Eco-Hydraulic Modelling of Flow, Water Quality (Heavy Metals) in the Kristalbad Artificial Wetland (Enschede, NL)

QU YITING
February, 2016

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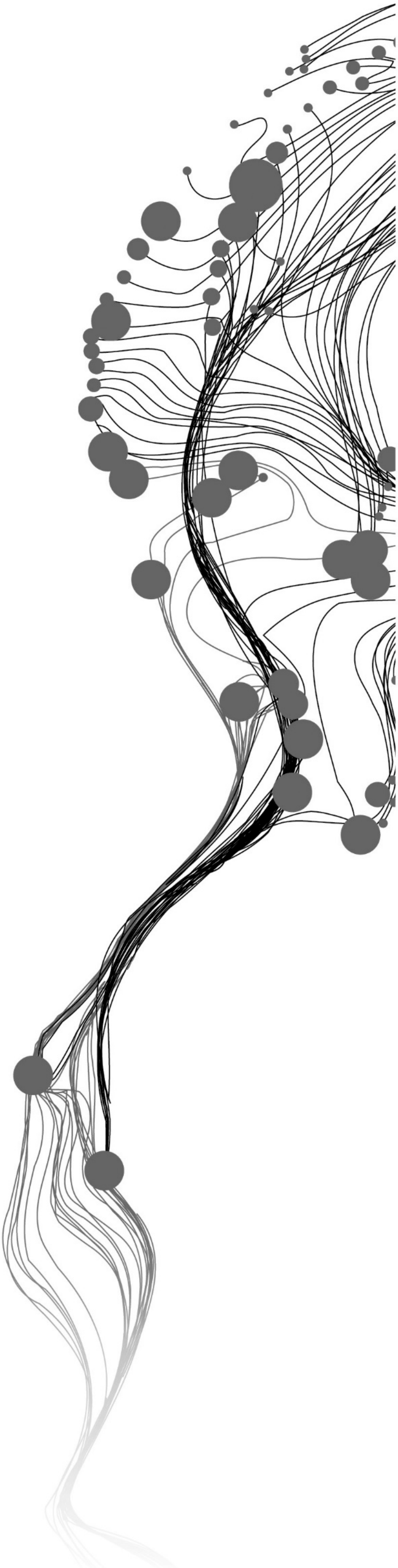
SECOND SUPERVISOR: Dr. Ir. S. Salama
External: Prof. Dr. X. Wang
CHAIR: Dr. M. Lubczynski



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Enschede, The Netherlands, February, 2016

Graduation Project (GP) submitted to the Faculty of Geo-Information Science and Earth Observation of the University of Twente in partial fulfilment of the requirements for the degree of Master in Geo-information Science and Earth Observation.
Specialization: Water Resources and Environmental Management

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ABSTRACT

Metals from domestic wastes and vehicle exhausts involved in water are treated by Waste Water Treatment Plant and will be further filtered by the Kristalbad system afterwards in Enschede in the Netherlands. The load of heavy metals is an important indicator of water quality in urban area. To estimate the heavy metals loads and carry out different scenarios under various flow conditions a hydrologic model is required. The study area Kristalbad is a multifunctional artificial wetland lying on the border of the municipalities of Enschede and Hengelo, beside the River Elsbeek draining the effluent from the sewage treatment plant in Enschede. The DUFLOW package is based on the one-dimensional partial differential equation that describes non-stationary flow in open channels and the sub model DUFLOW-METAL describes the fate of such common metals in urban as arsenic, copper, nickel, lead and zinc. As copper, nickel and zinc are usually of the highest amount in river such metals become the main focus in this study. In this research the functions and behaviours of Kristalbad on heavy metals under average flow, dry weather flow, wet weather flow and extreme condition will be studied with the sub model of DUFLOW, and also the sudden increase of metal for couple of hours will be simulated. The behaviour of the Kristalbad is analysed by comparing the simulated results under different scenarios and the function of it is assessed by calculating the removal efficiency of each part and the whole of the system.

Keywords: *urban water management, suspended matter, heavy metals, eco-hydraulic modelling, Geo-spatial data*

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1. INTRODUCTION

1.1. Background

The "Kristalbad" is a recently constructed artificial wetland infrastructure which came into use in 2012-2013. It is located between Hengelo and Enschede (Figure 1). It is a complex but challenging water management project because multiple water functions and ecosystem services are combined in such a limited area which are respectively storm water retention, water quality improvement, ecological connect, recreational and landscape management. The water in the Kristalbad comes largely from the urban sewage treatment plant effluent of Enschede-West and flows into the Elsbeek. This "water machine" was built for storm water retention and also intended to improve the water quality of the Elsbeek and downstream Bornse Beek systems. The system was inspired by proven methods of the Wetland Research Centre at the University of Halmstad in Sweden. The pond compartments of the Kristalbad are filled up alternately undergoing a diurnal filling – and - drainage cycle. Under the influence of light and air, biogeochemical processes in the water and sediment and aquatic vegetation there will be a purifying effect like breaking down and converting nutrients, carbon and other substances.

However, several questions in relation to its functioning, sustainability and impact still need to be answered. The hydraulic management (cycles) effects on the purification capacity of the system, growth of aquatic vegetation and the retention of other substances such as heavy metals, dissolved and particulate carbon still need to be observed and studied. The medium long term condition of the suspended matter coming from the Elsbeek and settling in the ponds, decomposition of aquatic weeds also requires further research. The growing conditions of aquatic plants and their effects on removing certain substances under the local circumstances are of great importance to the urban water quality. It is necessary to estimate the sensitivity and resilience of the system to externalities such as extreme weather events, high or low chemical loadings for assessing the functioning of the artificial wetland. Geospatial and satellite data may help with remote monitoring these water systems in additional to the traditional analysis approach under the simplified hydrologic model DUFLOW.

The present MSc studies will address a number of specific questions as phrased above. The research will be done in close cooperation with the regional water authority "Waterschap Vechstromen" and the municipality (Enschede city) in relation to the WWTP management.

In this study, focus is given to heavy metal contaminants in the wetland for which have been regarded as typical pollution source to receiving waters from urban catchments. For water quality managers are faced with many Dutch waters contaminants of heavy metals the metal load from the urban catchment area and resultant concentrations in the urban stream must be determined based on understanding the heavy metal absorption processes in Kristalbad.

The DUFLOW(Leidschendam, 1995) package is based on the one-dimensional partial differential equation that describes non-stationary flow in open channels. The sub model DUFLOW-METAL describes the fate of the metals arsenic (As), copper (Cu), lead (Pb), nickel (Ni), and zinc (Zn). Applications of the sub-model include studying the accumulation of heavy metals on the long-term in the bottom sediment and carrying out different management scenarios(Aalderink, 1997).

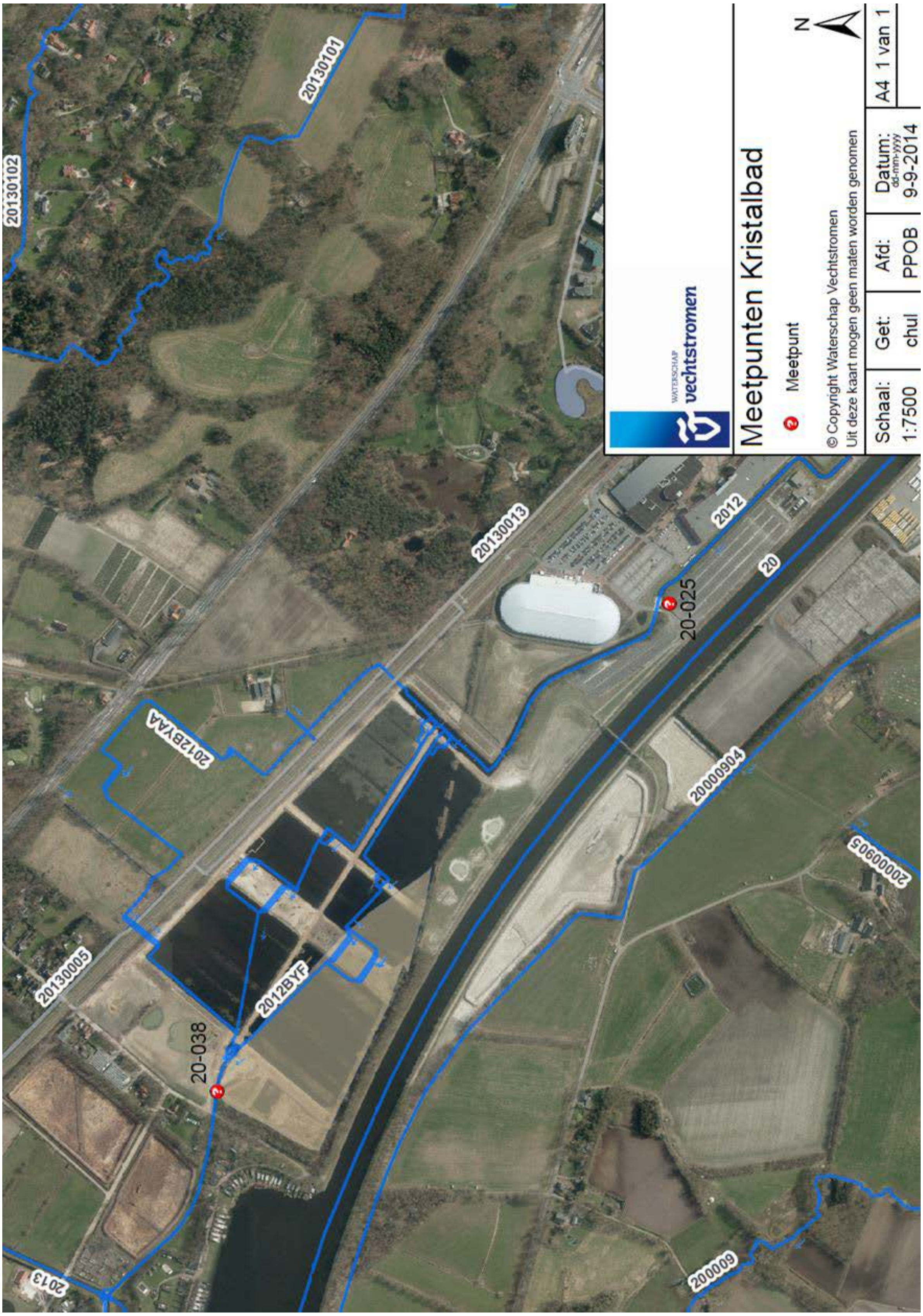


Figure 1 Overview of Kristalbad

1.2. Research Objectives

To assess the efficiency of the project Kristalbad, it's necessary to figure out the functioning and performance of the wetland. Heavy metal loads and suspended matter concentration is of great importance to indicate the water quality which requires a hydrologic model to estimate and predict.

- Analyze the heavy metal behavior and effect of the Kristalbad wetland system on removal in the water flows of the Elsbeek (carrying the effluents from the WWTP Enschede-west and draining through the wetland), using a simple mass balance and water quality process approach;
- Design an eco-hydraulic model for analyzing flow and heavy metal behavior in the Kristalbad, based on high resolution satellite and other geospatial data and generate a detailed geo-referenced physical eco-hydraulic modelling scheme of the wetland system;
- Evaluate the model suitability for simulating the Kristalbad wetland system and use the modelling system to evaluate flow and water management scenarios.

1.3. Research Problems and Questions

The wetland system consisting of three large ponds is hydraulically managed and alternatively filling and drying among the wetland ponds and diurnal water level changes in the system. The hypothesis here is that alternate filling and drying of the wetland ponds stimulates the removal of heavy metals.

The following research questions are to be answered to achieve specific objectives of the research:

- What impact does the Kristalbad have on heavy metal levels in waters of the Elsbeek draining the effluents from the WWTP Enschede-west?
- What major biogeochemical water quality processes occur in the wetland system respectively in relation to heavy metals?
- Is DMS suitable to simulate the heavy metal behavior and function of the artificial wetland?

2. LITERATURE REVIEWS

2.1. Reviews on Hydrologic Models

During the last two decades a couple of models were developed for constructed wetlands with differing purposes. Generally some groups of models can be distinguished: on one hand mechanistic models try to display the complex and diffuse interaction of occurring processes, on the other hand the same kind of models are used to investigate single processes (Daniel Meyer et al., 2015).

Table 1 Reviews on Hydrologic Models

Contributing modelling/simulation study	**Model used**	**Water flow**	**Biochemical processes**		**Additional processes**	**D**
			Species considered	Reactions		
Pálfy & Langergraber, 2013	HYDRUS/CW2D	Saturated and unsaturated (Richards eq.)	12<comma> incl. forms of COD<comma> N and P	9		2D
Morvannou, Choubert, Vanclooster, & Molle, 2014	HYDRUS/CW2D	Saturated and unsaturated (Richards eq.)	12<comma> incl. forms of COD<comma> N and P	9	Ammonium adsorption	2D
Pálfy & Langergraber, 2014	HYDRUS/CWM1	Saturated and unsaturated (Richards eq.)	16<comma> incl. forms of COD<comma> N and S	17	Heat transfer and root effects	2D
Rizzo et al., 2014	HYDRUS/CWM1	Saturated and unsaturated (Richards eq.)	16<comma> incl. forms of COD<comma> N and S	17	Ammonium adsorption	2D
Samsó & Garcia, 2013, and Samsó & García, 2013	BIO_PORE (COMSOL Multi-physics™)	Saturated (Darcy + adapting water table level)	18<comma> incl. forms of COD<comma> N and S	17	Root effects	2D
Forquet, Wanko, Molle, Mosé, & Sadowski, 2009, and Petitjean et al., 2012	Diph_M (MATLAB)	Unsaturated (two-phase flow)	forms of COD, NH4-N, oxygen	5		1D
Morvannou, Forquet, Vanclooster, & Molle, 2012	Dual-porosity model (DPM) in HYDRUS-1D	Saturated, unsaturated and preferential (Richards eq. + dual porosity)	0	0	Non-reactive tracer transport	1D

Claveau-Mallet, Wallace, & Comeau, 2012	PHREEQCP-hydroslag	Saturated	post treatment, no biochemical model	0	4 inorganic reactions	1D
Sani, Scholz, Babatunde, & Wang, 2013	Wang-Scholz-Model (COMSOL)	Vertical-flow wetlands with uniform water flow	no biochemical model	0	Clogging processes (particle setting)	1D
Zeng, Soric, Ferrasse, & Roche, 2013	RTD/GPS-X	Tanks in series with recycle and dead volumes under variable water content	12, incl. forms of COD, N (only soluble)	11	Interaction with biofilm growth	2D
D Meyer & Dittmer, 2014	RSF_Sim	Tanks in series with variable water content	no biochemical model	0	Transport, filtration, adsorption, degradation	1D,1.5D in future?

The most advanced reaction models are implemented in the Wetland Module of the HYDRUS software package (Langergraber & Šimuunek, 2005), based again on the mathematical formulation of the ASMs (Henze, 2000).

Duflow surface water hydrodynamic model aims to describe the behaviour of rivers in their natural conditions or state. As in all natural conditions inhomogeneities and inconsistencies do prevail, thus proving difficult to integrate all sub systems making up a single system. Despite that, Duflow within its limits generate results that can be applied in real life situations such as planning and construction of engineering structures, decision-making, and environmental conservation and wetlands management. The objective of this case study was to establish a design flood recommendable for mitigation by using Duflow surface hydrodynamic model. Various design flows are simulated against the different proposed structures hence, the optimal structure is finally recommended when economic, social and environmental constraints are considered in the decision making process. The measure of building a green-storage is the best and optimal structure for flood mitigation (Joleha, 2009).

