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REPORT

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Final Report on the Implementation of a Wetland Module for the Soil and Water Assessment Tool (SWAT)

Project acronym: Aquisafe II

by
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Present report was developed in compliance with the requirements of the quality management system DIN EN ISO 9001:2008

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Abstract

This report compiles the results of three consecutive work packages that have been worked on during the Aquisafe II project. The approach developed is based on the previous Aquisafe I project where the Soil Water Assessment Tool (SWAT) was used as an analytical instrument to develop mitigation strategies for N loads and concentrations in the Ic catchment. During Aquisage I we concluded that SWAT should include a wetland function with which the effect of artificially, constructed wetlands on solute N fluxes can be evaluated.

Chapter 1 compiles results of an extensive literature review that was made to identify potential wetland routines and processes that can be included in SWAT. The SWAT add-on to be developed should allow to individually test the effect on single wetlands (e.g. in a given hydrological response unit or subcatchment) as well as the effect of multiple wetlands on the landscape scale.

We therefore implemented a stand alone version of the new wetland module which is described in Chapter 2. Here we show the general functionality and individual components of the wetland module. The chapter ends with a virtual application of the modules using SWAT outputs copied from the Ic results. Additionally, a Monte Carlo based sensitivity analyses of the wetland module input parameters showed that the denitrification rate seems to be the most constrained parameter for the simulation of N turnover in the new wetland module.

A full implementation of the new wetland module is described in chapter 3. Here, the structural embedment of the wetland module in the SWAT architecture is described. To proof the functionality of the SWAT wetland module model runs were compared to the stand alone version to make sure that the module was correctly implemented. We conclude that the SWAT wetland extension is ready to be tested in real world catchments. Such a full test of the SWAT wetland model was planned towards the end of Aquisafe II. However, as data from the wetlands constructed within Aquisafe II were not available in due time, this last test of the SWAT module was possible.

Chapter 1

Modelling concepts for wetland systems – a literature review

1.1 Introduction

One goal of the project Aquisafe 2 is to find and enhance diagnostic tools to support the planning of mitigation systems to reduce diffuse pollution of river systems in agriculturally dominated regions. In the Aquisafe 1 project the model SWAT was identified to be a valuable tool in testing management scenarios in order to reduce nitrate pollution of surface water. The project also revealed short comings of the current representation of wetland systems in the SWAT model. The aim of this review is to provide an overview of existing approaches to model wetland systems. A suitable concept should be identified which could be easily integrated into the existing SWAT model. In consideration of the goals in the study at first a short theoretical review of wetland processes is given. Then, selected approaches, describing the water and nitrogen (N) balance of wetland systems, are presented and discussed, in order to identify a concept which could be integrated into SWAT. In the last part a recommendation is made how the selected concept of wetland modeling could be integrated into the SWAT model.

1.2 Nitrogen removal processes and wetland types

1.2.1 Nitrogen processes in wetland systems

Figure 1 summarizes the nitrogen related processes in a wetland system. Main inputs of N into the wetlands are point and nonpoint sources, precipitation and biological fixation of gaseous N2.

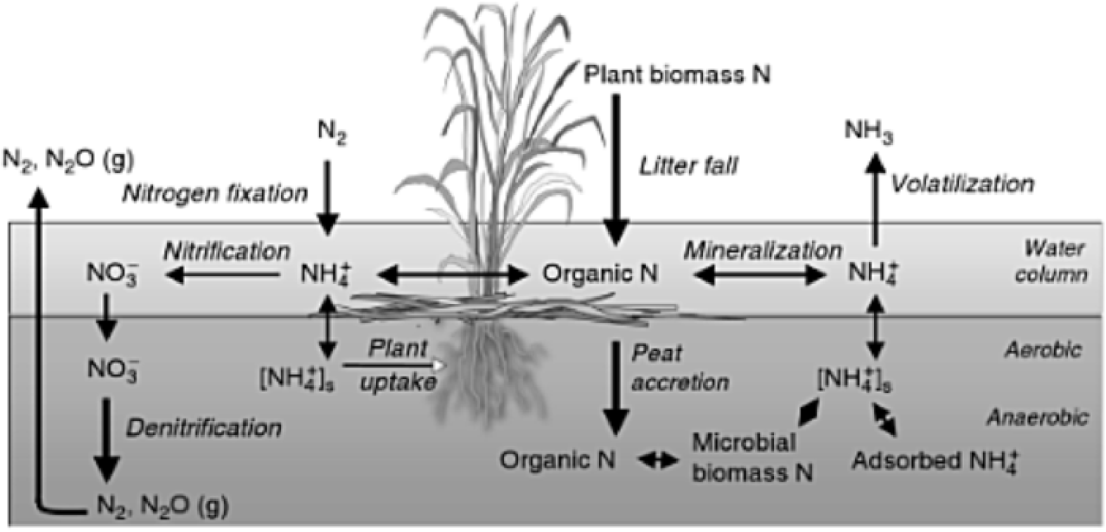


Figure 1 The nitrogen cycle in wetlands (Reddy and DeLaune, 2008)

Ammonification is the conversion of organic N to ammonium. A major portion of N in plant detritus and soil organic matter is associated with carbon (C), thus the process of ammonification is strongly related to organic C decomposition. Immobilization is the conversion or inorganic N compounds (NH4, NO3, NO2) to organic N forms (microbial biomass; plant uptake). These processes are controlled by substrate quality, C-N Ratio of the organic material which is subjected to decomposition, temperature, pH in the wetland soil and redox potential in the wetland water. Ammonium in wetlands could also be lost through volatilization. In this process the ionized form (NH4+) is converted into the unionized form (NH3) which is lost through exchange processes at the atmosphere-water interface. Ammonia volatilization is controlled by the ammonium concentration, buffer capacity (pH), floodwater depth, soil and water temperature, plant density and wind speed (Reddy and DeLaune, 2008).

Nitrification is the process in which ammonium is oxidized to nitrate. This process occurs under aerobic conditions in the wetland soil and the water column. Ammonium is oxidized by three types of microorganisms (chemoautotrophic bacteria, methane-oxidizing bacteria and heterotrophic bacteria) and fungi. Nitrification is controlled by the ammonium concentration, oxygen availability, pH, alkalinity, carbon dioxide, temperature, redox potential and abundance of nitrifying bacteria (Reddy and DeLaune, 2008).

