 5-17 illustrates the results of the parameter adjustment where a better fit can be achieved. The impact on the effluent concentration by a change from 0.4 to 1.2 [d<sup>-1</sup>] is highly significant. Further on a good adjustment could be achieved by a change to 1.2 [d<sup>-1</sup>].



Figure 5-17: Influence of the heterotrophic lysis rate on the simulated COD effluent concentration within the last 5 days of simulation

## 5.3.5 Final results

The final results are presented as median values over 5 days of simulation after reaching steady state. The measured influent and effluent values show median values from a sample size of 13. The standard parameter set of the biokinetic model CW2D are listed in the appendix (Table 10-5).

The first simulation was carried out using the standard biokinetic parameter set (Langergraber and Šimůnek, 2005) for the *sand, impounded* system (Table 5-4). The adjusted fractions of CR, CS and CI give a good fit to the overall measured COD effluent concentration. When looking at the nitrogen parameter it can be observed that the NH<sub>4</sub>-N effluent concentration is underestimated when  $\mu_{ANs} = 0.9$  [d<sup>-1</sup>] is used. With the adjustment of this parameter to a value of to 0.85 [d<sup>-1</sup>] a better fit can be achieved. The higher NO<sub>3</sub>-N removal within the model may be explained by a higher denitrification rate within the simulation, than within the measured PSCW experiment (Dal Santo, 2009). The standard maximum denitrification rate (Langergraber and Šimůnek, 2005) was not adjusted in this thesis.

Parameter	CR	CS	CI	COD	NH <sub>4</sub> -N	NO <sub>2</sub> -N	NO <sub>3</sub> -N
Unit	[mg.L <sup>-1</sup> ]						
Influent concentrations	274	100	20	394	93	0.008	0.59
Observed effluent concentrations	-	-	-	35	14.5	0.026	70.8
Simulated effluent concentrations							
Standard parameter $\mu_{ANs} = 0.9 \ [d^{-1}]$	0.2	8.3	27.5	36	10.37	< 0.003	55.47
Adjusted $\mu_{ANs} = 0.85 \ [d^{-1}]$	0.3	11.1	27.2	38.6	17.82	< 0.003	51.57

Table 5-4: Simulated effluent concentrations bevor and after the fitting process for the sandimpounded system

With the adjusted parameter, the simulation of the other two systems are carried out. This is based on the assumption, that in the PSCW laboratory experiment (Dal Santo, 2009) every system is operated under the same conditions. Table 5-5 and Table 5-6 are listing the results of the simulated systems using zeolite as filter media. For the first order exchange rate coefficient  $\alpha$ , needed within the adsorption process in HYDRUS, a value of 0.01 [d<sup>-1</sup>] was chosen.

With the adjustment of the maximum aerobic growth rate  $\mu_{ANs}$  within the *zeolite, impounded* system only a small change for the simulated NH4-N effluent concentration can be observed. The major impact to this change can be seen within the NO<sub>3</sub>-N effluent concentrations. This behaviour is explained by the lower nitrification rate based on the change of  $\mu_{ANs}$ . The fact that this doesn't lead to the same change of the NH4-N concentration in the effluent as observed in the *sand* - *impounded* system lies within the adsorption capacity of zeolite and therefor confirms the hypotheses by Dal Santo et al. (2010). While the system is loaded, NH<sub>4</sub>-N is adsorbed to the substrate and oxidised by the nitrifying bacteria during the resting period.

Table 5-5: Simulated effluent concentrations bevor and after the fitting process for the *zeolite-impounded* system

Parameter	CR	CS	CI	COD	NH <sub>4</sub> -N	NO <sub>2</sub> -N	NO <sub>3</sub> -N
Unit	[mg.L <sup>-1</sup> ]						
Influent concentrations	274	100	20	394	93	0.008	0.59
Observed effluent concentrations	-	-	-	29	0.06	0.52	51.8
Simulated effluent concentrations							
Standard parameter $\mu_{ANs} = 0.9 \ [d^{-1}]$	0.4	0.2	28.9	29.5	0.36	< 0.003	76.5
Adjusted $\mu_{ANs} = 0.85 \ [d^{-1}]$	0.2	0.1	29.6	29.9	0.27	0.05	66.1