2.2. Reviews on Heavy Metal Modelling

Elevated concentrations of heavy metals in natural soils and waters possibly deteriorate soil and water ecosystem functioning. Given the long times it takes for metal concentrations to reach steady state, the use of dynamic models should be considered to manage and evaluate the metal loads in time(Lofts et al., 2007). Moreover, key processes determining the fate of metals are related to properties such as pH and the concentration of dissolved organic matter (DOM), both being subject to changes due to external factors such as land use change, climate change and atmospheric deposition of nitrogen. Dynamic models help to understand the complex interactions of processes due to such external factors and give insight into the timescales at which changes take effect. Metal transfers in ecosystems are complex, but by identifying and quantifying key processes it is possible to produce useful descriptions of metal behaviour in soils and catchments with models that can be driven with limited data(Groenenberg, Tipping, Bonten, & Vries, 2015).

Smits (2004) presented a method to couple a surface-water-model built with Duflow, and a groundwater model built with MicroFem. The coupling software brings the results of both models in equilibrium with each other in an iterative way.

The model CHUM-AM (Chemistry of the Uplands Model—Annual Metals) was designed to describe metal behaviour in whole catchments including predictions of stream water concentrations (Tipping, Lawlor, & Lofts, 2006).

Wang, Yinglan, Jiang, Fu, & Zheng (2015) detected ten types of heavy metals during 2010–2013 for all ambient samples and point sources samples in Yunnan-Guizhou plateau and compared the multivariate approach (principle components analysis/absolute principle component score, PCA/APCS) and the chemical mass balance model (CMB) which shows that the identification of sources and calculation of source contribution based on the CMB were more objective and acceptable when source profiles were known and source composition was complex. The peak concentrations of many heavy metals (Cu, Ba, Fe, As and Hg) were found in the middle layer of sediment. However, the highest concentration of Pb appeared in the surficial sediment layer.

The sub model METAL of DUFLOW describes the behaviours of heavy metals. It is based on a model developed in the context of a Research on the Vecht (Duin, Portielje, & Aalderink, 1994). This model describes the fate of the metals arsenic (As), copper (Cu), lead (Pb), nickel (Ni), and zinc (Zn). The applications of the model are in the study of the accumulation of heavy metals on the long-term in the bottom sediment. The model is suitable to carry out different management scenarios. The model also can be used to examine the effect of changes in inlet strategies, in relation to the spread of contaminants. Another application is the prediction of the speed and degree of loading of soils. This is important, inter alia, to assess the usefulness of water decontamination. The model can predict for example, whether and how quickly sediment gets contaminated again after remediation.

3. DATA AND METHODS

3.1. Study Area Description

The Kristalbad is a recently constructed artificial wetland infrastructure which came into use in 2012-2013. It is located at 52.2472N, 6.8277E, on the border of the municipalities of Enschede and Hengelo, to the north of the Twente Canal and south of the Hengelosestraat/Enschedesestraat (Figure 1 Overview of Kristalbad). The railway Hengelo-Enschede cuts through the area. The Kristalbad has an area of 40 hectares and the area of the wet parts of which is approximately 34.7 hectares.

The project provides a solution to create runoff from Enschede at Hengelo the wide dispersal of the area, natural water treatment and the need for more recreation. The reasons for the refurbishment of the Enschede-North are bottlenecks in agriculture, water management, nature, landscape, recreation, environment and amenities. In addition, the city's need for a different organization of the outskirts emerged. The project is part of the 'development plan Enschede North'. In developing the Kristalbad is the multifunctional land between the two largest cities of central Twente.

It is a complex but challenging water management project because multiple water functions and ecosystem services are combined in such a limited area which are respectively storm water retention, water quality improvement, ecological connect, recreational and landscape management. The water in the Kristalbad comes largely from the urban sewage treatment plant effluent of Enschede-West and flows into the Elsbeek. This "water machine" was built for storm water retention and also intended to improve the water quality of the Elsbeek and downstream Bornse beek systems. The system was inspired by proven methods of the Wetland Research Centre at the University of Halmstad in Sweden. The pond compartments of Kristalbad are filled up alternately undergoing a diurnal filling – and - drainage cycle. Under the influence of light and air, biogeochemical processes in the water and sediment and aquatic vegetation there will be a purifying effect like breaking down and converting nutrients, carbon and other substances.

The main concern of the function is on purifying water. The water machine purifies water from the sewage treatment plant. The area consists of three sections (Figure 2). By sliding each of these sections successively each is full of water for a set time period, like 4 or 6 hours, flows away in the same set time period to get empty, and stands dry for another certain period (Figure 3).

The idea behind the water machine is that in dry weather flow (DWF) compartment I fills for four hours while compartments II and III emptying himself (from the Kampf & van den Boomen, 2013). After this compartment II filled compartments while I and III are empty. Finally fills compartment III himself and empty compartments I and II himself. This cycle is repeated every 12 hours. During the eight hours a compartment empties a portion of the fund will partially dry. This allows for the dynamic system in the Kristalbad. At high supplied flows or rainwater flow (RWF), the cycle will not be applied, because the water then will be on the thresholds of the distribution basin flow into the compartments. In this case the Kristalbad functions as retention. In practice it has been found that an empty and fill cycle of 12 hours is too short to allow the flood plain to get dry, the cycle will be a minimum of 32 hours. Since December 2014, the water machine is set so that a compartment fills for 1200 minutes (20 hours). Thus, the cycle currently stands at 60 hours instead of 12 hours.

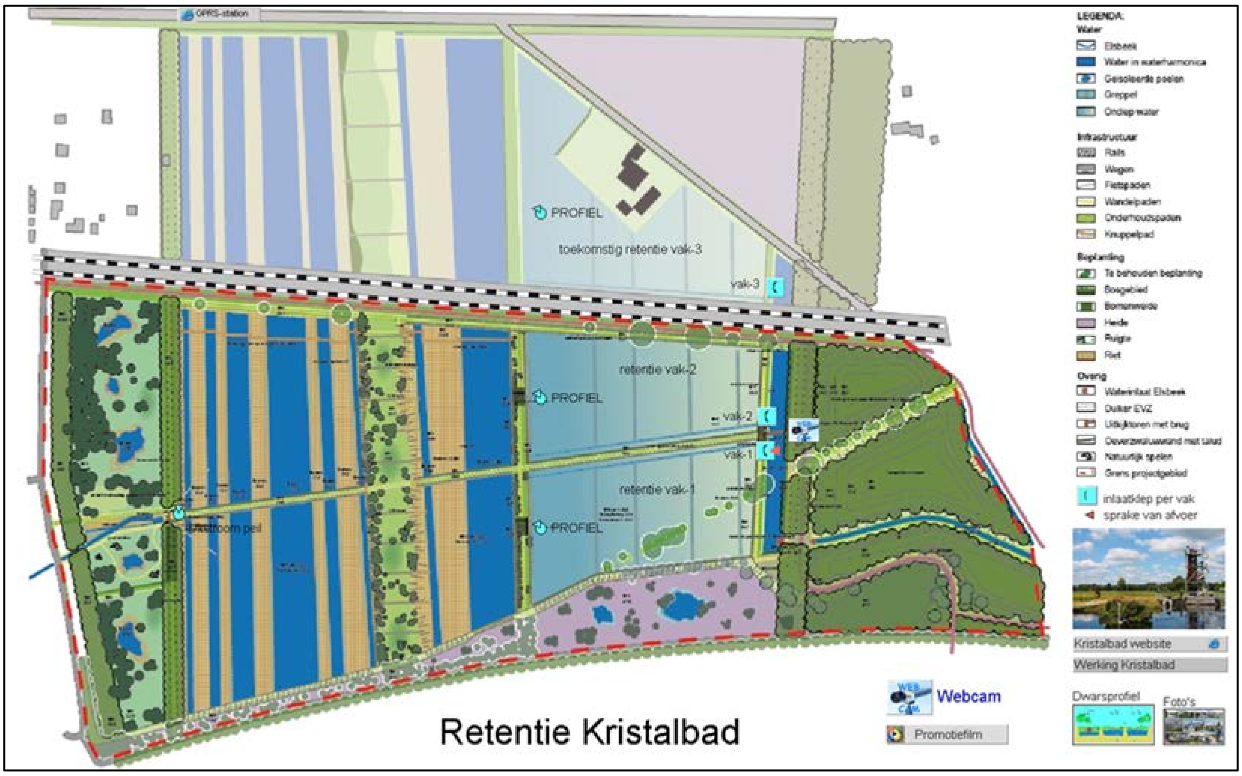


Figure 2 Schematization Information of Kristalbad

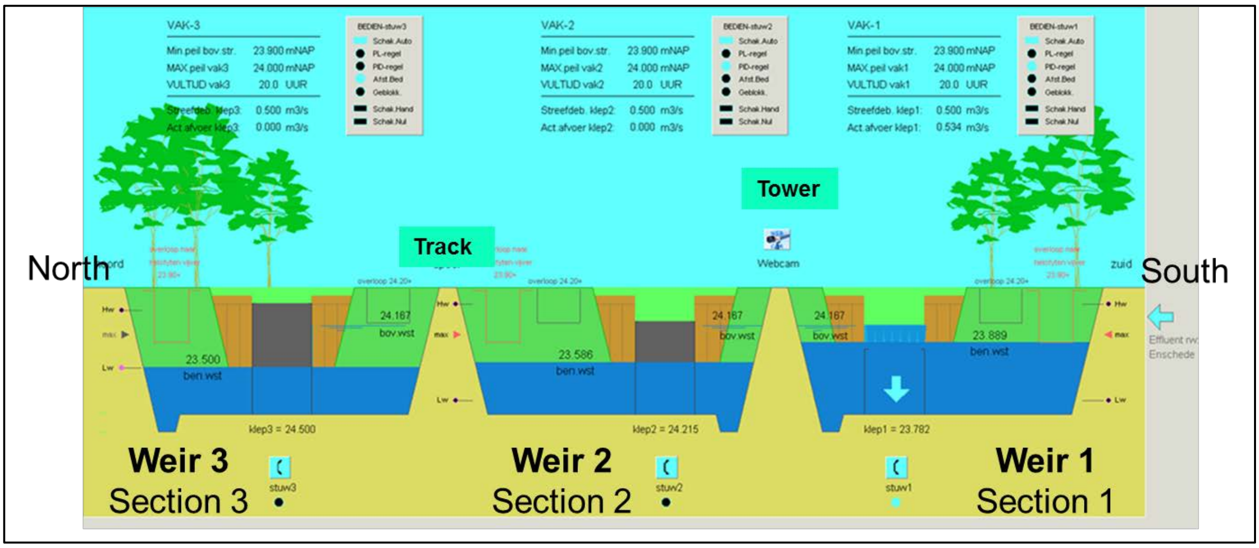


Figure 3 Water Buffer of Kristalbad (vertical scaling)

3.2. Data requirements

3.2.1. Geo-Spatial Data

To analyze the behavior and removal processes of heavy metals in Kristalbad, the flow and water level of Kristalbad will be estimated with DUFLOW flow model, the transport and removal efficiency of heavy metal is going to be simulated with the sub model METAL of DUFLOW.

Remote sensing data and Geo spatial data need to be pre-processed which includes importing images, choosing the study area, geometric correction, image enhancement and so on. As a result a detailed background map in '.dif' format can be created.

To design the model scheme high resolution remote sensing data is needed. Here the PAN image of SPOT 6 with resolution of 1.5m on May 24th in 2015 and multi spectral image of SPOT 6 with resolution of 6m on the same day is used. The DTM data of AHN 02 with resolution of 0.5m ((Waterschapshuis, 2015) is also used for the floor level part in the model scheme. GIS data in Shapefile format with spatial information and hydraulic structure details from water authority will help build a geo-referenced model and form a complex network.

3.2.2. Field Data

After the network is built in DUFLOW it requires a field check to see if the geo-referenced model exact or not. If there is any inaccuracy the calibration must be carried out according to field work.

Statistics from water authority and previous research are also needed. As can be seen in Table 2 the concentration of heavy metals of different sampling points in Kristalbad on 2014-11-28 has been analyzed in previous research in Kristalbad (Rebecca Naomi Ter Borg, 2015). From the same source is also the water level information.

Table 2 Analysis Results on Heavy Metal from Previous Research

Sampling Point	As	Cu	Pb	Ni	Zn	Dimension
Project Kristalbad water sample inlet	0.83	5.4	0.72	10	100	μg/m³
Project Kristalbad soil sample 1	<2	<2	<2	1.9	<10	mg/kg ds
Project Kristalbad soil sample 2	<2	<2	<2	1.5	<10	
Project Kristalbad soil sample 3	<2	<2	<2	2.5	<10	
Project Kristalbad soil sample 4	<2	<2	<2	1.9	<10	

The data mentioned above was sampled at the points in the Kristalbad shown in Figure 4:

Figure 4 Locations of the soil samples in the Kristalbad

3.3. DuFlow Model

3.3.1. DuFlow Modelling Studio (DMS)

The package as a whole is called Du(tch)flow. The computational core of this model is based on the FORTRAN computer code IMPLIC which is originally developed by the Rijkswaterstaat. In the Water Quality part the process descriptions can be supplied by the user. The DUFLOW package is based on the one-dimensional partial differential equation that describes non-stationary flow in open channels. For the flow model part the network will be built upon GIS data and remote sensing data and the water level and water flow will be simulated.

Duflow is designed to cover a large range of applications, such as propagation of tidal waves in estuaries, flood waves in rivers, operation of irrigation and drainage systems, etc.

3.3.2. Water transport Model

DUFLOW is based on the one-dimensional partial differential equation that describes non-stationary flow in open channels ((Abbott & Minns, 1998).

These equations, which are the mathematical translation of the laws of conservation of mass and of momentum, read:

Equation (1):

$$\frac{\partial \mathrm{B}}{\partial \mathrm{t}} + \frac{\partial Q}{\partial x} = 0$$

and

Equation (2):

$$\frac{\partial \mathrm{Q}}{\partial \mathrm{t}} + gA\frac{\partial H}{\partial x} + \frac{\partial(\alpha Q v)}{\partial x} + \frac{g|Q|Q}{C^2 AR} = a\gamma w^2 \cos(\Phi - \emptyset)$$

While the relation:

Equation (3):

$$\mathrm{Q} = \mathrm{v} \cdot \mathrm{A}$$

Holds and where:

t : time [s]

x: distance as measured along the channel axis [m]

H (x, t): water level with respect to reference level [m]

v (x, t): mean velocity (averaged over the cross-sectional area) [m/s]

Q (x, t): discharge at location x and at time t [m^3/s]

R (x, H): hydraulic radius of cross-section [m]

α (x, H): cross-sectional flow width [m]

A (x, H): cross-sectional flow area [m^2]

b(x, H): cross-sectional storage width [m]

B (x, H): cross-sectional storage area [m^2]

g: acceleration due to gravity [m/s^2]

C (x, H): coefficient of De Chézy [$m^{1/2}/s$]

$w(t)$: wind velocity [m/s]

$\Phi(t)$: wind direction in degrees [degrees]

$\emptyset(x)$: direction of channel axis in degrees, measured clockwise from the north [degrees]

$\gamma(x)$: wind conversion coefficient [-]

α: correction factor for non-uniformity of the velocity distribution in the advection term, defined as:

$$\alpha = \frac{A}{Q^2} \int v(y,z)^2 dydz$$

where the integral is taken over the cross-section A. [m^2]

The mass equation (Equation (1) states that if the water level changes at some location there will be the net result of local inflow minus outflow. The momentum equation (Equation (2) expresses that the net change of momentum is the result of interior and exterior the forces like friction, wind and gravity.