Through denitrification nitrate or nitrite is microbiologically reduced to nitrous oxide and dinitrogen (N2). This process is mediated by facultative bacteria under anaerobic conditions in the soil (resp. wetland soil). Denitrification is controlled by the oxygen content of the soil, the presence of nitrogen oxides (controlled by nitrate flux from aerobic zones to anaerobic sites), supply of electron donors, denitrification enzyme activity, temperature, pH (Reddy and DeLaune, 2008).

1.2.2 Natural wetlands

By definition wetlands can be described by the following three characteristics: (i) Wetlands are characterized by periodic or continuous inundation or saturation with fresh or saline water; (ii) they receive water of varying proportions from precipitation, groundwater or surface water; (iii) their soils have periodically anoxic conditions (e.g. hydric soils) and the vegetation is adapted to periods with low or no soil oxygen.

Wetlands can be classified based on vegetation, hydrological properties or their geomorphic setting. Table 1 summarizes the main types of wetlands based on hydrologic settings. An important feature of wetlands is their ability to improve or maintain water quality by trapping sediment and pollutants. This ability is correlated with the morphologic position, connectivity and water source of the wetlands. For example floodplain forests are highly connected and therefore possess a high potential to remove sediments or pollutants. On the other side depressional wetlands like fens or bogs which receive the water mainly via precipitation exhibit only a low potential for water quality improvement (Craft, 2005).

Table 1 Classification of natural wetlands based on hydrologic setting (adapted from Craft, 2005)

Geomorphic Setting	Water Source	Hydrodynamics	Exampl. of wetland type
Depression	Precipitation	Vertical	Potholes, vernal pools
Mineral soil flats	Precipitation	Vertical	Wet pine flats
Organic soil flats	Precipitation	Vertical	Peat bogs
Riverine	Surface water	Unidirectional, lateral	Floodplain forests
Estuarine fringe	Surface water	Bidirectional, lateral	Salt marshes, mangroves
Lacustrine fringe	Surface water	Bidirectional, lateral	Great lakes marshes
Slope	Groundwater	Unidirectional, lateral	Fens, seepage wetlands

1.2.3 Constructed wetlands

Constructed wetlands are either built for water quality remediation or to replace wetland dependent functions which were lost by destroying natural wetlands. Constructed wetlands are commonly used to filter or purify wastewater, storm water, mine drainage, animal waste and nonpoint runoff from agricultural lands.

Treatment wetlands are cells which contain various planting substrates and are planted with fast-growing hydrophytic vegetation. The type of substrate depends on the system of the treatment wetland. These wetland types are usually implemented as surface flow or subsurface flow wetlands (Craft, 2005, Kadlec, 2009).

In surface flow wetlands the water flows across the vegetated surface. Under the conditions of low flowing velocity the suspended solids settle at the wetland bottom. Nitrogen is mainly removed from the surface water through nitrification under aerobic conditions and through denitrification under unaerobic conditions in the wetland soils. The removal of phosphorus (P) is controlled by the sorption with Aluminium (Al) in acid soils and with Calcium (Ca) in neutral soils. Uptake of N and P by plants represents a temporal storage, since nutrients are released back to the water column after the death of plants, through the decay of the organic material. N and P are stored in the organic matter of the wetland soils (Craft, 2005).

In subsurface flow wetlands, the waste water moves laterally or vertically either through the soil or planting substrates. The planting substrate consists commonly of gravel or crushed rock to obtain a high hydraulic conductivity in the system and to prevent clogging with suspended materials. Advantages of subsurface flow wetland systems are the even distribution and flow rate of treatment water through the system, and also the reduced breeding opportunities for mosquitoes as well as the fewer nuisances of odor problems. A disadvantage is the lower effectiveness of N removal compared to surface flow systems because of the lower oxygen content in the system which inhibits nitrification (Craft, 2005). However, the effectiveness of the N removal of the wetland is dependent on the dominating N compounds in the inflowing water. If NO3 is the dominating N species, low oxygen content leads to denitrification and thusly to a removal of N from the water.

1.3 Modelling concepts of wetland systems

Several models, including lumped conceptual as well as semi-distributed more physically based, have been proposed to predict the impact of wetlands on nitrogen fate and turnover processes on the catchment scale. The following section summarizes the different concepts implemented.

1.3.1 HBV-N

Arheimer and Wittgren (2002) presented a basic wetland module integrated into the HBV-N model (Arheimer and Brand, 1998, 2000). In this mass balance approach wetlands are assumed as completely mixed batch reactors. Here the N-removal is dependent on the N-concentration in the wetland and a temperature dependent rate coefficient in a simple first-order equation. In the hydrological balance of the model wetlands are treated as small lakes with a generalized runoff-rating curve, where the outflow of the wetland is dependent on the stored water volume. Lakes are virtually situated at the outlet of those subbasins where wetlands should be considered. The areas of the wetlands are subtracted from the area of the arable land in the respective subbasin. In this approach the whole subcatchment drains into the wetland. The model was calibrated against measured data of 8 wetlands and then used in the study to evaluate the effects of potential wetlands on the nitrogen removal in a mesoscale catchment. The conclusion of this study was that the impact of wetlands was small and a large area of wetland is needed to reduce nitrogen loads in the investigated catchments. The authors also concluded that catchment modeling is a useful tool for the assessment of wetland creation plans.

1.3.2 SWAT

In the SWAT model wetlands are simulated as water bodies which are located within subbasins. Inflow and precipitation are added as input paths to the volume water stored in a wetland. Inflow is determined as a fraction of the subbasin area. Outflow from the wetland, evaporation and seepage through the wetland bottom are the possible output pathways of water. The surface area of the water body is calculated as a function of the stored water volume in the wetland and is used to calculate the precipitation which falls on the wetland as well as the amount which evaporates from the wetland. Seepage is calculated as a function of the surface area and the effective hydraulic conductivity of the wetland bottom. Outflow from the wetland occurs whenever the water volume exceeds the normal storage volume of the wetland. For the calculation nutrient transformations in the wetland a completely mixed system is assumed. The mass of a nutrient on a certain day is calculated with the mass of the nutrient entering the wetland on that day and the mass of the nutrient, which is already present in the wetland. The initial nutrient concentration is calculated with the initial mass and the initial water volume. The nutrient removal in the wetland is only considered by the removal via settling. Nutrient transformations (e.g. NH4 to NO3) are not considered. The mass of the removed nutrient is a function of the user defined settling rate as a fixed fraction independent of the water residence time in the wetland, the initial concentration of the nutrient during the time step and the area of the wetland respectively water body.