For the nitrogen parameters the simulation results of *the zeolite, free drainage* system (Table 5-6) show the same system behaviour as in the *zeolite, impounded* system. To fit the COD effluent concentrations the lysis rate of the heterotrophic bacteria,  $b_h$  [d<sup>-1</sup>], was increased from 0.4 to 1.2. Bevor the adjustment of the lysis rate also significantly higher simulated COD effluent concentrations within the *zeolite – free drainage* system than in the *zeolite – impounded* system can be observed, with 35.34 mg.L<sup>-1</sup> and 29.8 mg.L<sup>-1</sup>, with the biggest difference in the CS fraction. This supports the assumption, that denitrification is happening within an impounded drainage layer, as CS is consumed by the denitrification process. With the adjustment of the lysis rate, to reach a better fit between the simulated NO<sub>3</sub>-N concentrations is explained by the change of the maximum nitrification rate prior to the change of the lysis rate.

Table 5-6: Simulated effluent concentrations bevor and after the fitting process for the *zeolite-free drainage* system

Parameter	CR	CS	CI	COD	NH <sub>4</sub> -N	NO <sub>2</sub> -N	NO <sub>3</sub> -N
Unit	[mg.L <sup>-1</sup> ]						
Influent concentrations	274	100	20	394	93	0.008	0.59
Observed effluent concentrations	-	-	-	86	1.31	0.63	58.2
Simulated effluent concentrations							
Standard parameter $\mu_{ANs}$ = 0.9 [d^{-1}]; b_h~= 0.4~[d^{-1}]	0.2	6.6	28.1	34.9	0.13	0.028	78.1
Adjusted $\mu_{ANs} = 0.85 \ [d^{-1}]; \ b_h = 1.2 \ [d^{-1}]$	0.6	32.3	38.3	71.1	1.13	< 0.003	46.8

# 6. Summary and conclusions

Pilot-scale experiments have previously been performed on three two-stage constructed wetland systems. Measurements of the water flow and the wastewater constituents in the influent and effluent were carried out (Dal Santo, 2009). This master thesis shows the setup and calibration of the water flow and the degradation of the wastewater constitutes for every first stage of each system, namely *sand - impounded*, *zeolite - impounded* and *zeolite - free drainage*, defining the main filter material and the drainage conditions.

Generating the model domain based on the experimental data and boundary conditions was possible due to the features within HYDRUS (Šimůnek et al., 2012) and the implemented wetland module CW2D (Langergraber and Šimůnek, 2005). For the hydraulic simulation the lack of data on hydraulic conductivity saturated- and residual water content was overcome by the use of literature values and the implemented inverse solution to estimate these parameters within the chosen soil hydraulic model, the van Genuchten model without hysteresis (van Genuchten, 1980). A good fit of the cumulative-, and boundary flux of the measured and simulated data is achieved for all three systems. This is an important step as the reactions occurring in a CW are highly correlated with the hydraulic flow.

To determine the fractions of the COD influent (CR, CS, CI) was an important first step within the reactive transport model and provided a good fit for the impounded systems when comparing the simulated and measured COD effluent concentrations. For the *zeolite – free drainage* system the simulated COD effluent was still underestimated. Therefor only in this system the lysis rate for heterotrophic bacteria was adjusted.

Simulation results of the *sand* - *impounded* system show that by changing only one parameter, namely the maximum growth rate of *Nitrosomonas*  $\mu_{ANs}$ , the effluent concentrations of NH<sub>4</sub>-N and NO<sub>3</sub>-N can be fitted very well. To fulfil the assumption that all three systems are operated under the same conditions this fitted parameter is used for all three systems.

The results presented for the zeolite systems, namely *zeolite - impounded* and *zeolite - free drainage*, show to be true to this assumption for the nitrogen parameters. In order to implement the measured adsorption isotherm in HYDRUS the first-order rate coefficient for one-, or two-site non-equilibrium adsorption  $\alpha$  [d<sup>-1</sup>] needs to be given a value and was chosen properly.

For all parameter adjustments a trial and error approach was performed. This may be adequate, but also has shown to be time consuming. To run a simulation for 4800 hours the real calculation time lies within 24 to 48 hours depending on the time discretization and the density of the printed output. The complexity of a numerical solution within a biokinetic model addressing processes interacting with each other along the calculation time using a denes mesh of finite elements will always show to be time consuming. On the other hand, it can be pointed out that simulations of CW wetland behaviour are very appropriate to give a 100 time faster result on the systems behaviour when calibrated properly.