For the derivation of these equations it has been assumed that the fluid is well-mixed and hence the density may be considered to be constant.

The advection term in the momentum equation $\frac{\partial(\alpha Qv)}{\partial x}$ can be broken into $\alpha\left(2\,\frac{Q}{A}\,\frac{\partial Q}{\partial x} - \frac{Q^2}{A^2}\,\frac{\partial A}{\partial x}\right)$

The first term represents the impact of the change in discharge. The second term which expresses the effect of change in cross-sectional flow area is called the Froude term. In case of abrupt changes in cross-section this Froude term may lead to computational instabilities.

Equation (1 and Equation (2 are discretized in space and time using the four-point implicit Preissmann scheme.

A mass conservative scheme for water movement is essential for proper water quality simulation. If the continuity equation is not properly taken into account, the calculated concentration will not match the actual concentration. The mass conservative scheme is based on the fact that the error made in the continuity equation will be corrected in the next time step. Mass conservation is therefore guaranteed. The method used for this scheme is described in Booij, 1980.

For a unique solution of the set of equations additional conditions have to be specified at the physical boundaries of the network and at the sections defined as hydraulic structures. The user-defined conditions at the physical boundaries may be specified as levels, discharges or a relation between both, for instance a (tidal) elevation H, a discharge Q, or a so-called QH relation. At internal junctions the (implicit) condition states that the water level is continuous over such a junction node, and that the flows towards the junction are in balance since continuity requires:

Equation (4):

$$\sum_{J=1}^{JJ} Q_{i,j} + Q_i = 0$$

Where:

I: indication for the junction node

$Q_{i,j}$: discharge from node j to node i

q_i: additional or lateral flow to node i

The above equations are solved at each time step. They are transformed into a system of (linear) equations for the water levels. Equation (4 is not used in nodes where a water level is prescribed as boundary condition. In such a node no equation is needed because the water level is already known. Discharge boundary conditions are taken into account as the additional flow q_i.

To start the computations, initial values for H and Q are required. These initial values must be provided by the user; they may be historical measurements, obtained from former computations or just a first reasonable guess.

Additionally wind stress and rainfall conditions can be specified.

Various types of control structures can be defined such as weirs, culverts, siphons and pumping stations. Here in this study, weirs, culverts and general structures are defined for the network (Figure 5). At weirs and other structures discharges and levels can be controlled by manipulating the gates. DUFLOW allows for specification of such an operation using the so-called trigger conditions: depending on flow conditions at specified locations in the network, parameters such as the width of the weir, the level of the sill etc. can be adjusted during the computation. A common characteristic of structures is that the storage of water inside the structure is negligible compared with the storage in the open channels. The definition of flow direction in a structure is the same as the definition in ordinary channel sections, flow from the begin node to the end node is assumed to be positive. The discharge over a weir depends on the water level at both sides, the level of the sill, type of structures and the flow condition.

Figure 5 Hydraulic Structures in the Kristalbad

3.4. Water Quality Model: Model METAL

3.4.1. Processes and Transport in the Model METAL

Water quality managers are faced with many Dutch waters contaminants of heavy metals. The model METAL describes the behavior of heavy metals. It is based on a model developed in the context of a Research on the Vecht.

The following processes are described in the sub model *METAL*:

- Sorption of metal by solid (fraction < 16 mm), dissolved and particulate organic material (including algae)
- The effect of pH and chloride is taken into account for the calculation of the partition coefficient, but both cannot be modeled. However, there is the possibility to specify pH and chloride as the external variable
- Deposit of the heavy metals with sulfide under the sediment reducing conditions
- Dissolved and particulate organic material exchanges between soil and water column
- Heavy metals exchanges between bottom sediment and water column
- Net sedimentation and burial of sediment material

Besides the description of the sediment, water exchange, the transport of particulate, bound contaminants and the distribution of the pollution over a dissolved and a solids fraction bound, the behavior of suspended matter should also be described in this model. A simple approach is opted in the model for heavy metals as well as the model for organic contaminants where the behavior of a fraction of suspended solids in the water column is described assuming that sedimentation and resuspension are concurrent. However, a distinction is made between organic and inorganic suspended material. Resuspension flux itself is not calculated in this model. It should be specified by the user for the calculation. The interaction for organic contaminants with the bottom is described by means of the exchange with an active top layer in the model as well. The thickness of this layer is also assumed constant in this model. Compared with the model for organic contaminants the description of the sediment water exchange is somewhat more complex. The behavior of heavy metals in the active sediment top layer is different between oxidized and reduced layer. This is because the character of the adsorption of metal strongly depends on the redox conditions. The oxidized surface layer is often thin and contains only a small portion of the total amount of metal in the sediment, but this top layer determines the flux of the metal across the water- sediment interface. Among the active top layer is an inert layer with which the concentrations are assumed to be constant. The concept is schematically displayed in Figure 5.

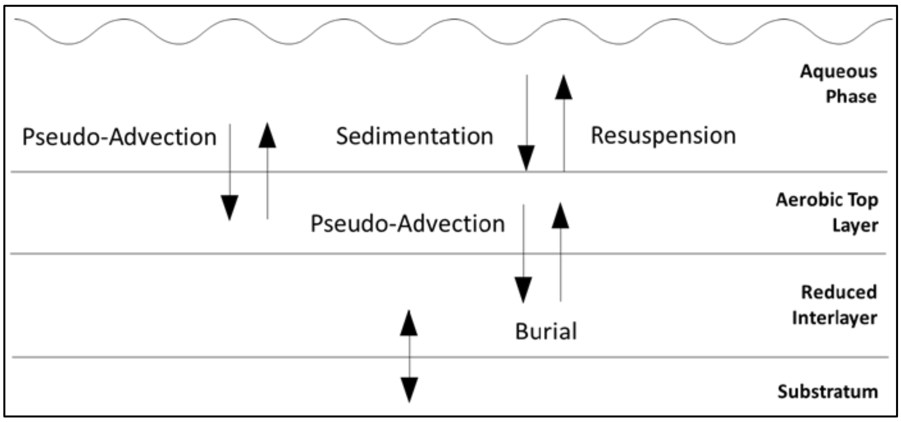


Figure 6 Behavior of suspended matter and Interaction of suspended particulate matter with the bottom

Since sorption plays an important role in the behavior of heavy metals, the behavior of sorbents is also described in detail. Balances are tracked by floating substance, particulate and dissolved organic matter, and algae.

Figure 6 shows an overview of the transport processes in the model. Exchange of dissolved metal as well as the DOC bound metal is described with a diffusion term. The diffusion takes place over all the three boundary layers in the system. The same also applies to the pseudo- advective transport which occurs as a result of net sedimentation or net resuspension. Due to the pseudo-advection the boundary layer shifts. Pseudo advection is also used for the metals which are adsorbed to the sediment. However, this exchange process does not apply to the water column -sediment top layer boundary. Finally the exchange of suspended solids bound metals over the interface between the water column and sediment top layer is described. Such exchange is controlled by sedimentation and resuspension.

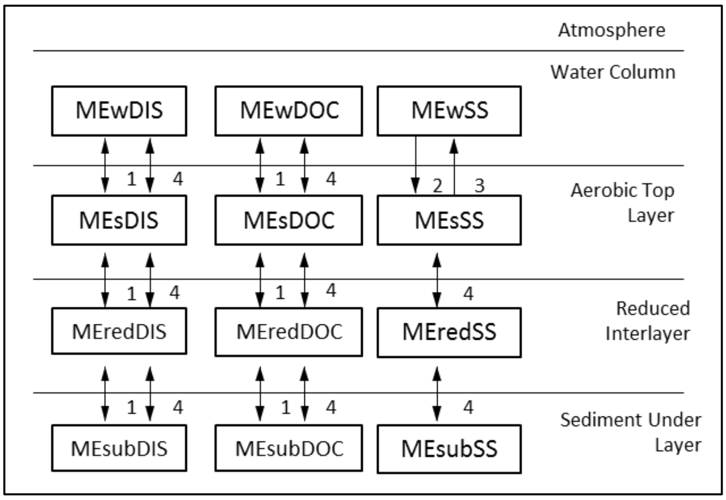


Figure 7 Schematic Overview of Processes and Transport in the Model METAL

[1] Diffusive exchange, [2] Sedimentation, [3] Resuspension, [4] Pseudo-advection

The specific entry for the METAL sub model consists of 4 parts which are respectively: initial conditions (Table 3), boundary conditions (Table 4), parameters (Table 5) and external variables (Table 10). Some of the parameters need to be calibrated.

3.4.2. Initial Conditions

For the water column five state variables can be defined. For each of these variables, the state must be specified at time zero. The initial state is often estimated on the basis of measurements. However, this is always not easy for complex networks. In such cases, an estimation of the initial conditions can be made by performing a preliminary simulation. The concentration of AOCW can be estimated from the chlorophyll -a content where the carbon / chlorophyll ratio in the algae is assumed as a constant. The POCW content can possibly be estimated from the glow loss of the floating substance.

In addition to the state variables for the water column in this model three state variables for the bottom are also defined. For these variables a good estimate of the initial conditions is of great importance. Since the processes in the bottom and also the exchange with above the water column proceeds very slowly, an erroneous choice of the initial concentration in the bottom will influence the results of a simulation. It is advisable to follow the progress of the simulated concentrations of these substances in the bottom for which is easy to follow. If one system is assumed in balance, concentrations in bottoms may not change greatly after years of constant load. In addition to a wrong choice of initial concentrations or load a wrong estimation of process or exchange rates can also give rise to highly varying concentrations in the sediment.

Finally, for the concentrations of DOC, POC and the heavy metals in the sublayer an initial condition should also be specified. It is believed that these levels remain constant. In the model it subjects to any process. In fact, this can be defined as an external variable. However, they are included as state variables since in this way it is easier to assign a value to such concentrations for each section. This also applies to the variable S, the total content of inorganic sulfur in the bottom. The total inorganic sulfur is only used to determine whether the metal sulfide in the reduced sub-layer is important or not. If the total S content is higher than a certain threshold value, it is believed that the concentration of dissolved metal is determined by the solubility product of the metal sulfide. In the model a fixed limit of 3.0 g S / kg sediment is observed.

Table 3 Initial conditions for water column required in METAL model as entry

Type	Source	Name	Typical Value
Water Column	Measurement / Estimation	ME_WTOT (As, Cu, Pb, Zn, Ni)	g ME.m^{-3}
		POC_W	g POC.m^{-3}
		DOC_W	g DOC.m^{-3}
		AOC_W	g AOC.m^{-3}
		SS_W	g SS.m^{-3}
Sediment	Measurement / Estimation	ME_sTOT (As, Cu, Pb, Zn, Ni)	g ME.m^{-3}
		$ME_{red}T$	g ME.m^{-3}
		$ME_{sub}T$	g ME.m^{-3}
		DOC_B	g DOC.m^{-3}
		POC_B	g POC.m^{-3}
		DOC_{SUB}	g DOC.m^{-3}
		POC_{SUB}	g POC.m^{-3}
		S	g S.m^{-3}

3.4.3. Boundary Conditions

Both of the edges to simulate system and all discharges in the system serve as five state variables of the water column parameters are to be specified. The system boundary is often estimated on basis of measurements. If data is not sufficient the system boundary should be accurately defined. This boundary must be selected in a way that the boundary conditions do not influence the result of the calculation at the interested point.

Point source discharges are also considered as boundary conditions in Duflow. For all the state variables the quality of the discharge must be given. This means the quality must be assigned to all the water enters the system. Basically it comes down to that a quality boundary condition should also be assigned to all boundary conditions of the water transport model.

The initial conditions for the POCW can also be estimated from the loss on ignition of the suspended matter. The AOCW content is calculated from the chlorophyll-a concentration. However it can be assumed that for many point sources the chlorophyll content is equal to zero.

According to the balance equations total metal concentrations will be sufficient for the heavy metal with the given total content in discharges and in the system boundaries.

Table 4 Boundary conditions required in METAL model as entry

Type	Source	Name	Typical Value
System Boundary	Measurement / Estimation	ME_WTOT (As, Cu, Pb, Zn, Ni)	g $ME.m^{-3}$
		POC_W	g $POC.m^{-3}$
		DOC_W	g $DOC.m^{-3}$
		AOC_W	g $AOC.m^{-3}$
		SS_W	g $SS.m^{-3}$
Point Discharges	Measurement	C_WTOT (As, Cu, Pb, Zn, Ni)	$g.m^{-3}$
		POC_W	g $POC.m^{-3}$
		DOC_W	g $DOC.m^{-3}$
		AOC_W	g $AOC.m^{-3}$

3.4.4. Parameters

Table 5 Parameters required in METAL model as entry

Name	Description	Source	Typical Value
α	POC fraction released by dying algae	Literature[1]	0.5 – 1.0
DZ1	Thickness aerobic top layer of sediment	Measurement/estimation	0.05-0.02 m
DZ2	Reduced sediment thickness interlayer	Measurement/estimation	0.05-0.02 m
$\boldsymbol{E_Z}$	Effective diffusion constant	Literature[5]	5.10^{-5} $m^2.day^{-1}$
FC	Carbon / dry substances ratio	Literature[1,3]	0.52 g C. g $Substance^{-1}$
FWX	Percentage of particulate matter < 16 μm		System specific
FBX	Percentage of sediment particles < 16 μm		System specific
MESulf	Constant concentration of dissolved metal in sufficient inorganic S	Literature	See Table 6
$\boldsymbol{K_{ME}SSW}$	Partition coefficient of airborne substances in the water column	Literature	See Table 9
$\boldsymbol{K_{ME}DOC}$	Partition coefficient of DOC	Literature	See Table 7

$K_{ME}SS$	Partition coefficient based on adsorption equivalents	Literature	See Table 8
$K_{hyd,W}$	Hydrolysis rate of POC in water	Literature[1,3]	10^{-2}-10^{-3} day^{-1}
$K_{hyd,B}$	Hydrolysis rate of POC in sediment		10^{-4}-10^{-3} day^{-1}
$K_{d,min,W}$	Mineralization speed of POC in water	Literature[1,3]	10^{-2}-10^{-3} day^{-1}
$K_{d,min,B}$	Mineralization speed of POC in sediment		10^{-4}-10^{-3} day^{-1}
POR	Porosity of top layer	Measurement/estimation	System specific
ϱANO	Density of inorganic substance	Literature	2600.10^3 $g.m^{-3}$
ϱORG	Density of organic matter	Literature	1000.10^3 $g.m^{-3}$
V_{SN}	Sedimentation rate of organic matter	Literature[1,4]	0.3 – 2.0 $m.day^{-1}$
V_{SP}	Sedimentation rate of algae		0.05 – 0.1 $m.day^{-1}$
V_{SS}	Sedimentation rate suspended solids		2-10 $m.day^{-1}$

Sources: [1] Jorgensen & Gromiec, 1989, [2] Sven Erik Jorgensen, 2013, [3] Bowie & Tech, 1985, [4] Brown & Barnwell, 1987, [5] Portielje, 1994

The thickness of the oxidized surface layer DZ1 depends on the depth of penetration of oxygen and nitrate. Under this layer there is a layer where iron is reduced. This is important since heavy metals are mainly attached to Fe (III) - (hydr) oxides which are formed under oxidizing conditions. In the reduced layer where iron presents as Fe (II) the complexes are more soluble, and under the condition where sufficient inorganic sulfur presents the concentrations of the metal in dissolved form usually determine the solubility product of the corresponding metal sulfide. The metal sulfides precipitate in the pores of the reduced layer and form an insoluble complex.