1.3.3 SWIM

Hattermann et al. (2006) presented an extension of the SWIM model which represents wetlands and riparian zones for river basin modeling. The original SWIM model was built on the SWAT model and MATSALU (Krysanova et al., 1998) where the hydrological components of SWIM were taken from SWAT. Major differences between SWIM and SWAT are the spatial aggregation and the nitrogen turnover processes. With the presented extension the following features where implemented in SWIM:

(1) Daily groundwater table dynamics at the hydrotope level
(2) Assessment of nutrient retention in groundwater and interflow
(3) Implementation of water and nutrient uptake by plants from groundwater
(4)

Groundwater recharge is calculated using an exponential delay function and groundwater table dynamics are explicitly considered by a linear storage approach. The N removal in wetlands and riparian zones follows a linear approach depending on the residence time and the content of organic material. Denitrification is not modeled as a process but described by a linear decay function. Here mean residence time of the water package and the half-life of nitrogen in different geologic formations are important parameters. The explicit plant uptake of nitrogen depends on the rooting depth of the simulated plants. This module has been tested and applied to a mesoscale catchment in Germany. The study showed that wetlands and riparian systems are effective in reducing nitrogen fluxes to the river systems and that plant N uptake from groundwater is mainly responsible for this effect. However, a long term N plant uptake effect is restricted to areas that are used for grazing or hay making such as floodplains where plant material is regularly removed. In wetlands that are not further managed, N plant uptake is reversible and can lead to a delayed N loss. The authors concluded that restoration of wetlands and riparian zones will help to control non-point source pollution in watersheds.

1.3.4 MIKE11-WET

The model MIKE 11 WET (Dorge, 1994) is an add-on module to the MIKE 11 river model system. The model is fully distributed (water and nitrogen balance are explicitly calculated for each grid cell) and consists of two submodules regarding hydrology and biological processes. The wetland hydrology is calculated based on the hydraulic pressure in the saturated zone as well as the hydraulic conductivity of the substrate and hydrologic forcing functions (precipitation and evaporation). In the biological submodule the whole turnover processes of nitrogen from mineralization and nitrification are explicitly modeled based on abiotic forcing functions such as irradiance and temperature. The model is limited to fully water saturated conditions in the soil. Other important assumptions in the model are: nitrogen for plant production is not limited; nitrogen cycle is independent of the phosphorus and carbon cycle; nitrogen turnover is limited to the root zone (Dorge, 1994). The conclusion was that the model is able to consider site-specific nutrient removal and retention processes for single wetlands.

1.3.5 WETTRANS

WETTRANS (Trepel and Kluge, 2004) is a matrix model which connects flow paths and nitrogen transformation with a quasi-stationary mass balance approach. In this approach the inflow and outflow pathways of a wetland as well as the incoming and outgoing nitrogen concentrations are stored in a matrix. With each outflow pathway (e.g., subsurface outflow, ditch outflow, drain outflow and river outflow) a specific transformation coefficient for nitrogen is associated. The model simulates at annual time steps assuming quasi-stationary conditions for the studied wetland.

1.3.6 WETSAND

The WETSAND model (Kazezyilmaz-Alhan et al. 2007) is stand-alone model for solute transport dynamics in wetlands. It is used to investigate the effects of restored wetlands on the water quality of storm water runoff. The wetland water quantity is calculated by using the diffusion wave equation. In the water quality submodel concentration of nitrogen compounds and total phosphorus are calculated by using a one dimensional advection-dispersion-reaction equation with first order loss rates for the specific nutrient species. In the case of nitrogen for each nitrogen compound one equation is used which are finally coupled. Kazezyilmaz-Alhan et al. (2007) coupled the WETSAND additionally with the model SWMM 5 (Rossman, 2005) by using the outputs of SWMM 5 as boundary conditions. SWMM 5 is a storm water management model developed for urban areas. The conclusion of this study was that the model (WETSAND) could be used to simulate the fluctuations of the magnitude of nutrient concentrations and water volume for different wetlands.

1.3.7 WWQM

The WWQM-model by Chavan and Dennett (2008) was developed to describe a surface flow constructed wetland. The model consists of four submodels considering hydrology, nitrogen, phosphorus and total suspended solids. The hydrological submodel follows generally the same water balance approach as the wetland module implemented in SWAT. In the nitrogen submodule all processes are modeled as first-order reactions. The nitrogen balance in this approach includes: (1) mineralization of organic nitrogen to ammonium; (2) volatilization of ammonia; (3) transformation of ammonium to nitrate; (4) denitrification; (5) plant uptake and release of nitrogen; (6) particulate settling and resuspension and (7) diffusion of dissolved forms. The study showed that the model was able to simulate the processes measured at a pilot scale constructed wetland.

1.3.8 CW2D

Toscano et al. (2009) coupled the CW2D model (Langergraber, 2001, Langergraber and Simunek, 2005) to the HYDRUS-2D (Simunek et al. 1999) software to simulate the hydraulic behavior and effluent pollutant concentrations of a pilot-scale two stage subsurface constructed wetland for the treatment of municipal waste water. CW2D describes the biogeochemical transformation and degradation processes in subsurface flow constructed wetlands. The model considers compounds of organic material, nitrogen and phosphorus. The modeled transformation processes include hydrolysis, nitrification, mineralization of organic matter and denitrification. These processes are simulated as Monod-type rate expressions with kinetic parameters which are all considered as temperature dependent. The temperature dependence of all kinetic parameters is calculated by using the Arrhenius equation (Langergraber and Simunek, 2005). HYDRUS-2D uses the Richard's equation to describe saturated and unsaturated water flow and the advection-dispersion equation for heat and solute transport. The conclusion of the study (Toscano et al. 2009) was that the coupled model was able to represent the observed processes at the pilot-scale constructed wetlands. The authors also concluded that the hydraulic behavior of the considered system has to be correctly described in order to achieve a good representation of the modeled effluents.

1.4 Model comparison

In the previous chapter several approaches for modeling natural and constructed wetlands have been presented. Table 2 compares the described models with respect to their ability to simulate the main processes governing N turnover in wetland systems.