In the process of reaching steady state conditions, several problems occurred. While for COD and the nitrogen parameters steady state could be assumed after 200 days of simulation, this was not true for the bacterial community. As for now, no growth limiting functions are implemented in the wetland module. To overcome the problem, adjustments to lysis rates of the heterotrophic and autotrophic can be an option but also will lead to a change with the simulated effluent concentrations.

Another problem occurred with the repeating behaviour of the simulated effluent concentrations generating a peak at always the same time. When performing a simulation using initial condition from a time step just bevor this occurrence, trying to generate the same system behaviour, the results showed a different behaviour, e.g. the same behaviour when starting the simulation from the chosen overall initial conditions. It can be assumed that this leads to numerical problems, which will need further research.

Based on the results of the thesis it can be concluded that:

- The measured volumetric effluent flow rates could be simulated for all three CW systems.
- With the chosen influent fractions for COD, a good match with measured COD effluent concentrations could be reached for the impounded systems; to match COD effluent concentrations for the free drainage system, adjustments to lysis rate of heterotrophic bacteria were needed.
- Measured and simulated effluent concentrations for the *sand impounded* system have been fit using the maximum growth rate for *Nitrosomonas*  $\mu_{ANs}$ . This adjustment also shows good results within the other two systems.
- When simulating adsorption for NH<sub>4</sub>-N, responsible for short-term retention of NH<sub>4</sub>-N in between loadings (as described by Dal Santo et al., 2010), a goof match between measured and simulated effluent concentration for the zeolite systems could be achieved.
- The difference in COD removal in systems with impounded and free drainage layer could be simulated and can be explained by enhanced denitrification in the impounded drainage layer.

# 7. Outlook

To improve future simulation studies certain data requirements should be met by the experimental or fully implemented constructed wetland system. For the hydraulic flow simulation, measurement addressing the properties of the filter media should be carried out in order to define parameters for the soil hydraulic model. For the biokinetic simulation parameters of the wastewater such as COD, nitrogen (NH<sub>4</sub>-N, NO<sub>2</sub>-N, NO<sub>3</sub>-N) are an important basic data set as should be the development of measurement techniques to determine the kinetic parameters. Within the study mentioned above, Pálfy et al. (2015) points out that simulations were carried out using literature values and that measured data such as soil hydraulic parameters, adsorption capacity and others, would be more appropriate. Morvannou et al., (2011) developed a method to characterize nitrification kinetics such as the maximum growth rate by using a respirometric tool. Along with this development came a confirmation of the assumption of Langergraber (2001) that bacteria in active sludge systems and CWs are similar and that parameters of the biokinetic models for CWs can be derived from ASMs. Langergraber et al. (2007) compared measurements and simulations on heterotrophic bacteria. Adjustments to the lysis rate within CW2D showed good results and steady state conditions could be achieved. This should be a next step within the performed simulation study but implemented as a second step after the fractionation of the COD influent. For the HYDRUS wetland model a clogging model would be the next step. This would also limit the bacterial growth to the size of the pore space generating a more realistic behaviour of the system as performed by Samsó and García (2013).

Including more processes will lead to an even more complex model and help to improve the knowledge on the behaviour of constructed wetlands and its processes. This complexity will also help to create simpler models as design tools helping to improve a more sophisticated way of designing CWs than the rule of thumb approach. In a recent study done by Pálfy et al. (2015), shows the possibility of using a complex biokinetic model such as CW2D to revile week points of a preliminary design and to help to develop an optimized system for a specific site. The simulation performed in this study points out the weakness of a CW implemented as a polishing stage for a sequence batch reactor effluent and facilitates the design of an effective system. This clearly shows the practicable use of complex models in the evaluation- and design process of CWs.

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# 10. Appendix

# 10.1 CW2D biokinetic model

Table 10-1: Stoichiometric coefficients for ammonium nitrogen (Langergraber and Šimůnek, 2005)

Table 10-2: Stoichiometric coefficients for ammonium nitrogen (Langergraber and Šimůnek, 2005)