Table 6 provides an overview of the maximum soluble metal concentration in the pore water with excessive sulfide. From the table it appears that the precipitation with sulfide plays an important role for Cu and Pb. The concentrations of these metals are indeed very low. The precipitation with sulfide does not play a significant role for Arsenic. In the reduced layer the adsorption of As is therefore determined by complex formation of DOC and adsorption of the solid.

Table 6 Dissolved metal concentration in the pore water by forming metal sulfides

Metal	Constant concentration of dissolved metal
Cu	0.003
Zn	0.01
Ni	0.025
Pb	0.003

The penetration depth of oxygen is usually in the range of 0.5 - 2.0 cm, and depends on the effective diffusion coefficient and the aerobic mineralization consumption of oxygen in the pore water. Of course the oxygen concentration in the above water is also important.

Although the oxidized surface layer is thin and therefore only represents a small proportion of the total amount of the heavy metals in the water bottom this layer is important for the fluxes of dissolved metal over the sediment - water interface. Namely the thickness of this layer determines the concentration gradient at the interface.

The partition coefficients of metals in DOC are calculated from the stability of the complexes of the metal with humus. This amounts for copper 7.5, nickel 4.8, lead 5.6 and zinc 4.7 (Buffle, 1990). It has been taken as a starting point that humus is the main component of dissolved organic carbon. The stability constant is given by:

Equation (5):

$$K_{0.3} = \frac{[MEHUM]}{[ME] \cdot [HUM]}$$

Where:
$K_{0.3}$: the equilibrium constant is (-)
[MEHUM]: the concentration of the metal humus complex (= 1)
[ME]: the concentration of dissolved metal ($g \cdot m^{-3}$)
[HUM]: the concentration of humus (g DOC $\cdot m^{-3}$)

Table 7 shows the calculated partition coefficients of metal in DOC. The conversion of equivalents to mass is adopted that the mass of per mole humus amounts 1000 equivalents and humus is composed of 50% carbon. The water system model Vecht (Duin et al., 1994) showed that the calculated value for Cu was too high. A value of 0.5 $m^3 \cdot g$ DOC^{-1} was determined by calibration.

Table 7 Partition Coefficients for DOC

Metal	Partition Coefficients $m^3 \cdot g$ DOC^{-1}
As	$10 \cdot 10^{-6}$
Cu	24 (Vecht 0.5)
Zn	0.10
Ni	0.10
Pb	1.02

The partition coefficients of solids in the bottom are calculated in the model. These can be optionally adjusted for pH and chloride. The table below gives some typical values of the constants in these equations.

Table 8 Uncorrected partition coefficients on the basis of adsorption - equivalents (KMESS ') and the correction factors for pH (a) and salinity (b)

Variable	KMESS'(l/eq·10^{-6})	a	b
As	0.003	0	0
Cu	0.085	1.25	$-5.39 \cdot 10^{-5}$
Ni	0.010	-	
Pb	0.231	1.176	$-6.59 \cdot 10^{-5}$
Zn	0.020	1.358	$-8.06 \cdot 10^{-5}$

In literature the partition coefficients of suspended solids in the water column vary greatly. In Table 9 some values are given to be applied in a number of models. The model Heavy Metals has been developed and applied to study at the Vecht. The partition coefficients for Cu, As and Zn for the Vecht are determined by calibration.

Table 9 Some values for the partition coefficients of suspended silt in the water column ($m^3 \cdot g^{-1}$)

Variable	Horizon range	Horizon medi0.044an	SOM3	DBW/RIZA	ZWMET
As	0.003-0.029	0.014	0.0002	0.01	0.1
Cu	0.026-0.052	0.044	0.11	0.05	0.050
Ni	0.003-0.016	0.008	-	0.008	0.008
Pb	0.092-0.468	0.177	0.6	0.640	0.64
Zn	0.027-0.13	0.042	0.1	0.11	0.22

Koelmans & Radovanovic (1996)have developed a model that predicts the overall partition coefficients for a number of metals (Cd, Cu, Pb, Ni and Zn) in the water column on the basis of a number of separate macro chemical environment variables (such as: chloride, pH, EC and sulfate) and characteristics of the floating sludge (e.g. organic carbon, total Fe and Mn content, CEC, etc.). Besides the complex model which requires detailed input from a large number of environmentally variables Koelmans and Radovanovic also present some simple regression equations where a reasonable estimate of the partition coefficient can be obtained.

3.4.5. External Variables

The dispersion constant serves as the external variable to be entered. The production rate of algal biomass (AOC) is not described in the model and should be specified by the user. This could possibly be calculated by means of one of the eutrophication models and are entered as a function of time. A distributed resource is considered in the balance equation for all metals. It can be used, for example, to bring the atmospheric depositions or other non-point sources into account.

Table 10 External variables required in METAL model as entry

Name	Description	Source	Typical Value
D	Dispersion constant	Literature	System specific
F_{res}	Resuspension flux	Literature	System specific
ME_{atm}	Diffuse source	Mass balance	System specific
P_{AOC}	Production speed AOC	Literature	System specific

In addition to the output of the state variables a large number of the processed values in the model can be worked out as a function. A number of potentially interesting variables are listed in Table 11.

Table 11 Overview of a number of variables as functions to carry out

Symbol	Description	Unity
ϱSSW	Suspended solids water column density	$g.m^{-3}$
ϱSSB	Solid sediment density	$g.m^{-3}$
V_R	Pseudo - advective transport speed due to resuspension	$m.day^{-1}$
V_S	Pseudo - advective transport speed due to sedimentation	$m.day^{-1}$
$Fc_{SS,B}$	Organic matter fraction in the water column	-
$Fc_{SS,W}$	Organic matter fraction in the water sediment	-
FSPOC	POC content in solid bottom	$g\ POC.\ g\ substance^{-1}$
$ME_W DIS$	Concentration of metal dissolved in water column	$g.m^{-3}$
$ME_W DOC$	Concentration of DOC associated metal in water column	$g.m^{-3}$
$ME_W SS$	Concentration of SS associated metal in aerobic top layer	$g.m^{-3}$
$ME_{red} DIS$	Concentration of dissolved metal in the reduced intermediate layer	$g.m^{-3}$
$ME_{red} DOC$	Concentration of DOC associated metal in the reduced intermediate layer	$g.m^{-3}$
$ME_{red} SS$	Concentration of SS associated metal in the reduced intermediate layer	$g.m^{-3}$
$ME_{DIS} W$	Concentration of dissolved metal (DIS + DOC) in water column	$g.m^{-3}$
$ME_{DIS} S$	Concentration of dissolved metal (DIS + DOC) in pore water aerobic top layer	$g.m^{-3}$
$ME_{DIS} RED$	Concentration of dissolved metal (DIS + DOC) in pore water of the reduced interlayer	$g.m^{-3}$
$ME_{SS} W$	Metal content in floating sludge	$g.kg^{-1}$
$ME_{SS} S$	Metal content in bottom sludge of aerobic top layer	$g.kg^{-1}$
$ME_{SS} RED$	Metal content in bottom sludge of reduced interlayer	$g.kg^{-1}$

The interactions involved without transport processes, advection and dispersion, need to be supplied by the quality model development part of the program. These are stored in the process description file *.mod. The resulting set of equations has to be compiled using DUPROL. After compilation a *.mob file is created which can be read by DUFLOW.

3.5. Modelling Scenarios

The general scheme for modelling in this study is shown as Table 12. At first a very simplified model as M1 is used for a first approximation and evaluation of the flow and transport rates in the system. M2 is still a simplified steady state model where topography (i.e. floor and surface levels) as well as major flow regulating structures namely weirs, culverts and general structures are implemented. In this third model, using the schematization of M2, varying flow conditions will be simulated and evaluated. For the flow model scenario of dry weather with low discharge as well as scenario under wet weather with high discharge has been simulated. For water quality part in M1 only simple track model and decay model with constant concentration and under spill condition have been simulated. The METAL model is only simulated in M3 and M2under complex realistic network with varying dynamic flow.

As a result there will be the following scenarios to be discussed: the basic average scenario with average discharge and metal loads, scenario dry and wet with relatively low or high discharge and average metal loads, scenario extreme with sudden increase in discharge with average metal loads and metal accident scenario with sudden increase in metal loads under average discharge.

Table 12 Modelling Work Flow

Model	Water Quality sub-models	Scenarios	
M1(Simple) Steady state	M1_TRAC M1_DEC	Flow	Dry weather（Low discharge） Wet weather（High discharge）
		Water Quality	Constant track and decay model (low concentration, high concentration) Spill
M2 (Real Structure) Steady state	M2_TRAC M2_DEC	Flow	Dry weather（Low discharge） Wet weather（High discharge）
		Water Quality	Constant Metal (low load, high load) Spill
M3 (Dynamic)	M3_TRAC M3_DEC M3_METAL	Simulated Varying Dynamic flow	

3.6. Field work

The method used is a combination of hydrologic modelling, literature research, use of monitoring results of the past years. A calibration on the network of the flow model requires field check.

4. NETWORK SETUP AND MODEL ENTRY

4.1. Network Setup

4.1.1. Model building: Simplified Steady state model (M1)

At first a very simplified network (Figure 7) is used for a first approximation and evaluation of the flow and transport rates in the system. It assumes:

- Realistic dimensions of channels and pond volumes, lengths, derived from high resolution geo data and field checks;
- Steady state (constant flow Qadd inputs; QH or QL out)
- No gravity bed slope (zero bottom level; piston flow Qadd);
- No implementation of flow regulating structures

It is used for the initial evaluation of flow rates and velocities, residence times and substance concentrations using

- Steady state flow conditions
- Different discharges (from WWTP Enschede West) and
- A simple tracer 1D and transport model of a substance

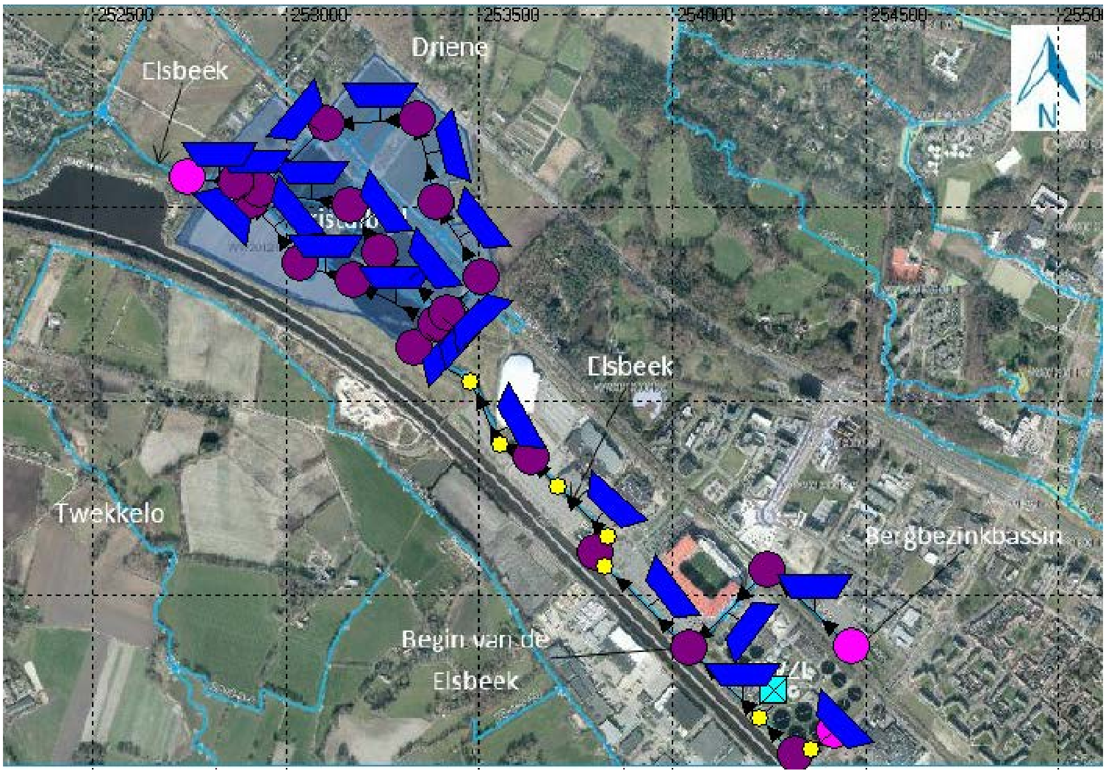


Figure 8 Simple Schematization of the flow network in DMS

The network was built based on GIS data information from the "Vechtstromen" Water authority (aan-afvoervakken) and accompanying files in combination with a detailed image background using (Figure 8) (digital aerial image data from Geoweb (©RWS, 2013]).

The flow section lengths were derived from the GIS data and background; the cross sections were derived based on field on-site visits and other information.

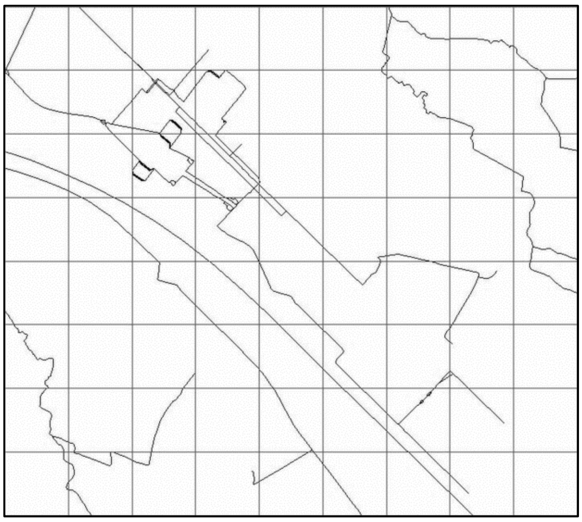


Figure 9 Background map based on GIS data

Hereafter, the network objects and how they were implemented in Duflow DMS are succinctly described.

- *Network schematization: part A (WWTP Enschede West)*

The part A (Figure 9) includes 5 nodes(NOD 0,1,2,4,15), 4 sections (SEC 0,3,7,21), 4 cross sections (CSC 0,1,2,23), 2 scheme points (SCH 5,9) and 1 discharge point(DIS 0).