The modeling approaches listed in Table 2 differ from simple submodules integrated into hydrological models considering the mesoscale (HBV-N and SWIM) to fully distributed models for the microscale to mesoscale (MIKE11-WET). Additionally stand alone models are presented which mostly describe constructed wetlands (WETSAND, WWQM, CW2D). All models differ in the representation of the hydrological and nitrogen balance as well as in the detail of the implementation of the considered processes.

Besides the presented models various other approaches exist to describe wetland water and nutrient balances. Examples include models that were developed with the STELLATM visualization and modeling tool (Verhoeven and van der Peilj, 1999, Martin and Reddy, 1997). These models are mainly used for scientific purposes in studying processes in wetland systems and not applicable for scenario predictions with an integrated watershed model. Dittrich et al. (2007) presented a model to describe the water balance of large wetlands in the Spreewald, Germany, as a case study. Langergraber et al. (2009) provide an intensive overview of existing modeling approaches in describing subsurface flows in constructed wetlands. The author identified two differentiated objectives in modeling constructed wetlands: mechanistic models which are used to gain knowledge about wetland dynamics and functioning and simple and robust models for design purposes. However, none of the presented approaches fit to the concept of the SWAT model. This is either due to the description of the nitrogen cycle which is in some cases too complex for the integration in SWAT (see the STELLATM approaches) or the process description is too coarse due to the spatial resolution of the approach (Dittrich et al. 2007). Cui et al. (2005) linked a modified version of DNDC (Li et al. 1992) with the hydrological model MIKE-SHE (Refsgaard and

Table 2 Summary of hydrology and nitrogen dynamics in the presented models

Model	Hydrology	Ammonification	Nitrification	Denitrification	Remarks
HBV-N	Treated as small lakes with own runoff-curve, subasin area	Not considered	Not considered	Not considered	N removal by simple first-order equation depending on

	drains into the wetland				temperature and N concentration
SWIM	Water table dynamics, upland area drains into wetland or riparian zone	Not considered	Not considered	Linear decay function	Plant uptake depending on plant rooting depth
SWAT	Dynamic water budget, user defined fraction of the subbasin drains into the wetland	Not considered	Not considered	Not considered	Nutrient removal considered via settling as fixed ratio
MIKE11-W	Vertical and lateral flow to adjacent grid cells, area above drains into the wetland	Explicitly for each grid cell	Explicitly for each grid cell	Explicitly for each grid cell	Immobilization and adsorption also considered
WETTRANS	Not considered	Not considered	Not considered	Not considered	Matrix flow path model
WETSAND	Horizontal and vertical flow by Darcy's equation, upland area drains into the wetland	Advection-convection equation with first order rate constants	Adversion-convection equation with first order rate constants	Adversion-convection equation with first order rate constants	
WWQM	Dynamic water budget approach, fraction of upland area drains into the wetland	First order equation with rate constants depending on temperature and moisture of wetland soils	First order equation with rate constants depending on temperature and moisture of wetland soils	First order equation with rate constants depending on temperature	Ammonia volatilization also considered; Plant uptake also considered
CW2D	Coupled to HYDRUS 2D, Wetland system connected to point sources	Monod-type rate expressions	Monod-type rate expressions	Monod-type rate expressions	Kinetic parameters dependent on temperature calculated with Arrhenius equation

Storm, 1995) in order to calculate greenhouse gas emissions from forested wetlands. The disadvantage of this approach is the high data demand due to the distributed spatial resolution of MIKE-SHE. Hence, this approach is not suitable for calculating wetland dynamics at the mesoscale. Lamers et al. (2007) used the standalone version of Wetland-DNDC (Cui et al., 2005) to calculate emissions of nitrous oxide from water logged soils. The process description of the nitrogen and carbon balance in this model is too complex for an easy integration or coupling with the SWAT-model. Liu et al. (2008) described a sophisticated way to enhance the descriptions of the water balance of wetland systems in the SWAT-model. Since this approach only covers the water balance and the nutrient cycles are not affected this approach is not suitable for the modeling purposes within the Aquisafe 2 project.

The aim of this review is to find a simple but robust approach for wetland simulation, which could be integrated into the SWAT model. The above described approaches of HBV-N and SWIM provide simple approaches of an integrated modeling of wetland dynamics at the watershed scale. But these approaches do not consider all governing processes of the nitrogen cycle in the wetland and are thus not qualified to be integrated into SWAT. The approach used by MIKE11-W takes into account all processes of the nitrogen cycle but in this case the representation is too detailed for an implementation into a watershed model investigating the mesoscale, which would result in a huge data demand and computational effort. The WETTRANS model provides a matrix approach which is not suited to be implemented into a numerical watershed model, because of its process description and the temporal scale of the considered processes. The standalone models WETSAND and CW2D also provide too detailed process descriptions and are not suitable to be integrated into SWAT due to the different spatial representation of the processes related to the N-cycle. The hydrologic dynamics in the WWQM model resembles the existing hydrologic approach for Wetlands in SWAT. The submodule of the nitrogen cycling considers all main processes of nitrogen dynamics in wetland systems to a degree which is acceptable for the mesoscale. Due to these facts we conclude that the approach of the WWQM model is suitable to be integrated in the SWAT-model.

1.5 Suggested improvement of the current SWAT approach

To improve the prediction accuracy and consideration of N turnover processes of the SWAT model in wetland applications, we suggest the following approach. Compared to the approach currently implemented in SWAT, we suggest an explicit consideration of the nitrogen cycle in wetland systems. The module will consist of 3 nitrogen pools (organic N, Ammonia and Nitrate) and the processes mineralization, nitrification /denitrification and volatilization are explicitly simulated. Another advantage of the new approach is that it can be easily extended for the consideration of phosphorus and sediments.

1.5.1 Basic assumptions and concept of implementation:

At the first stage the following assumptions are made:

- Wetlands in SWAT should be located right before the outlet of the subbasin;
- Water enters the wetland only as stream discharge (point source) or by precipitation; stream discharge and quality is dependent on computed discharge and nutrient composition (amounts) of the upland area in the respective subbasin;
- Plant growth, transpiration, nitrogen uptake and release by plants will not be considered for simplicity.

These assumptions are especially made with respect to the designed constructed wetlands of the Ic catchment, France. In case other wetland types are considered we suggest including also further processes. The most relevant processes that are not included here are (i) a connection between the wetland and groundwater flow, lateral subsurface flow or surface runoff, (ii) N plant uptake and feedbacks between N stored in wetlands and plant growth.