$$\begin{split} \nu_{1,P} &= i_{P,CS} - (1 - f_{Hyd,CI}) \cdot i_{P,CR} - f_{Hyd,CI} \cdot i_{P,CI} \\ \nu_{2,P} &= 1/Y_{H} \cdot i_{P,CR} - i_{P,BM} \\ \nu_{3,P} &= 1/Y_{H} \cdot i_{P,CR} - i_{P,BM} \\ \nu_{4,P} &= 1/Y_{H} \cdot i_{P,CR} - i_{P,BM} \\ \nu_{5,P} &= i_{P,BM} - (1 - f_{BM,CR} - f_{BM,CI}) \cdot i_{P,CS} - f_{BM,CR} \cdot i_{P,CR} - f_{BM,CI} \cdot i_{P,CI} \\ \nu_{6,P} &= -i_{P,BM} \\ \nu_{7,P} &= i_{P,BM} - (1 - f_{BM,CR} - f_{BM,CI}) \cdot i_{P,CS} - f_{BM,CR} \cdot i_{P,CR} - f_{BM,CI} \cdot i_{P,CI} \\ \nu_{8,P} &= -i_{P,BM} \\ \nu_{9,P} &= i_{P,BM} - (1 - f_{BM,CR} - f_{BM,CI}) \cdot i_{P,CS} - f_{BM,CR} \cdot i_{P,CR} - f_{BM,CI} \cdot i_{P,CI} \\ \end{split}$$

B	N. Componentis	1 02	~ 8	cs CS	94	5 XH	%ANs	XANb	8 NH4N	9 NOIN	N03N	11 N2N	11 B
	1012 CT 2010 T	£03			- gcob		1000	1			-Na		4
		C)		Heterotroph	ic organisati						1.27		ŝ
	Hydralysis Acrebic growth of heterotrophs on	1 - 1/Y <sub>n</sub>	$\frac{1-f_{ny,m}}{-1R_n}$	7	Distan.	-			na Na				22
-0	read by biodegradable COD Nitrate-based growth of heterotrophs		$-WY_{B}$			а			NA		$/({}^{\mathbf{E}}A - \mathbf{I}) -$	$(1 - Y_{\rm H})/$	14
-	on routing appropriate COD N triad-based gas with of hotentro phy		-1/V <sub>ii</sub>			-			10 per	$V_{m} = V_{m} V_{m}$	11.08T	NTA - L	4*a
10	tur raturg interest and one COLP		fauce	1 - faure -	fina	ī			N <sup>5</sup> A	1-(11 <sup>4</sup>		LI III	450
		10	Aut	otrophic organise	us 1-Minu	Semunas	ŝ				1000		
•	Accelor growth of NURDSamouts on memoryline	-(343 - Y					-		il.	-1/V	107,004		100
-	Lysis of Miresemenen	4	fina A	$1 - f_{\rm NMCR} = f_{\rm NMCR}$	fina ans 2 <i>-Nitr</i>	obacter	7		WIN				¢,
**	A sechic growth of Nitrebucter on mittle Lysis of Nitrebucter	$-(1.14 - Y_{\rm ANA})$	faur	1 - finze - finze -	fisici	2		- 7	n <sub>te</sub>	-I/YAM	1/Yan		14

Table 10-3: Stoichiometric matrix of reactions in CW2D (Langergraber and Šimůnek, 2005)

Table 10-4: Reaction rates in CW2D (Langergraber and Šimůnek, 2005)

R Process / Reaction rate rcj
Heterotrophic organisms
1 Hydrolysis
$K_{h} \cdot \frac{c_{CS}/c_{XH}}{K_{X} + c_{CS}/c_{XH}} \cdot c_{XH}$
2 Aerobic growth of heterotrophs on readily biodegradable COD
$c_{O2}$ $c_{CR}$
$K_{Het,O2} + c_{O2}$ $K_{Het,CR} + c_{CR}$ $J_{N,Het} + c_{XH}$
3 NO3-growth of heterotrophs on readily biodegradable COD
$K_{DN,D2}$ $c_{ND3}$ $K_{DN,ND2}$ $c_{CR}$
$\mu_{DN} \cdot \frac{\mu_{DN}}{K_{DN,02} + c_{02}} \cdot \frac{\mu_{DN}}{K_{DN,N03} + c_{N03}} \cdot \frac{\mu_{DN,N02}}{K_{DN,N02} + c_{N02}} \cdot \frac{c_R}{K_{DN,CR} + c_{CR}} \cdot f_{N,DN} \cdot c_{\chi}$
4 NO2-growth of heterotrophs on readily biodegradable COD
K <sub>DN 02</sub> CN02 Ccn
$\mu_{DN} \cdot \frac{c_{N,DN}}{K_{DN,DN} + c_{DN}} \cdot \frac{c_{N,DN}}{K_{DN,DN} + c_{N,DN}} \cdot \frac{c_{N,DN}}{K_{DN,DN} + c_{N,DN}} \cdot c_{N,N}$
5 Lysis of heterotrophs
$b_{\mu} \cdot c_{\nu\mu}$
Autotrophic organisms 1 - Nitrosomonas
6 Aerobic growth of Nitrosomonas on NH4
C <sub>02</sub> C <sub>NH4</sub> C <sub>IP</sub>
$\frac{\mu_{ANs}}{K_{ANs,O2} + c_{O2}} \frac{K_{ANs,NH4} + c_{NH4}}{K_{ANs,IP} + c_{IP}} \frac{c_{XANs}}{K_{ANs}}$
7 Lysis of Nitrosomonas
b <sub>HAN5</sub> · c <sub>XAN5</sub>
Autotrophic organisms 2 - Nitrobacter
8 Aerobic growth of Nitrobacter on NO2
$c_{02}$ $c_{NO2}$
$\frac{\mu_{ANb}}{K_{ANb,O2} + c_{O2}} \frac{1}{K_{ANb,NO2} + c_{NO2}} \frac{J_{N,ANb}}{K_{ANb}} \frac{c_{XANb}}{c_{XANb}}$
9 Lysis of Nitrobacter
$b_{HANb} \cdot c_{XANb}$
Conversion of solid and liquid phase concentrations
$c_{XY} = \frac{\rho}{\theta} \cdot s_{XY}$ , where $Y = H, ANs, ANb$
Factor for nutrients
$f_{N,x} = \frac{c_{NH4}}{K_{x,NH4} + c_{NH4}} \cdot \frac{c_{IP}}{K_{x,IP} + c_{IP}} , \text{ where } x = Het, DN, ANb$