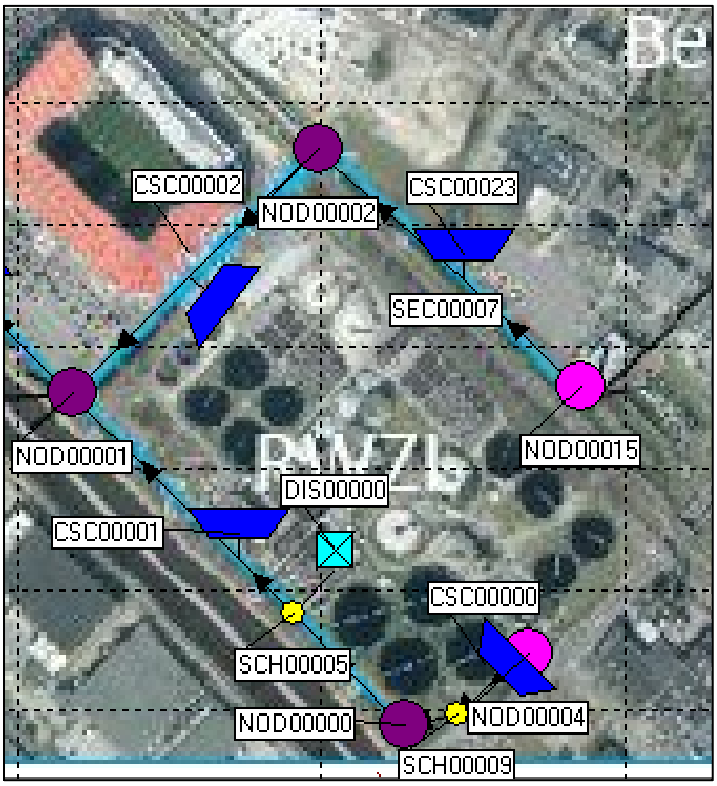


Figure 10 Simple Schematization of Part A

NOD 3 and NOD 15 are the start points of the flow model which are respectively at the south and east of the WWTP (Figure 10). The discharge point is along the Elsbeek.

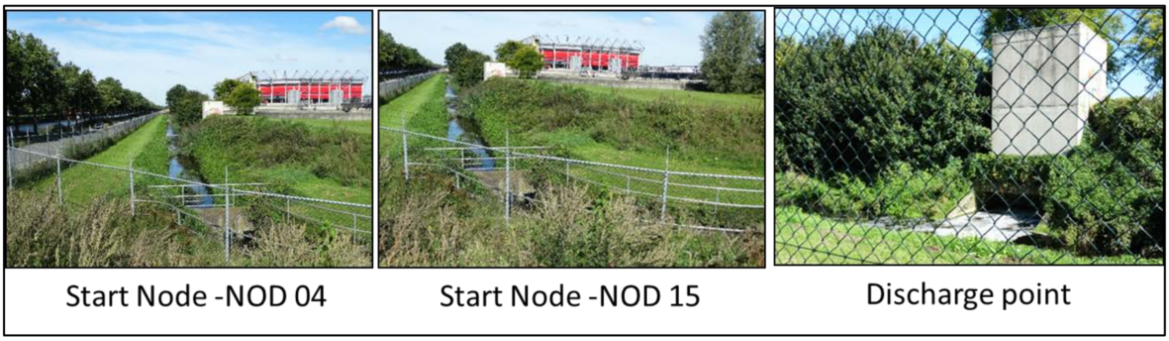


Figure 11 Photos of Key Points of Part A in the Network

SEC00003 and SEC00000 connect one of the start point NOD0004 to the joint node NOD0001 with the respective lengths of 46m and 194m. The cross sections (CSC0000 and CSC00001) for this part are both set as scheme *River 1* (Figure 11).

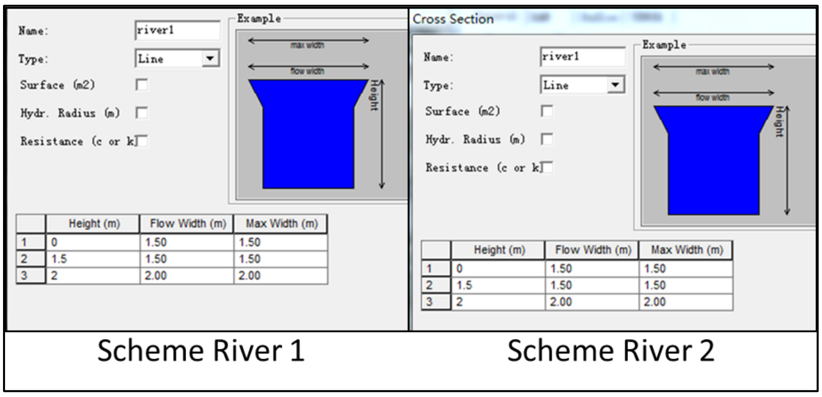


Figure 12 Cross Section Schemes for Part A and Part B

SEC00007 and SEC00021 connect the other start point NOD00015 to the joint point NOD00001 and the lengths of which are separately 129m and 150m. The turning point NOD00002 connects these 2 sections. The cross section for section NO. 7 (CSC0023) is still set as the scheme *River 1* while after the turning point the other section (CSC00002) becomes wider with the cross section scheme as *River 2* (Figure 11).

- ***Network schematization: part B (middle part and weir)***

The part B (Figure 12) starts as a confluence from NOD00001 passing by NOD00022 and NOD00018 and ends at NOD00003. Sections No.2 (150m), No.14 (118m) and No.15 (103m) are involved with the same cross section settings as scheme *River 2*.

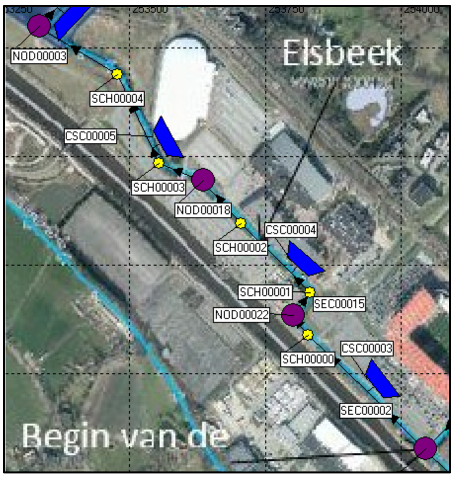


Figure 13 Simple Schematization of Part B

- *Network schematization: part C: Kristalbad wetlands*

There are 3 pond systems and an outlet system involved in this part (Figure 13). Along the direction of the flow from the south to the north are respectively pond system No.1, No.2 and No.3. The confluence flows into these systems through the intake channel (Figure 14) which connects the beginning points (NOD00003, NOD00006 and NOD00007) of 3 ponds with SEC00004 (47m), SEC00005 (23m) and SEC00006 (47m). The cross section settings for this channel are still as Scheme River 2.

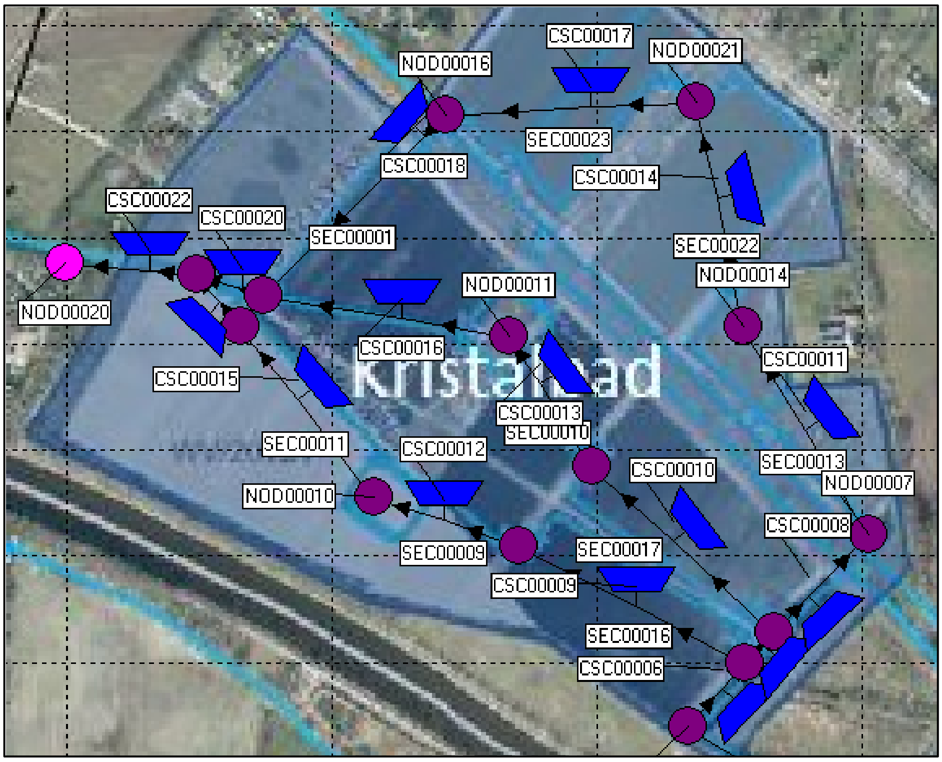


Figure 14 Schematization of Part C

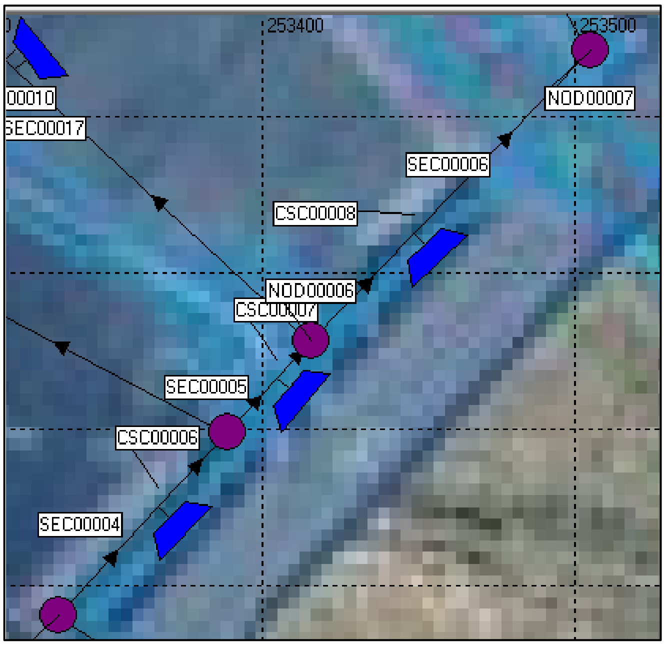


Figure 15 Schematization of the Intake Channel for Part C

For Pond system 1 (vak_1): Pond_11 → Pond_12 → Pond_13

Pond_11 is between NOD00005 and NOD00008. The length here (SEC00016) is about 114m with cross section CSC00009 described in Figure 15:

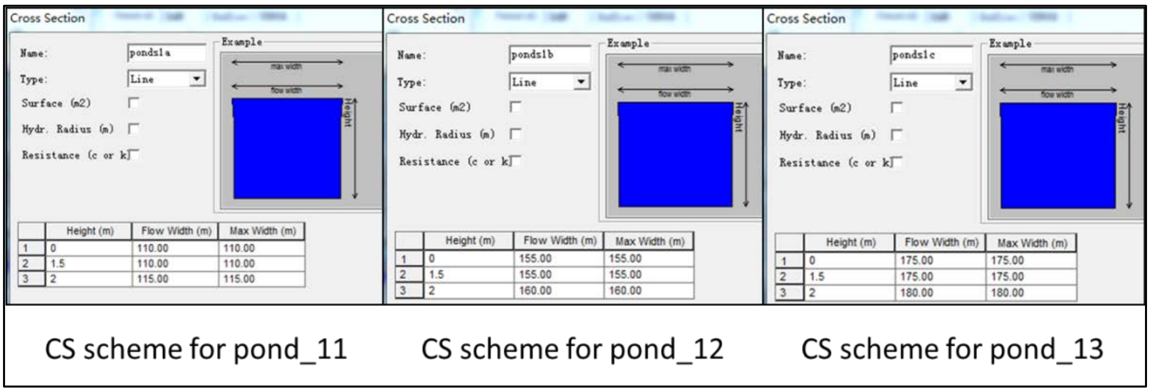


Figure 16 Cross Section scheme for pond_1

Pond_12 is from NOD00008 to NOD00010 as long as 75m with the cross section simulated as CSC00012 with the scheme in Figure 15. Pond_13 begins at NOD00010 and ends at NOD00012 with the length of 118m and a cross section CSC00015 modeled like Figure 15.

For Pond system 2 (Vak_2): Pond_21 → Pond_22 → Pond_23

Pond_21 is between NOD00006 and NOD00009. The length here is about 128m with cross section CSC00010 scheme as Figure 16:

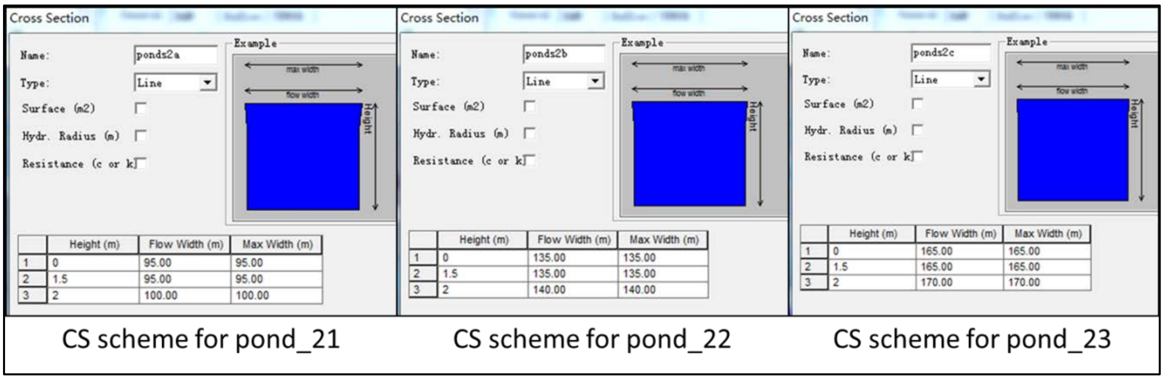


Figure 17 Cross Section scheme for pond_2

Pond_22 is from NOD00009 to NOD00011 as long as 92m with the cross section simulated as CSC00013. Pond_23 begins at NOD00011 and ends at NOD00013 with the length of 103m and a cross section modeled like CSC00016 (Figure 16).

Pond system 3 (Vak_3): Pond_31 → Pond_32 → Pond_33

Pond_31 is between NOD00007and NOD00014. The length here is about 114m with cross section CSC00011 (Figure 17):

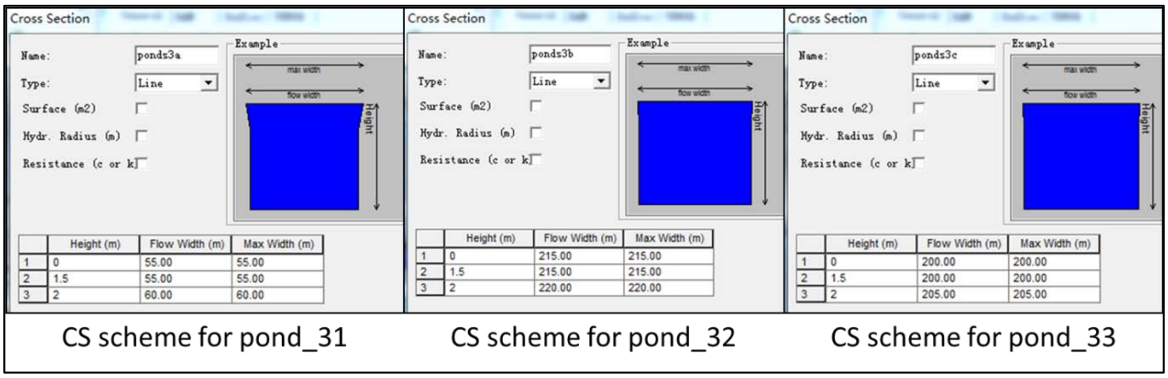


Figure 18 Cross Section Scheme for pond_3

Pond_32 is from NOD00014 to NOD00021 as long as 123m with the cross section simulated as CSC00014. Pond_33 begins at NOD00021 and ends at NOD00016 with the length of 103m and a cross section CSC00017 modeled like scheme ponds3c (Figure 17).