The new wetland routine should be implemented as a new subroutine in the code. Through a yes/no switch in the *.bsn-file the decision can then be made whether the new or the original wetland-module is used. The new Aquisafe-module should be called in the main subbasin loop to make sure that all parameters which are needed are updated every time step.

The necessary wetland storage parameters should be taken from the original approach and the respective *.pnd-file. In this file the new parameters regarding the rate constants for the nitrogen balance should be added and read from the respective *.pnd-file.

1.5.2 Water balance:

The water balance in the suggested approach is comparable to the already implemented approach. The water volume of the wetland is computed as given in Eq. (1). The water volume stored in the wetland is added by water which is flowing from the subbasin channel to the wetland. Evaporation and outflow from the wetland describe water losses. Outflow only occurs if the water volume in the wetland exceeds the storage capacity of the wetland (Eq. (2)).

(1) $$Q_{actual(t)} = Q_{PS(t)} + \left(P_{(t)} - E_{(t)}\right) * A - Q_{out(t)}$$

$Q_{PS(t)}$ *Flow from point sources at time step t; in this case from the incoming channel [m^3]*

$Q_{actual(t)}$ *Net water flow into the wetland at time step (t) [m^3]*

$P_{(t)}$ *Precipitation [m] at time step t*

$E_{(t)}$ *Evaporation from the wetland [m] at time step t*

A Wetland area [m^2]

$Q_{out(t)}$ *Outflow of the wetland [m^3] at time step t*

(2a) $$VOL_{w(t)} = VOL_{w,max} - VOL_{w(t-1)}$$

(2b) $$Q_{out(t)} = \max[0;\ Q_{PS(t)} + \left(P_{(t)} - E_{(t)}\right) * A - VOL_{w(t)}$$

$VOL_{w(t)}$ *Water volume that can be stored in the wetland at time step t [m^3]*

$VOL_{w,(t-1)}$ *Water volume stored in the wetland at the preceding time step [m^3]*

VOLw,max Maximum water volume that can be stored in the wetland [m3]

Water traveling time through the wetland is an important factor in the settling, turnover and decay of nitrogen. The travel time respectively the hydraulic retention time for the wetland is computed following Eq. (3)(Chavan and Dennett, 2008).

(3) $$HRT = 0.84 * \frac{V}{Q_{ou(t)}} * (1 - e^{\left(-0.59*\frac{L}{W}\right)})$$

HRT Hydraulic retention time for the wetland [d]

V Volume of the wetland [m^3]

$Q_{out(t)}$ *Outflow of the wetland [m^3] at time step t*

L Length of the wetland [m]

W Width of the wetland [m]

1.5.3 Nitrogen balance:

Based on the approach by Chavan and Dennett (2008) the nitrogen balance in the new module consists of three pools representing organic nitrogen, ammonia and nitrate. Transformations from one nitrogen species to another are represented by first order reaction equations. Chavan and Dennett (2008) also provide a way to calculate the rate constants of the considered transformation processes depending on water temperature and pH-value of the environment. In general these calculations could also be implemented into the new SWAT-module, since all needed parameters are provided by the model. The transformation processes are also dependent on the retention time or travelling time of the respective water package through the wetland. In the stage of testing the proposed approach we suggest to calibrate the rate constant and compare the results to values reported in literature and measured data of the pilot scale experiments in Aquisafe 2. Additionally the storage capacity of the different nitrogen pools needs to be evaluated by the pilot scale experiments or by a further literature study. In the stage of implementation and model testing we suggest to calibrate this parameter.

Eq. (4) describes the balance of the organic nitrogen pool. Organic nitrogen is mineralized into ammonia or leaves the wetland by outflow. Organic Nitrogen can only get into the wetland system via inflow.

(4) $$OrgN_{w(t)} = OrgN_{w(t-1)} + OrgN_{in(t)} - OrgN_{out(t)} - OrgN_{\min(t)}$$

$OrgN_{w(t)}$ *Organic nitrogen in the wetland [kg] at time step t*

$OrgN_{w(t-1)}$ *Organic nitrogen in the wetland [kg] at the preceding time step t*

$OrgN_{in(t)}$ *Organic nitrogen going into the wetland [kg] at time step t*

$OrgN_{out(t)}$ *Organic nitrogen going out of the wetland [kg] at time step t*

$OrgN_{min(t)}$ *Organic nitrogen mineralized in the wetland [kg], transferred to NH_4 Pool at time step t*

The following equations describe the way how Eq. (4) is solved internally in the SWAT-Code. At the beginning of the time step the organic Nitrogen pool is updated by using

Eq. (5a). In the next step the amount of the mineralized organic nitrogen is calculated (Eq. (5b)). At the end of the time step the organic nitrogen pool is updated by using Eq. (5c).

(5a) $OrgN_{w(t,b)} = OrgN_{w(t-1)} + OrgN_{in(t)}$

(5b) $OrgN_{\min(t)} = OrgN_{w(t,b)} * k_{min}$

(5c) $OrgN_{w(t,e)} = OrgN_{w(t,b)} - OrgN_{out(t)} - OrgN_{\min(t)}$

k_{min} Mineralization rate constant [1/day]

$OrgN_{w(t,b)}$ Organic nitrogen in the wetland [kg] at the beginning of time step t

$OrgN_{w(t,e)}$ Organic nitrogen in the wetland [kg] at the end of time step t

Eq. (6) describes the balance of the ammonia pool. Inputs into the ammonia pool are due to inflows by water and the amount of organic N which is ammonified during the time step. Ammonia either leaves the wetland with the outflowing water, is volatilized or nitrified.

(6) $NH4_{w(t)} = NH4_{w(t-1)} + NH4_{in(t)} + OrgN_{\min(t)} - NH4_{out(t)} - NH4_{vol(t)} - NH4_{nit(t)}$

$NH4_{w(t)}$ Ammonia in the wetland [kg] at time step t

$NH4_{w(t-1)}$ Ammonia in the wetland [kg] at the preceding time step t-1

$NH4_{in(t)}$ Ammonia going into the wetland [kg] at time step t

$NH4_{out(t)}$ Ammonia leaving the wetland [kg] at time step t

$NH4_{vol(t)}$ Ammonia volatilized in the wetland [kg] at time step t

NH4nit(t) Ammonia nitrified in the wetland [kg], transferred to NO_3-pool at time step t

The following equations describe the way how Eq. (6) is solved internally in the SWAT-Code. At the beginning of the time step the ammonia pool is updated by using Eq. (7a). In the next step the amounts of the volatilized and nitrified ammonium is calculated (Eq. (7b and 7c)). At the end of the time step the ammonium pool is updated by using Eq. (7d).