	Description [unit]	Value
Hydrolysis	Ale state la	for 20°C (10°C)
Kh	hydrolysis rate constant [1/d]	3 (2)
Kx	saturation/inhibition coefficient for hydrolysis [gCOD <sub>CS</sub> /g COD <sub>BM</sub> ]	0.1 (0.22) *
Heterotrophi	c bacteria (aerobic growth)	22200
Цн;	maximum aerobic growth rate on CR [1/d]	6 (3)
b <sub>H</sub>	rate constant for lysis [1/d]	0.4 (0.2)
Khet. O2	saturation/inhibition coefficient for So [mg O2/L]	0.2
Klet, CR	saturation/inhibition coefficient for substrate [mg COD <sub>CR</sub> /L]	2
Khet, NH4N	saturation/inhibition coefficient for NH4 (nutrient) [mg N/L]	0.05
Klet, IP	saturation/inhibition coefficient for P [mg N/L]	0.01
Heterotrophi	c bacteria (denitrification)	4000000.0X
H <sub>DN</sub>	maximum aerobic growth rate on CR [1/d]	4.8 (2.4)
Khet. 02	saturation/inhibition coefficient for So [mg O2/L]	0.2
Khet NO3N	saturation/inhibition coefficient for NO3 [mg N/L]	0.5
Klet.NO2N	saturation/inhibition coefficient for NO2 [mg N/L]	0.5
Khet, CR	saturation/inhibition coefficient for substrate [mg COD <sub>CR</sub> /L]	4
Khet, NH4N	saturation/inhibition coefficient for NH4 (nutrient) [mg N/L]	0.05
Khet, IP	saturation/inhibition coefficient for P [mg N/L]	0.01
Ammonia oxi	dising bacteria (Nitrosomonas spp.)	and a second
HANIS	maximum aerobic growth rate on S <sub>NH</sub> [1/d]	0.9 (0.3)
BANS	rate constant for lysis [1/d]	0.15 (0.05)
KANS 02	saturation/inhibition coefficient for So [mg O2/L]	1
KANKNH4N	saturation/inhibition coefficient for NH4 [mg N/L]	0.5
KANAP	saturation/inhibition coefficient for P [mg N/L]	0.01
Nitrite oxidisi	ing bacteria (Nitrobacter spp.)	
HAND	maximum aerobic growth rate on S <sub>NH</sub> [1/d]	1 (0.35)
bAND	rate constant for lysis [1/d]	0.15 (0.05) *
KAND.02	saturation/inhibition coefficient for So [mg O2/L]	0.1
KAND,NO2N	saturation/inhibition coefficient for NO2 [mg N/L]	0.1
KAND, NH4N	saturation/inhibition coefficient for NH4 (nutrient) [mg N/L]	0.05
KANDUP	saturation/inhibition coefficient for P [mg N/L]	0.01

Table 10-5: Kinetic parameters in CW2D (Langergraber and Šimůnek, 2005)