Flow from Pond 3 and Pond 2 join at NOD 00013 and then join the flow from Pond 1 at NOD00019 (Figure 18).

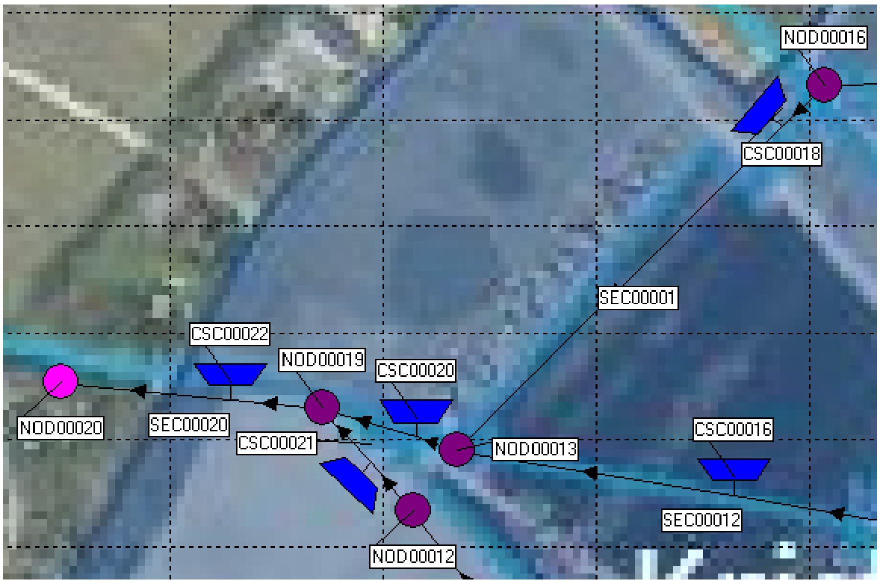


Figure 19 Schematization of the outlet system of Kristalbad

As can be seen in Figure 18 SEC00001 is 28m long with the cross section of CSC00018 set as Scheme Lake (Figure 19):

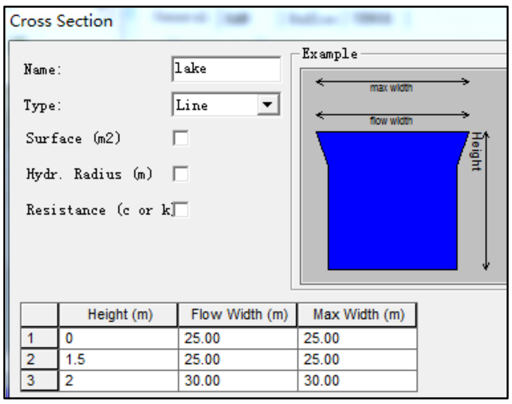


Figure 20 Scheme Lake

Distance between NOD00013 and NOD00019 is 20m, between NOD00012 and NOD00019 is 29m and between last 2 nodes is 93m. All of the rest cross sections including CSC00020, CSC00021 and CSC00022 are all set as Scheme River 1.

4.1.2. Model Building: Steady state model_2 (M2)

In M2 (Figure 20) topography, i.e. floor and surface levels, are implemented; as well as major flow regulating structures, namely weirs, culverts and general structures. Floors and surface levels come from AHN 02 data. Detailed information on weirs, culverts and general structures are from GIS data from water board and field measurements. Flow and water levels are according to gravity slope and structure contractions, crown, crest heights. In this model, evaluation of more realistic water levels, flow rates and residence times can be pursued.

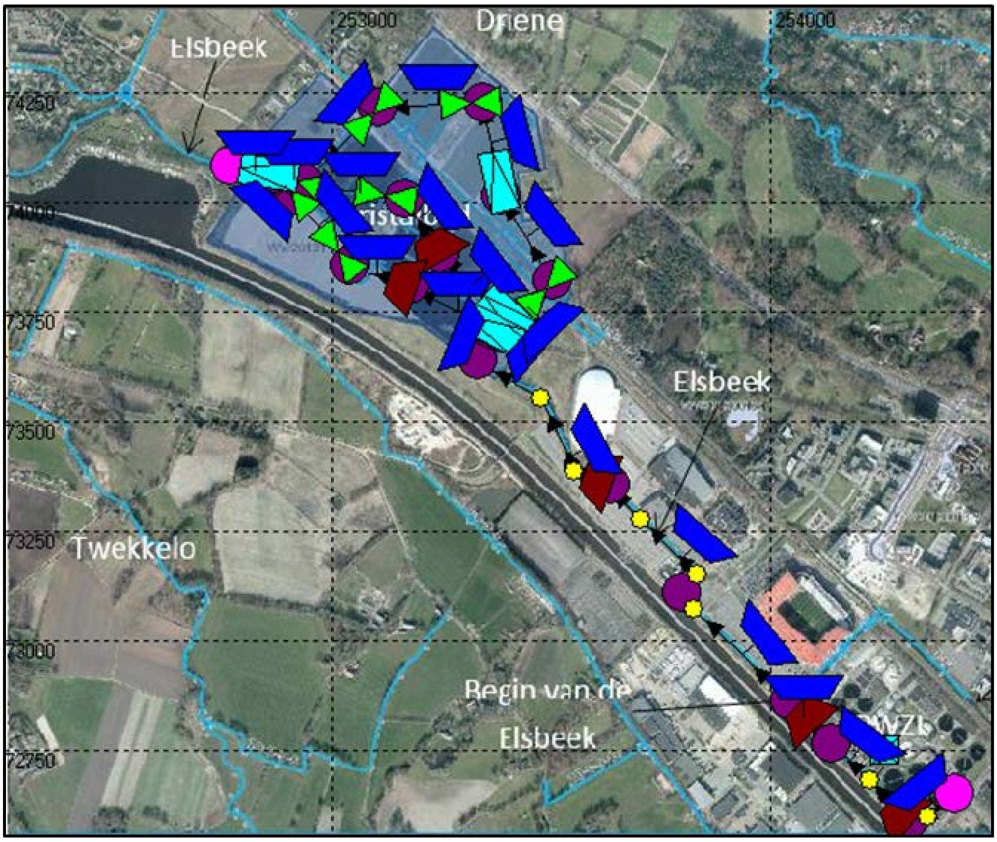


Figure 21 Realistic Schematization of Kristalbad

In M2, Part A (Figure 21) is simplified as the deleted part doesn't affect the results and 2 weirs are added. One weir is added near NOD00000 coded as WEI00000 with shape height of 27.82m, crown width of 2.5m and crown height of 26.3m; the other, WEI 00001, is of 27.72m in shape height, 2.5m in crown width and 26.15m in crown height.

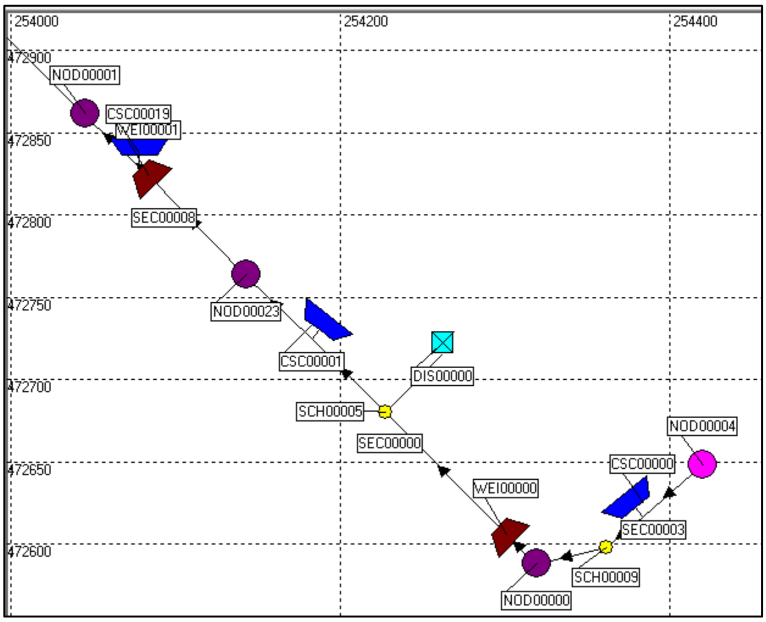


Figure 22 Part A of Kristalbad in M2

As is shown in Figure 22 WEI00002 is added on the last section of Part B. The shape height is 26.64m, the crown width is 10.3m and the crown height is 25.12m.

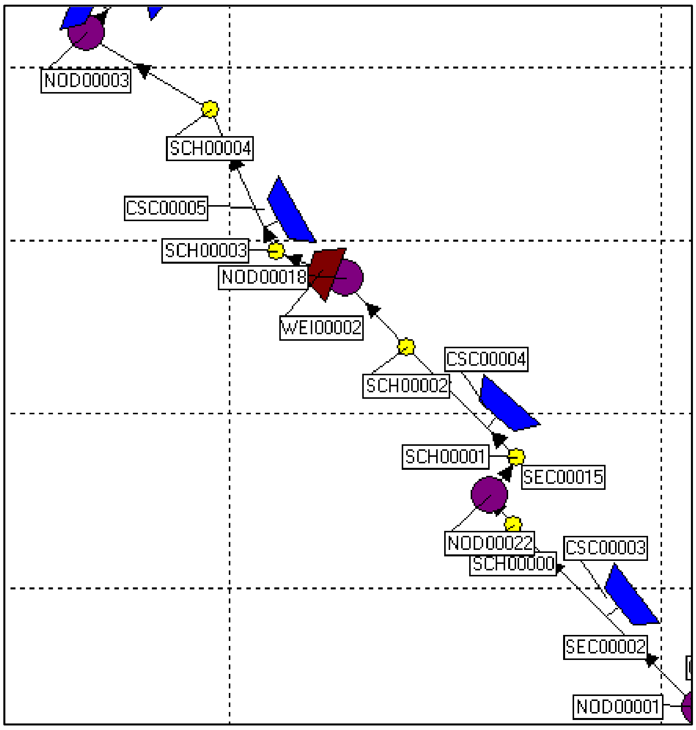


Figure 23 Part B of Kristalbad in M2

As is shown in Figure 23 general structures, weirs and culverts are assigned to the system. For Pond 1 a general structure GST00003 is modeled at the intake of the system, and a weir WEI00004 is set at the begging of Pond_12. On this weir, the shape height is 24.42m, the crown width is 0.3m and the crown height is 23.92m. There are 2 culverts at the two ends of Pond_13. For the begging one, CLV00000, the tube width is 1.25m, the height is 22.493m and the length is 43.3m. As for the ending one, CLV00003, the 3 parameters are respectively 0.2m, 21.091m and 11.78m.

As far as Pond_2 is concerned there is a general structure at the intake GST00002; one weir WEI00003 at the begging of Pond_22 with shape height of 24.38m, crown width of 0.3m and crown height of 23.95m;

two culverts at each end of Pond_23, CLV00002 and CLV00004. Tube width of CLV00002 is 1.25m, height is 22.514m and length is 43.23m. The other tube is 0.3m wide, 21.021 high and 14m long.

There are 3 culvert systems in Pond_3. The one at the intake is 0.5m wide, 23.843 m high and 41.08m long; the one at the end of Pond_32, known as CLV00006, is 1.25m in width, 22.457m in height and 41.87m in length; the 3 parameters for the one at the end of Pond_33 CLV00005 are respectively 1.5m, 21.145m and 2.92m. Furthermore there is a general structure at the begging of the Pond_32.

There is also a general structure at the outlet of the whole system which is known as GST00001 in the system.

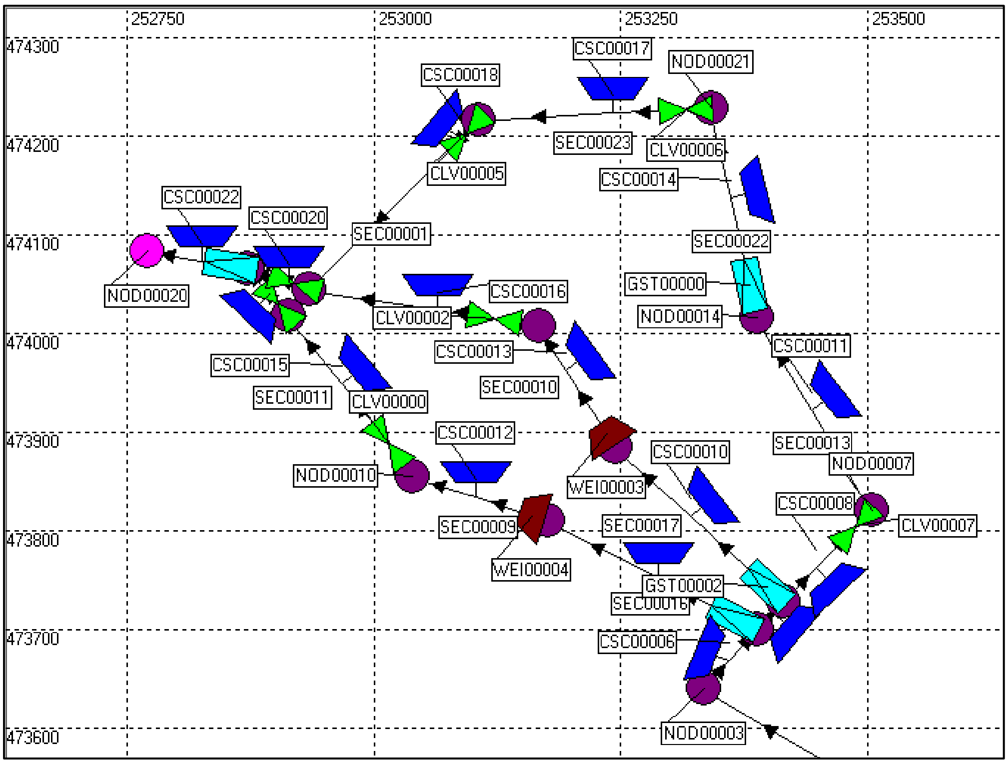


Figure 24 Part C of Kristalbad in M2

4.2. Model Entry for METAL

4.2.1. Initial Condition

To simplify the model the initial conditions for all the scenarios are set as the same based on measurement data. The discharge at time zero is 0.3 m3/ s and the level is 0.5m. The concentrations of copper, nickel and zinc are assigned to 0.005 mg/L. In fact as the quality model is adopted from the Vecht River system which speaks well for the average condition of metals in water in the NL the initial conditions for the Kristalbad are kept as default.

4.2.2. Boundary Conditions

The flow data of discharges point of WWTP are the analyzed results from previous work and water levels of the outlet of the Kristalbad system are from AHN02 data.

An overview of the residence times at various flow rates is shown in Table 13. The residence time of the water in the Kristalbad is an average of 4.4 days. The daily volume in the Kristalbad is about 173.500 m3. During DWF there will be approximately 25,000 m3 of effluent via the Elsbeek the Kristalbad inflows. If this is the case, the residence time in the Kristalbad would be longer. The hydraulic residence time is 6.9 days. The natural degradation of materials will have a larger share in a longer residence time in the Kristalbad.