(7a) $NH4_{w(t,b)} = NH4_{w(t-1)} + NH4_{in(t)} + OrgN_{\min(t)}$

(7b) $NH4_{vol(t)} = NH4_{w(t,b)} * k_{vol}$

(7c) $NH4_{nit(t)} = NH4_{w(t,b)} * k_{nit}$

(7d) $NH4_{w(t,e)} = NH4_{w(t,b)} - NH4_{out(t)} - NH4_{vol(t)} - NH4_{nit(t)}$

k_{vol} Volatilization rate constant [1/day]

k_{nit} Nitrification rate constant

$NH4_{w(t,b)}$ Ammonia in the wetland [kg] at the beginning of time step t

$NH4_{w(t,e)}$ Ammonia in the wetland [kg] at the end of time step t

Eq. 8 describes the balance of the Nitrat-pool. The wetland system could gain nitrate via inflow and by nitrifying ammonia. Nitrate could be lost via outflow and denitrification.

(8) $$NO3_{w(t)} = NO3_{w(t-1)} + NO3_{in(t)} + NH4_{nit(t)} - NO3_{out(t)} - NO3_{den(t)}$$

$NO3_{w(t)}$ Nitrate in the wetland [kg] at time step t

$NO3_{w(t-1)}$ Nitrate in the wetland [kg] at the preceding time step t

$NO3_{in(t)}$ Nitrate going into the wetland [kg] at time step t

$NO3_{out(t)}$ Nitrate leaving the wetland [kg] at time step t

NO3den(t) Nitrate denitrified in the wetland [kg] at time step t

The following equations describe the way how Eq. (8) is solved internally in the SWAT-Code. At the beginning of the time step the nitrate pool is updated by using Eq. (9a). In the next step the amount of the denitrified nitrate is calculated (Eq. (9b)). At the end of the time step the nitrate pool is updated by using Eq. (9c).

(9a) $$NO3_{w(t,b)} = NO3_{w(t-1)} + NO3_{in(t)} + NH4_{nit(t)}$$
(9b) $$NO3_{den(t)} = NO3_{w(t,b)} * k_{den}$$
(9c) $$NO3_{w(t,e)} = NO3_{w(t,b)} - NO3_{out(t)} - NO3_{den(t)}$$

k_{den} Denitrification rate constant [1/day]

$NO3_{w(t,b)}$ Nitrate in the wetland [kg] at the beginning of time step t

$NO3_{w(t,e)}$ Nitrate in the wetland [kg] at the end of time step t

The implementation of the proposed approach should be followed by an intensive sensitivity and uncertainty analysis in order to test the new module.

Chapter 2

Development of a wetland module (stand alone version)

2.1 Introduction

The first version of the presented module was developed as a stand-alone wetland model and written in the Python programming language. It uses climate data to predict evapotranspiration and SWAT predictions of runoff and loads of different N-species as boundary conditions. This approach allows investigating the module capabilities independently from the rest of the model and it also eases the implementation of potential changes of the module. After thorough testing of the Python based wetland module and final acceptance of its design by the Aquisafe II consortium, the code will be translated into the Fortran language and implemented into the SWAT code.

Hereafter follows a description of the mechanisms implemented in the module code. Then, the results of a conceptual first application are analysed. Finally, a conclusion on the achievements and next development steps are presented at the end of the document.

2.2 Model description

SWAT is a semi-distributed model and considers the catchment as a succession of nested sub-catchments. It computes the different water and nutrient balances at a daily (discrete) time step for each of these entities. That is why a certain order of occurrence of processes had to be chosen even though they are likely to occur simultaneously (see also Julich et al., 2010). However, we assume that the averaging of process rates over the considered time step will have no impact on the modelling results.

The actual mitigation zones were planned to be implemented along streams. In order to ease the implementation of the module in the SWAT model architecture itself, a wetland has to be defined as a buffer between two successive upstream and downstream sub-catchments. In other words, water and nutrients flowing out of an upstream SWAT sub-catchment contribute to the corresponding wetland balances before eventually flowing out into the next downstream SWAT sub-catchment.

2.2.1 Water balance

First, the water balance of a wetland is computed for each time step. Water volume increases with precipitation and inflow and decreases with evaporation and outflow. For each time step, the actual water volume contained into the wetland is updated according to the Eq. (1).

$$V_t = V_{t-1} + L \cdot W \cdot \left(P_t - E_t\right) \cdot 10^{-3} + Q_{in,t} - Q_{out,t} \qquad (1)$$

In Eq. (1), Vt is the water volume [m³] in the wetland at the end of time step t, Vt-1 is the water volume [m³] at the end of the previous time step t-1. The product of the length L [m] and the width W [m] of the wetland corresponds to the area of the wetland surface [m²]. It is used to transform the total amount of daily precipitation Pt and the daily evaporation Et [mm] into the same unit of other water volumes [m³]. The variables Qin,t and Qout,t represent the volume of water flowing in and out from the wetland on time step t respectively [m³/d]. Inflow Qin,t is provided by the SWAT model whereas the outflow Qout,t is computed within the model such as

$$Q_{out,t} = \max\left(0; L \times W \times \left(P_t - E_t\right) \cdot 10^{-3} + Q_{in,t} - V_{\max} + V_{t-1}\right) \quad (2)$$

where L is the length and W is the width of the wetland [m], Vmax is the maximum volume of the wetland and other notations correspond to those in Eq. (1).

2.2.2 Nitrogen balance

Water flowing in and out of the wetland transports nutrients. Moreover, the module takes into account the nitrogen (N) turnover processes which have been identified as critical in wetlands: mineralisation, nitrification, volatilisation and denitrification (Julich et al., 2010). Four different pools of N (which are also computed by SWAT) are considered: organic N (ON), ammonium N (NH4-N), nitrite N (NO2-N) and nitrate N (NO3-N). The two latter species are actually combined in a single pool. The ratio of nitrite to nitrate content is updated at the beginning of each time step and assumed to remain constant during this time. The considered N transformation turnover processes are summarised in Figure 1.