Table 10-6: Temperature dependence, stoichiometric parameters, composition parameters and parameters describing oxygen transfer in CW2D (Langergraber and Šimůnek, 2005)

Parameter	Description [unit]	Value
Temperature d	ependences (activation energy [J/mol] for Arrhenius equation)	
Tdep het	Activation energy for processes caused by XH [J/mol]	47800
Tdep aut	Activation energy for processes caused by XA [J/mol]	69000
Tdep Kh	Activation energy Hydrolyses [J/mol]	28000
Tdep KX	Activation energy factor KX for hydrolyses [J/mol]	-53000 *
Tdep_KNHA	Activation energy for factor KNHA for nitrification [J/mol]	-160000 *
Stoichiometric	parameters	
fina ci	production of CI in hydrolysis	0.0
FBM CR	fraction of CR generated in biomass lysis	0.1
fam ct	fraction of CI generated in biomass lysis	0.02
YHet	yield coefficient for XH	0.63
YANS	vield coefficient for XANs	0.24
YAND	yield coefficient for XANb	0.24
Composition pa	arameters	
IN CR	N content of CR [g N/g COD <sub>CR</sub> ]	0.03
INCS	N content of CS [g N/g COD <sub>CS</sub> ]	0.04
INCI	N content of CI [g N/g COD <sub>c1</sub> ]	0.01
IN.BM	N content of biomass [g N/g COD <sub>BM</sub> ]	0.07
IP CR	P content of CR [g P/g COD <sub>CR</sub> ]	0.01
IP.CS	P content of CS [g P/g COD <sub>CS</sub> ]	0.01
IP CI	P content of CI [g P/g COD <sub>ci</sub> ]	0.01
IP.BM	P content of biomass [g P/g COD <sub>BM</sub> ]	0.02
Oxygen		10000
cO2_sat_20	saturation concentration of oxygen [g/m <sup>3</sup> ]	9.18
Tdep cO2 sat	activation energy for saturation concentration of oxygen [J/mol]	-15000
	to point on into [1/d]	240

angergraber (2007)

# 10.2 R-Code

The used \*.R files are include within the DVD attached in the back of the printed version.

The following R-Code addresses the chosen observation nodes within the model domain. The output file is created by HYDRUS during the simulation (ObsNod.out). For illustration reasons the printed code only addresses two observation nodes but can be extended to the needed amount.

#### 

#### START OF CODE

#direct access to HYDRUS files ==> OBSERVATION NODES
#gives you graphs as shown in the HYDRUS results

#print function -> run in seperat file

```
'zeichne <- function(time, x_1,x_2)
```

```
{
```

```
ycoord <- max(x_1,x_2)
```

```
plot(time,x_1,type="l",ylim=c(0,ycoord))
```

```
lines(time,x_2,col="2")
```

```
lines(time,x 3,col="3")
```

```
lines(time,x 4,col="4")
```

```
lines(time,x_5,col="5")
```

```
lines(time,x_6,col="6")
```

```
lines(time,x 7,col="7")
```

#gives a simple legend for the observation nods

```
legend(0,ycoord, #coordinates upper left corner equal to the def of x and y axis c("1","2"), # puts text in the legend
```

```
lwd=c(0.5), # NA provides no line at first legend print
col=c(1,2,3,4,5,6,7), # gives the legend lines the correct color and width
bty="y")
```

}

#when using RStudio, set working directory as shown below, #to run code: ctrl+A and ctrl+enter to run the complete code

#### Appendix

#set working directory to actual hydrus file, e.g. .../temp/FILENAME of interest #be aware that HYDRUS shortens the file name in the temp folder setwd("C:/hydrus/Temp/~Hydrus3D\_2xx/FILENAME)

#read observation node file NOD <- read.table("ObsNod.out", header=T, sep="",dec=".", skip="5")</pre>

#while simulation is not finished - erase last row drop<-nrow(NOD) NOD<-NOD[-drop,]</pre>

#create time vector
time <- NOD\$time</pre>

#variables for max. 7 Observation nodes // to get same views as in HYDRUS
# \_1...# of Obersvation Nod // s infront ... sorbtion