Table 13 Residence times in the Kristalbad at different flow rates

WWTP Flow	Residence Time (days)
DWF 25000 – 30000 m³/day	6.9 - 5.9
RWF 70000 – 118000 m³/day	2.5 – 1.0
Year Average (2013) 40059 m³/day	4.3
Summer Average (2013) 39469 m³/day	4.4
Average Residence Time	**1 - 4**

As the most common and obvious metals in urban are copper, nickel and zinc, such metals are the focus in this study. To observe the behavior of the Kristalbad under different flow conditions the loads are set to be the same as which under the average flow with average metal concentration (Table 2).

Table 14 Average Concentrations and Loads of Metals of WWTP

Metal	As	Cu	Ni	Pb	Zn
Conc. (μg/L)	0.83	7.9	10	0.72	90.5
Load (g/s)	0.000399	0.00366	0.00464	0.00033	0.041956

The extreme flow condition refers to the discharge increases for a while and falls back to the normal level afterwards. In the study the extreme scenario is s simulated one where the discharge increased from 0.4629 m3/s, which is equal to the constant discharge of the average scenario, at 05:00 on October 1st gradually to 1.6m3/s and then drops to 0.4629m3/s again at 17:00 the same day (Figure 31). Such scheme is applied as the boundary condition to both the beginning of the Elsbeek and the WWTP discharge point. The metal amounts follow the average settings.

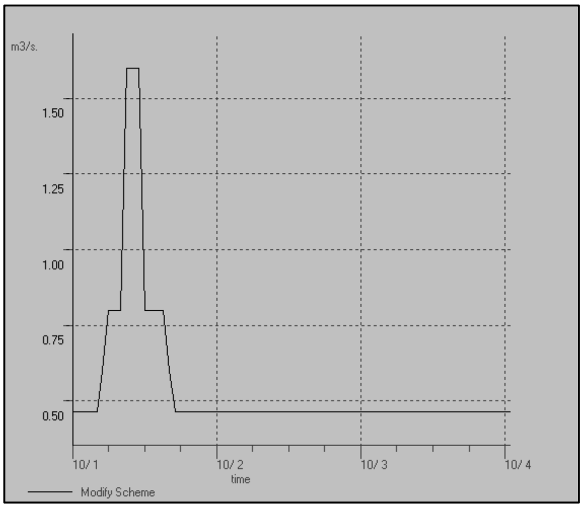


Figure 25 Discharge Scheme of Extreme Scenario

To simulate a metal accident the loads of copper and zinc are set as ten times as the average level casted for about 2 hours (Table 16).

Table 15 Metal Loads Scheme under Meatal Accident

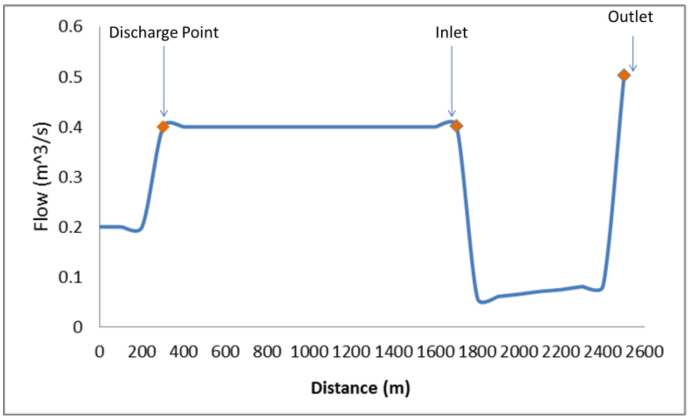
Time	Cu Load (g/s)	Zn Load (g/s)
2015/10/01 00:00 - 2015/10/01 03:00	0.00366	0.04196
2015/10/01 04:00 - 2015/10/01 05:00	0.0366	0.4196
2015/10/01 06:00 - 2015/10/01 05:00	0.00366	0.04196

4.2.3. Calculation Settings

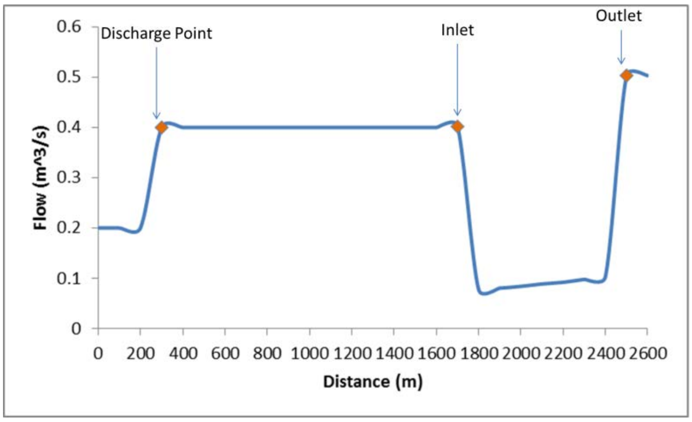
For the water movement a time step of five minutes is used. This has been experimentally determined. For the quality it can be calculated with a time step of 10 minutes. In this case the maximum allowable step time for the quality is also determined by trial and error. In this case, the maximum allowable time step is determined by the sedimentation of suspended solids (2.0 m·day-1). Output interval is selected as half an hour. The time series is set as from 2013-10-01 00:00:00 to 2013-10-08 00:00:00 for Scenario Average, Dry and Wet; for Scenario Extreme and Scenario Metal Accident it begins at 00:00 on October 1st and ends at 00:00 on October 4th. The space step is adjusted to 20 meters and the theta for hydraulic calculation is adjusted to 0.75 to keep the flow stable. The size of this file in these simulations is also limited by a limited number of variables to carry (to select output variables in the calculation settings dialog). As the output for all the sections is requested it is possible to ask for the length of profiles on concentration. In this study the outputs required are the loads of copper, nickel and zinc in water column.

5. SCENARIOS AND ANALYSIS

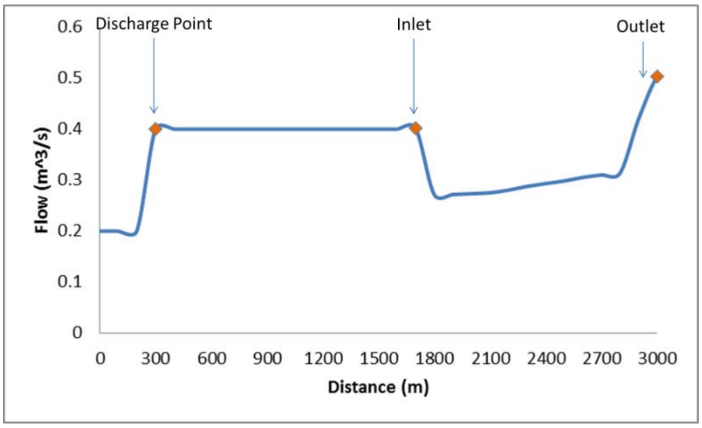
There are 3 routes involved in relation to the space related graph, namely Pond_1, Pond_2 and Pond_3. Take the scenario under extreme flow event when reached balance as an example (Figure 24): for all 2 routes the parts before the inlet point and after the outlet point are the common part namely the Elsbeek channel and the parts between the inlet and the outlet points are actually the separated ponds; for Pond_1 and Pond_2 the Kristalbad ponds end at the distance of 2500m, while Pond_3 ends where the distance equals 3000m.



Pond_1



Pond_2



Pond_3

Figure 26 The Kristalbad System Structure in Space Related Graph

5.1. Kristalbad Behaviors with Metals under Different Flow Condition

With the close loads of copper and nickel the behaviors and varying tendencies of these two metals are quite alike under all kinds of scenarios throughout the whole progresses which can be seen from space related graphs (Figure 25), so that only copper and zinc are going to be discussed in details.

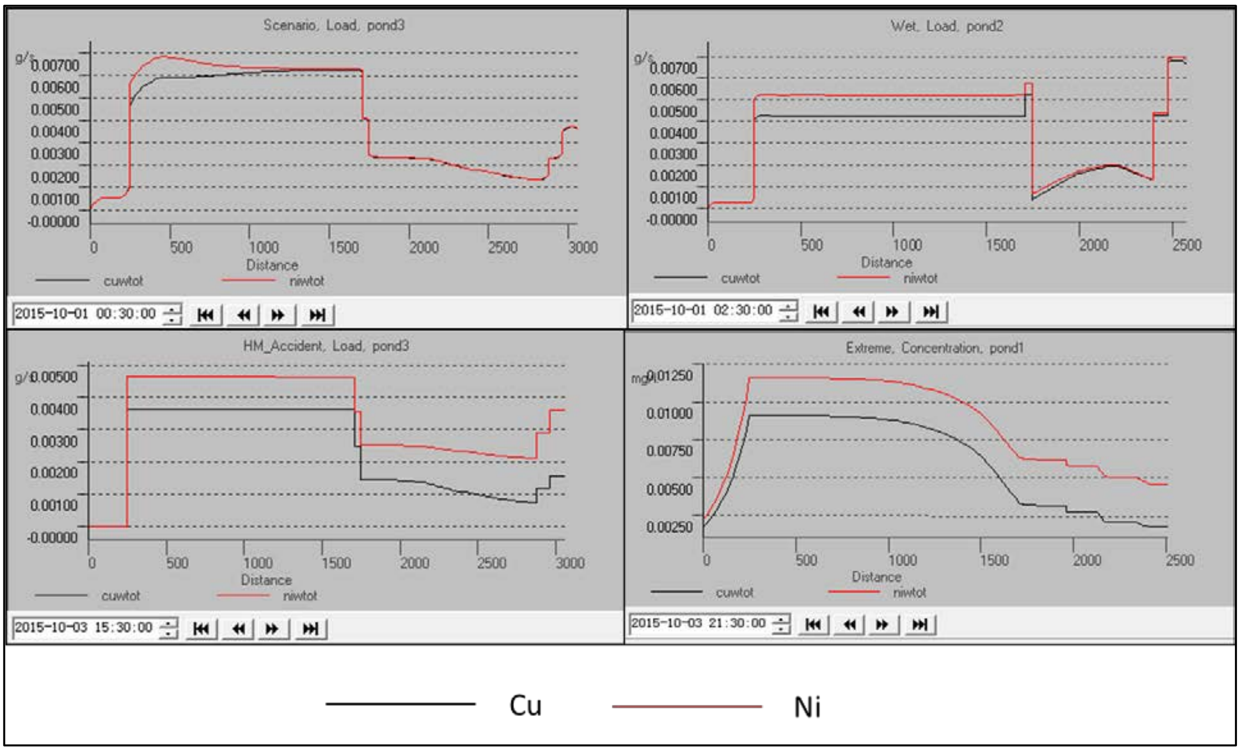


Figure 27 Comparisons between Cu and Ni on Total Loads/ Concentrations in Water Column under Different Scenarios across the Kristalbad

Copper varies in similar relatively simple patterns under the constant flows of both average and dry condition. While under wet weather condition where the discharge is relatively high the situation is a bit more complicated.

5.1.1. Average Flow

Under the average scenario it takes 3.5 hours for zinc in the part of Elsbeek channel before the inlet to reach steady and 3 hours for copper as regards to the loads of the metals in discussion after the constant loads of metal contaminant from the WWTP casted into the river. As the great difference in loads zinc behaviors differently from copper in getting constant throughout the inflow channel. As is shown in Figure 28 as immediately as the metals casted into the river copper transports quickly to the other end while zinc load increase gradually from the very beginning to the inlet of the Kristalbad. After a while copper loads of different parts of the channel along the river decrease at the same time, but the beginning part decreases more low than the ending part; and the zinc load along more portion of the river gets to the same constant value as the discharge point. At last there is a little decrease in both metal loads throughout the inflow channel and the channel reaches the steady state. Then the water with constant loads of metals will split into three ponds.

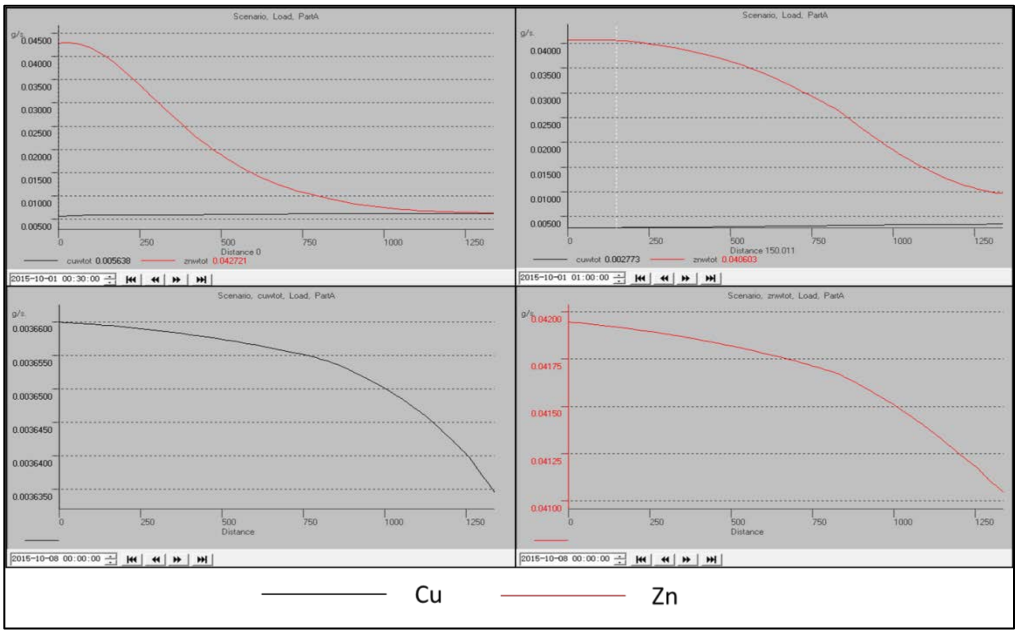


Figure 28 Copper and Zinc Loads Getting Constant throughout the Inflow Channel

As can be seen in Figure 29 from left to right are respectively the space-distributions of loads of copper in water column of route Pond_1, Pond_2 and Pond_3 under average flow at the steady state. The X axis is the distance with the unit of meter and the Y axis refers to the loads of the metal with the unit of gram per second. The sudden decreases indicate the water flow into the Kristalbad system. Different from route Pond_1, the inlet sections connecting three parts of the Kristalbad burdened some loads which explained the buffers in Pond_2 and Pond_3 between inlet point and the sections in ponds. The same can be applied to the outlet system as well. There are obvious decreases in all the three ponds, but the load drops off relatively even at the first half to the last half in pond_3. This is probably because the general structures of pond_1 and pond_2 are at the beginning of the sections while which of pond_3 is in the middle of the sections. The slight buffers in all the three ponds in loads correspond to the culverts involved.

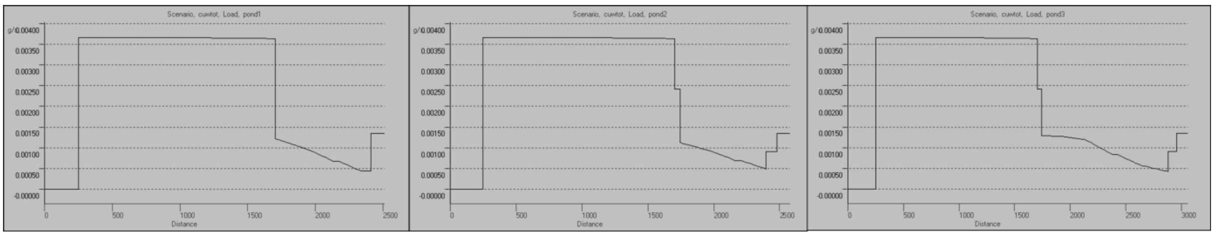


Figure 29 Space Distribution of Total Loads of Copper in Water Column of 3 Routes under Average Flow Condition

Although the load of zinc is much higher than the load of copper the difference between zinc and copper the purification behaviors of them are similar (see Figure 29 and Figure 30) only for zinc in pond_3 the removal efficiency is almost 100% which is also the reason there is one less buffer zone in pond_2 compared to copper there.