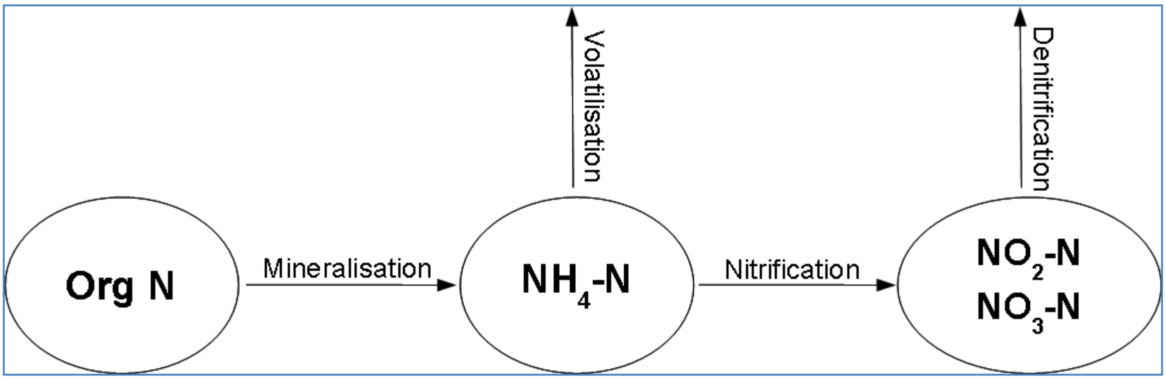


Figure 1 Turnover processes considered in the new wetland module

Pools are all expressed in [kg N] as it is the unit used in the SWAT model. The wetland is assumed to be a well-mixed water body and therefore we consider the different N-species concentrations to be uniform in it as well as in the outflow. The different turnover processes are governed by the N-species availability (i.e. concentration in the wetland), a temperature factor Tf,t, (Eq. 4) adapted from the INCA model (Whitehead et al., 1998) as well as a user input free dimensionless factor which controls the process rates.

$$T_{f,t} = 1.047^{(T_t - 20)} \quad (4)$$

In Eq. (3), Tf,t is the value of the dimensionless temperature factor at time step t computed as a function of the corresponding daily average temperature Tt [°C]. At the beginning of a time step each N store is updated with the amount of the corresponding species flowing in and which becomes directly available for the internal N cycle (Eq. (5) to (8)).

$$ON_{t,b} = ON_{t-1} + ON_{in,t} \quad (5)$$

$$NH_4N_{t,b} = NH_4N_{t-1} + NH_4N_{in,t} \quad (6)$$

$$NO_2N_{t,b} = NO_2N_{t-1} + NO_2N_{in,t} \quad (7)$$

$$NO_3N_{t,b} = NO_3N_{t-1} + NO_3N_{in,t} \quad (8)$$

In Eq. (5) to (8), the variables ON, NH4N, NO2N and NO3N correspond to the organic N, ammonium N, nitrite N and nitrate N, respectively. They are expressed in [kg]. The subscript t,b corresponds to the different stores at the beginning of the time step, the subscript t-1 is assigned to the store content at the end of the previous time step and the subscript in,t is assigned to the amount of different N species flowing into the wetland from the directly upstream catchment.

The daily process rates are then calculated for each time step according to Eq. (9) to (12).

$$m_t = k_m \cdot T_{f,t} \cdot \frac{ON_{t,b}}{V_t + Q_{out,t}} \quad (9)$$

$$n_t = k_n \cdot T_{f,t} \cdot \frac{NH_4N_{t,b}}{V_t + Q_{out,t}} \quad (10)$$

$$v_t = k_v \cdot T_{f,t} \cdot \frac{NH_4N_{t,b}}{V_t + Q_{out,t}} \quad (11)$$

$$d_t = k_d \cdot T_{f,t} \cdot \frac{NO_2N_{t,b} + NO_3N_{t,b}}{V_t + Q_{out,t}} \quad (12)$$

In Eq. (9) to (12), mt, nt, vt and dt represent the computed mineralisation, nitrification, volatilisation and denitrification rates [kg m-3 d-1] at time step t, respectively. The dimensionless variables km, kn, kv and kd represent the user input maximal specific rates [d-1] for mineralisation, nitrification, volatilisation and denitrification, respectively. They are corrected by the temperature factor Tf,t previously computed according to Eq. (4). The variables ONt,b [kg], NH4Nt,b [kg] NO2Nt,b [kg] and NO3Nt,b [kg] represent the organic N, ammonium N, nitrite N and nitrate N stores at the beginning of the time step as computed in the Eqs. (5) to (8), respectively. The term Vt+Qout,t corresponds to the total water volume available for dilution during the time step t.

Finally, concentrations are updated according to the simplified N cycle (Fig. 1). The wetland is supposed well-mixed and the outflow has the same chemical signature than the wetland itself which makes it easy to calculate loads. The amount of the different N species in the wetland is updated as the product of the corresponding final concentrations by the water content of the wetland at the end of the time step. In both the outflow and the wetland, the previously computed ratio of nitrite to nitrate is used to update both pools.

2.3 Module test

The first test of the wetland module is realised in a very conceptual way. A large wetland is simulated at the outlet of the ‘Ic amont’ catchment, a 14.5 km² upstream sub-catchment of the Ic catchment. Its surface is set to correspond to the total surface area which may be converted to wetlands over the next years in the Ic, i.e. 1% of the agriculturally used catchment agricultural cover, corresponding to 12 ha. This simulation gives an overview of the cumulative effect of the different wetlands to be implemented. The module is fed with the output of the SWAT model calibrated over a four year period from 1/1/2006 to 31/12/2009. Corresponding boundary conditions of the wetland are presented in Figure 2. A good agreement between model predictions and observed data in the general dynamics guarantees reliability of the input data.