#node 1

#node 2

h_1 <- NO	D\$hnew ;	h_2 <-	NOD\$hnew.1;	
theta_1 <-	NOD\$theta ;	theta_2 <-	NOD\$theta.1;	
02_1 <-	NOD\$Conc ;	02_2 <-	NOD\$Conc.13	;
sO2_1 <-	NOD\$Sorb ;	sO2_2 <-	NOD\$Sorb.13;	
rOM_1 <-	NOD\$Conc.1;	rOM_2 <-	NOD\$Conc.14	;
srOM_1 <-	NOD\$Sorb.1 ;	srOM_2 <-	NOD\$Sorb.14;	
sOM_1 <-	NOD\$Conc.2;	sOM_2 <-	NOD\$Conc.15	;
ssOM_1 <-	NOD\$Sorb.2 ;	ssOM_2 <-	NOD\$Sorb.15;	
iOM_1 <-	NOD\$Conc.3;	iOM_2 <-	NOD\$Conc.16	;
siOM_1 <-	NOD\$Sorb.3 ;	siOM_2 <-	NOD\$Sorb.16;	
hetOM_1 <-	NOD\$Conc.4;	hetOM_2 <-	NOD\$Conc.17	;
shetOM_1<-	NOD\$Sorb.4 ;	shetOM_2<-	NOD\$Sorb.17;	
aNS_1 <-	NOD\$Conc.5;	aNS_2 <-	NOD\$Conc.18	;
saNS_1 <-	NOD\$Sorb.5 ;	saNS_2 <-	NOD\$Sorb.18;	
aNB_1 <-	NOD\$Conc.6;	aNB_2 <-	NOD\$Conc.19	;
saNB_1 <-	NOD\$Sorb.6 ;	saNB_2 <-	NOD\$Sorb.19;	
NH4_1 <-	NOD\$Conc.7;	NH4_2 <-	NOD\$Conc.20	;
sNH4_1 <-	NOD\$Sorb.7 ;	sNH4_2 <-	NOD\$Sorb.20;	

#### Appendix

NO2_1 <-	NOD\$Conc.8;	NO2_2 <-	NOD\$Conc.21	;
sNO2_1 <-	NOD\$Sorb.8;	sNO2_2 <-	NOD\$Sorb.21;	
NO3_1 <-	NOD\$Conc.9;	NO3_2 <-	NOD\$Conc.22	;
sNO3_1 <-	NOD\$Sorb.9;	sNO3_2 <-	NOD\$Sorb.22;	
N2_1 <-	NOD\$Conc.10	;N2_2 <-	NOD\$Conc.23	;
sN2_1 <-	NOD\$Sorb.10;	sN2_2 <-	NOD\$Sorb.23;	
IP_1 <-	NOD\$Conc.11	;IP_2 <-	NOD\$Conc.24	;
sIP_1 <-	NOD\$Sorb.11;	sIP_2 <-	NOD\$Sorb.24;	
Tr_1 <-	NOD\$Conc.12	;Tr_2 <-	NOD\$Conc.25	;
sTr_1 <-	NOD\$Sorb.12;	sTr_2 <-	NOD\$Sorb.25;	

#create different plots which are plotted using the "zeichne" function

#three examples shown below

#also possible to print less observation node data. it will cause an error but do the plotting anyway

#plot O2 concentration over the domain zeichne(time,O2\_1,O2\_2)

#plot Nitrosonomas concentration over the domain
zeichne(time,saNS\_1,saNS\_2)

#plot het.MO concentration over the domain
zeichne(time,shetOM\_1,shetOM\_2)

#samples of plots
plot(time,NH4\_7,type="l",col="1")
#xlim=c(35,45),ylim=c(10,20)
plot(time,NO3\_7,type="l")

COD\_7 <-rOM\_7+sOM\_7+iOM\_7 plot(time,COD\_7,type="I") plot(time,saNS\_1,type="I")

#### 

#### END OF CODE

The following code addresses the effluent output file created by HYDRUS (effluent.out)

#when using RStudio, set working directory as shown below, than ctrl+A and ctrl+enter to run the complete code

#set working directory to actual hydrus file, e.g. .../temp/FILENAME
setwd("C:/hydrus/Temp/~Hydrus3D\_2xx/FILENAME")

#read effluent file
EFFLUENT <- read.table("effluent.out", header=F, sep="",dec=".", skip="4")</pre>

#while simulation is not finished - erase last row drop<-nrow(EFFLUENT) EFFLUENT<-EFFLUENT[-drop,]

#table to vector of each effluent conc.