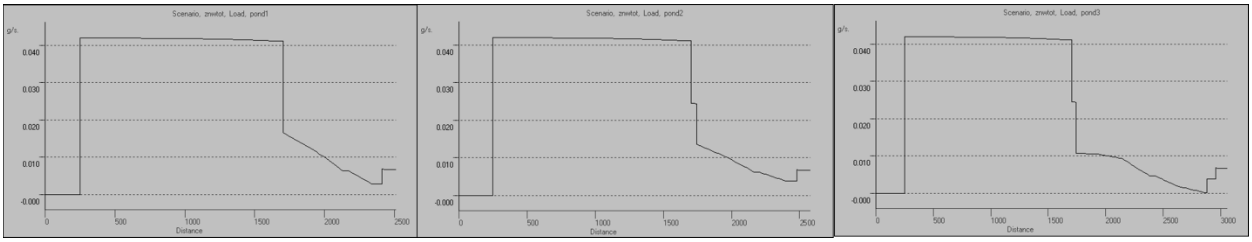


Figure 30 Space Distribution of Total Loads of Zinc in Water Column of 3 Routes under Average Flow Condition

5.1.2. Dry Flow Scenario and Wet Flow Scenario

The dry flow condition almost follows the average flow pattern. It still takes 3 hours for copper throughout the channel to get steady but for zinc it changes to 4.5 hours.

Under wet weather flow zinc transports following the average and dry pattern while the situation for copper becomes quite different. It still takes 6.5 hours for copper throughout the channel to get steady but for zinc it takes only 5 hours this time. Copper moves alike in Pond_1 and Pond_2 but Pond_3. Figure 29 presents the copper transport in pond_1 which also can be regarded as the copper movement in pond_2 and Figure 30 shows that in pond_3. Copper moves very fast as the flow is high so that for a while the outlet load is higher than the inlet. The direct cause for this is mostly that pond_3 does not function well enough to release the quickly casted load of copper in short time. It takes two days for the constantly casted copper to finally go down.

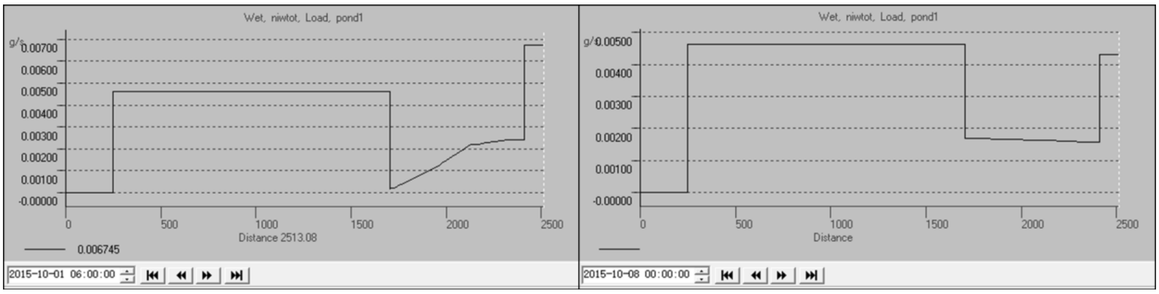


Figure 31 Copper Transport in Pond_1 under Wet Weather Flow

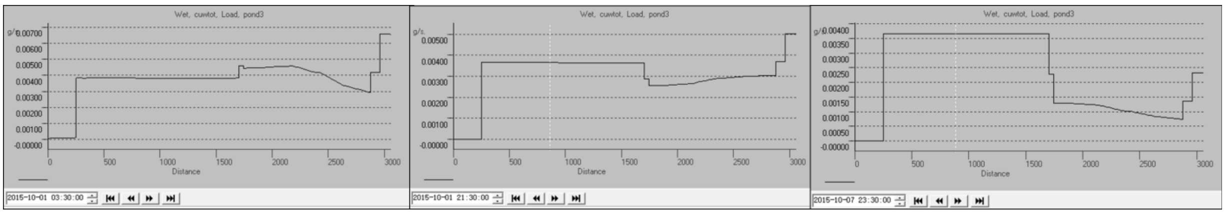


Figure 32 Copper Transport in Pond_3 under Wet Weather Flow

5.1.3. Extreme Flow Scenario

The loads vary corresponding to the discharge variation in time. Similar to the situation under wet scenario the when discharge increases Pond_3 does not perform as good for copper as the other two ponds or the zinc purification efficiency in short time, but the whole system keeps decreasing copper load effectively (Figure 32). It is obvious that when discharge rises up the beginning part of the system reacts at first; when discharge falls down the same part of the system gets steady at first as well (Figure 32). It takes 5 hours for both copper and zinc loads to get steady after the discharge gets back to constant.

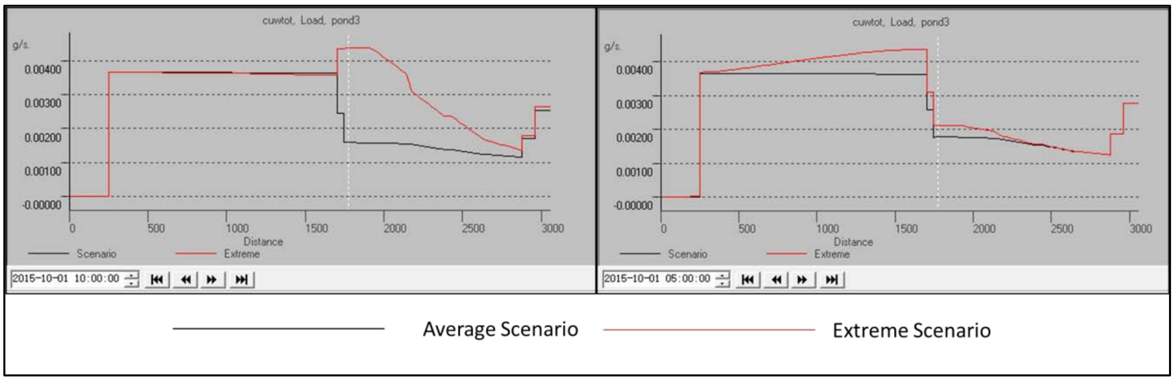


Figure 33 Comparison between Average Scenario and Extreme Scenario on Copper Transportation in Pond_3

5.1.4. Removal Efficiency

The removal efficiency of the system in copper and zinc is shown in Table 17. Compared to copper The Kristalbad works better for purifying zinc than for copper. Generally speaking Pond_3 is the most efficient among all the three ponds. This is because Pond_3 covers larger area of water along longer distance and is equipped with more complicate hydraulic structure. But higher discharge affects the function of the system negatively, especially for pond_3 to remove copper.

Table 16 Removal Efficiency of the System in Copper and Zinc

Scenario	Scheme	Cu			Zn		
		Influent Load (mg/s)	Effluent Load (mg/s)	Efficiency (%)	Influent Load (mg/s)	Effluent Load (mg/s)	Efficiency (%)
Average Flow	Pond_1	1.166	0.434	62.779	15.509	2.886	81.391
	Pond_2	1.116	0.494	55.735	13.471	3.913	70.952
	Pond_3	1.287	0.428	66.744	10.74	0.135	98.743
	The Kristalbad	3.66	1.342	63.333	41.9527	6.783	83.832
Dry Flow	Pond_1	1.183	0.22	81.403	16.446	1.301	92.089
	Pond_2	1.137	0.386	66.051	13.479	2.443	81.876
	Pond_3	1.27	0.329	74.094	9.797	0.039	99.602
	The Kristalbad	3.66	0.919	74.891	41.9527	3.73	91.109
Wet Flow	Pond_1	1.373	0.97	29.352	16.563	7.632	53.921
	Pond_2	0.988	0.625	36.741	12.746	5.295	58.458
	Pond_3	1.283	0.737	42.557	12.203	2.098	82.808
	The Kristalbad	3.66	2.329	36.366	41.9527	14.927	64.419
Extreme Scenario	Pond_1	3.66	2.329	36.366	16.562	2.753	83.378
	Pond_2	1.204	0.435	63.87	13.649	3.681	73.031
	Pond_3	1.088	0.492	54.779	10.673	0.034	99.681
	The Kristalbad	1.33	0.556	58.195	41.952	6.418	84.702

5.2. Kristalbad Behaviors under Metals Accident

The simulated results for the two metals in 3 ponds are relatively similar. Figure 33 shows the transport of copper throughout Pond_3 as an example. The loads increase as soon as the sudden high load of copper appears in water column. The peak of copper load moves with the metal spells from the WWTP to the other end of the system while the value of which keeps dropping till the system gets the steady states as the average level. It takes about 45 hours for the Kristalbad to completely recover from such simulated accident. With increasing element of metal loads all parts of the Kristalbad contribute positively to purifying metals in water compared to the situation with an increasing element of discharge.

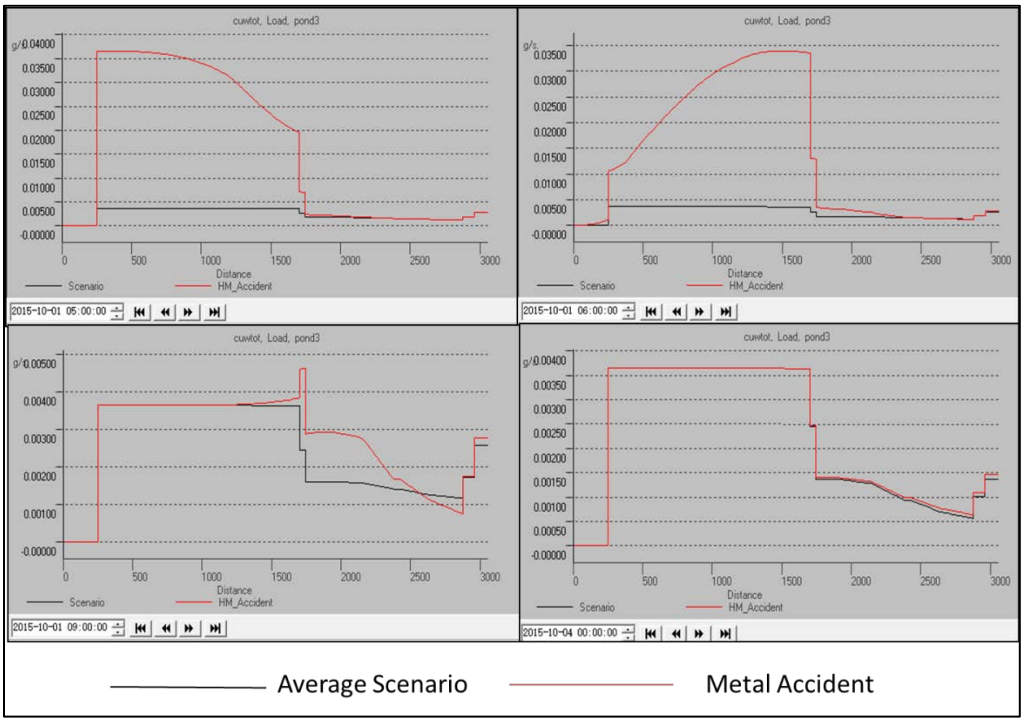


Figure 34 Copper Transport in Metal Accident Scenario

6. CONCLUSIONS AND RECOMMENDATIONS

6.1. Conclusions

In this study a prototype modelling system for analyzing the behavior of heavy metals form a WWTP was developed; a semi-detailed system was designed, incorporating the channels and ponds and also a number of the more important hydraulic structures were represented.

The sizing of the system was determined by adopting real dimensions and making use of Geo-spacial data such as digital aerial photo background, the AHN accurate elevation model (0.5m), and detailed GIS geodatabase information from the water authority. Field work and surveying was also done to verify the system dimensions and functioning.

The water quality model Metal built on the basis of the Vecht river system (Duin et al., 1994) was linked to the flow model in Duflow. This model allows analysis the behavior of 5 heavy metals i.e. As, Ni, Cu, Pb and Zn in water column and the sediment phase of the channels and ponds. The processes and transports involved in the model include the sorption of metal by solid (fraction < 16 mm), dissolved and particulate organic material (including algae); the effect of pH and chloride; deposit of the heavy metals with sulfide under the sediment reducing conditions; dissolved and particulate organic material exchanges between soil and water column; heavy metals exchanges between bottom sediment and water column; and the net sedimentation and burial of sediment material.

Use was made of measurements of (2013, 2014) heavy metal concentrations in water and sediment (pond systems 1 and 2) done by the Water authority. This permitted to use realistic values for model initial and boundary quality conditions for concentrations.

Observed average, dry and wet weather flows were adopted in the model runs. Due to renewal works of the ITC Geoscience or GS laboratory (incl. retirement of lab head) and installation of new equipment's, no active field sampling and lab measurement data could be gathered and executed during the MSc period. Just recently (February, 2016), a new ICP-OES Perkin Elmer was installed in the lab, the instrument typically used and needed for analysis of those elements. Therefore a number of theoretical (but with realistic parameter settings) scenarios' were run in Duflow, namely Scenario Extreme and Scenario Metal Accident.

Using this prototype model, the releases of heavy metals in the residual effluent from the Enschede West WWTP municipal waste water treatment plant were simulated. The aim was to analyze the behavior of the metals and to investigate the retention in the Kristalbad, and the removal efficiency. With the limited real data as input for the model it reached steady with proper adjustment of calculation settings. It can be concluded that the DuFlow model works fine for simulating the Kristalbad system.

The two main heavy metals in urban area Cu and Zn were initially used. We observed a quite different behavior between the two metals which can be explained by their chemical reactivity and behavior of these two elements in aqueous and sediment media. When the Kristalbad works functionally well, it takes longer time for zinc to get steady than copper does. No matter under what kind of weather condition zinc does not overload the ponds; but the situation is quite different in pond_3 for copper under both constant high flow and sudden increase of flow condition. And the removal efficiency is always higher for zinc than for copper.

Regarding the functioning of the Kristalbad compared to copper the Kristalbad works better for purifying zinc than for copper. Generally speaking Pond_3 is the most efficient among all the three ponds. This is because Pond_3 covers larger area of water along longer distance and is equipped with more complicate hydraulic structure. But higher discharge affects the function of the system negatively, especially for pond_3 to remove copper.

6.2. Recommendations

For the network detailed flow (effluent) data from the WWTP and level data (from the water authority) in the Kristalbad system can be used to further optimize the model. The general structures involved in the model can be more specific regarding the parallel structure. With such two elements the cycle of the Kristalbad may also be presented.

For the water quality model mass balance approaches combined with sampling data and laboratory determinations of heavy metals may now be used to further calibrate and validate the model. One difficulty in the detailed water quality model process of heavy metals will be the effect of hydraulic structures on the element behavior. Although some processes (e.g. extra oxygen intake at weirs) can be simulated in Duflow, it will remain a challenge to verify all effects (incl. sediment) of the different structures in the system on the overall behavior of the water quality in the system.

As far as the analysis based on a realistic metal model with sufficient data is concerned, the contribution of aquatic plants to breaking down and converting heavy metals along with the light, air and alternating water levels influence on breaking down and conversion of heavy metals should be looked further into.

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