- time <- EFFLUENT\$V1 O2 <- EFFLUENT\$V2 rOM <- EFFLUENT\$V3
- sOM <- EFFLUENT\$V4
- iOM <- EFFLUENT\$V5
- NH4 <- EFFLUENT\$V9
- NO2 <- EFFLUENT\$V10
- NO3 <- EFFLUENT\$V11
- N2 <- EFFLUENT\$V12
- P <- EFFLUENT\$V13
- tracer <- EFFLUENT\$V14
- COD <- rOM+sOM+iOM

#get the right print frame (max and min x-axis,y-axis values)

x <-length(time)

t <-time[x] minNH4 <- min(NH4) maxNH4 <- max(NH4) minNO3 <- min(NO3) maxNO3 <- max(NO3) maxCOD <- max(COD) minCOD <- min(COD)

#plot

plot(time,NH4,type="l")

plot(time,COD, col =1,type="l",xlim=c(0,t),ylim=c(minCOD,maxCOD), main="COD", xlab=expression("time" ~(hours)), ylab=expression("effluent concentration" ~~ (~mg~.~L^{-1})))

plot(time,NO3, col =1,type="l",xlim=c(0,t),ylim=c(minNO3,maxNO3), main="NO3-N", xlab=expression("time" ~(hours)), ylab=expression("effluent concentration" ~~ (~mg~.~L^{-1})))

plot(time,NH4,col =1,type="l",xlim=c(0,t),ylim=c(minNH4,maxNH4),main="NH4-N", xlab=expression("time" ~(hours)), ylab=expression("effluent concentration" ~~ (~mg~.~L^{-1})))

plot (time,COD, col =1,type="l",xlim=c(1000,t),ylim=c(minCOD,60), main="COD", xlab=expression("time" ~(hours)), ylab=expression("effluent concentration" ~~ (~mg~.~L^{-1}))) lines(time,rOM, col =2,type="l") lines(time,sOM, col =3,type="l") lines(time,iOM, col =4,type="l")

#statistical summary of all components summary(rOM) summary(sOM) summary(iOM) summary(COD)

summary(NH4)

summary(NO2)

summary(NO3)

#### 

END OF CODE

# 10.3 Content of the DVD

Folders:

- HYDRUS simulation files: h3d2 format working directories for all three systems, divided into subfolders for flow simulation and reactive transport simulation
- Input Data: hydraulic flow and final effluent concentrations provided by Dal Santo (2009), HYDRUS input Data
- R-Files: generated R-statistic files for the analysis, evaluation and statistical calculations of the simulation data including the used \*.csv sheets.

Files:

• PDF-version of this master thesis: Pucher 2015 Simulation of vertical flow filters for the treatment of domestic wastewater using sand and zeolite as filter material.pdf

# 11. Curriculum Vitae

Contact information

		Bernhard Pucher bernhard.pucher@gmail.com
Education		
	2013 – after date	Master program Water Management and Environmental Engineering, University of Natural Resources and Life Sciences (BOKU University), Vienna
	2005 – 2013	Bachelor program Civil Engineering, University of Natural Resources and Life Sciences (BOKU University), Vienna
	2004 – 2005	Civil Service with the Austrian Red Cross
	2004	High School degree, HTL Braunau, School for Electrical Engineering
Trainings		
	2015	HYDRUS wetland module short course (2 days),
		University of Natural Resources and Life Sciences, Vienna
	2015	Modelling constructed wetlands with BIO-PORE and the Hydrus wetland module (3 days),
		6 <sup>th</sup> International Symposium on Wetland Pollutant Dynamics and Control, 13 <sup>th</sup> to 18 <sup>th</sup> September 2015, York, UK
Work experier	nce	
	since 2008	Freelancer with Artex Art Services / Vienna Art Handling
	2013/7 – 2013/8	Internship with IBZ Civil Engineering, Braunau
	2003 – 2012	Several internships in shift operational labour conditions (KTM, AMAG, BORBET Austria, Wacker Chemie)
Further skills		
	Languages	German (native), English (excellent)
	IT proficiency	HYDRUS 2D/3D wetland module, AutoCAD 2015, SWMM, R-Statistic, ArcGIS 10
		Windows and Mac OS operating system, Microsoft Office, Adobe Photoshop
		Basic programming skills in C, C++ and Java
Interests		Road cycling, Cyclo-cross, Discgolf, Outdoor activities, Travelling

# 12. Affirmation

I certify, that the master thesis was written by me, not using sources and tools other than quoted and without use of any other illegitimate support.

Furthermore, I confirm that I have not submitted this master thesis either nationally or internationally in any form.

Vienna, 17<sup>th</sup> of November 2015