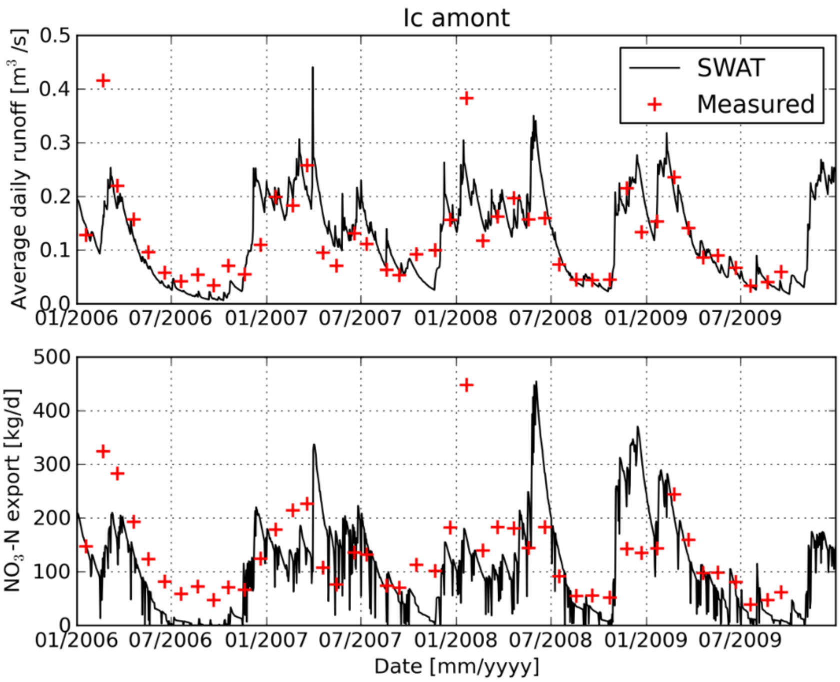


Figure 2 Boundary conditions (top: daily water inflow, bottom: daily nitrate N inflow) of the wetland module as provided by SWAT for the outlet of the Ic amont sub-catchment

The depth of this hypothetic large wetland is set to 1.2 m which is of the same order than the wetlands to be constructed. In order to proportionally keep the same shape of the wetland, i.e. a 2:1 ratio of length to width, wetland dimensions are set to 490 m length and 245 m width, respectively.

The module relies on some free parameters governing the turnover processes in the wetland. With the lack of observation data, parameter values remain hard to quantify. In order to get an idea of the expected wetland denitrifying potential, we performed a Monte-Carlo simulation based sensitivity and uncertainty analysis. For a total of 10,000 model runs, parameters governing the turnover processes are randomly altered between chosen minimum and maximum bounds indicated in Table 1.

Table 1 Parameter ranges used in the Monte-Carlo procedure

Parameter	Description	min value	max value
k_m	Mineralisation constant rate [d^{-1}]	0.001	1
k_v	Volatilisation constant rate [d^{-1}]	0.001	1
k_n	Nitrification constant rate [d^{-1}]	0.001	1
k_d	Denitrification constant rate [d^{-1}]	0.001	1

The range of simulated global nitrate retention rates is shown in Figure 3, where the red curve represents the daily nitrate N inflow into the wetland as predicted by SWAT. The daily nitrate N outflows predicted for each of the different 10,000 wetland model runs are merged into the shaded area which represents the predictive uncertainty associated with the module parameters. The outflow of NO3-N is always less than or equal to the NO3-N inflow on the same day. This confirms that the wetland module is well designed and behaves like a natural wetland with mostly denitrifying conditions.

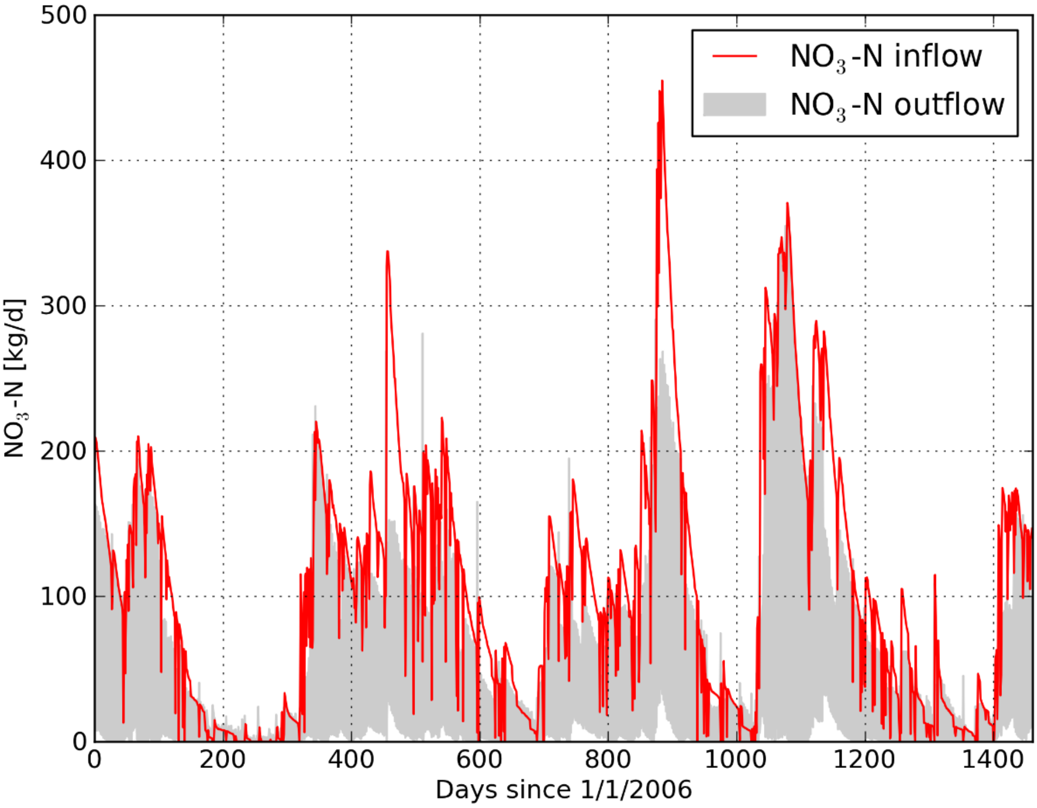


Figure 3 Nitrate N balance into the hypothetical large wetland at the outlet of the Ic amont sub-catchment

Dotty plots in Figure 4 express the average NO3-N retention rate as a function of the different parameter values in order to assess the global sensitivity of the module. It is clear that the only really sensitive parameter is the denitrification rate kd. The highest nitrate retention rate achieved is about 813 mg N m-2 d-1. These values are in good agreement with published ones which range between -123.2 and 2493.0 mg N m-2 d-1 (Périllon and Matzinger, 2010). This makes the prediction plausible.

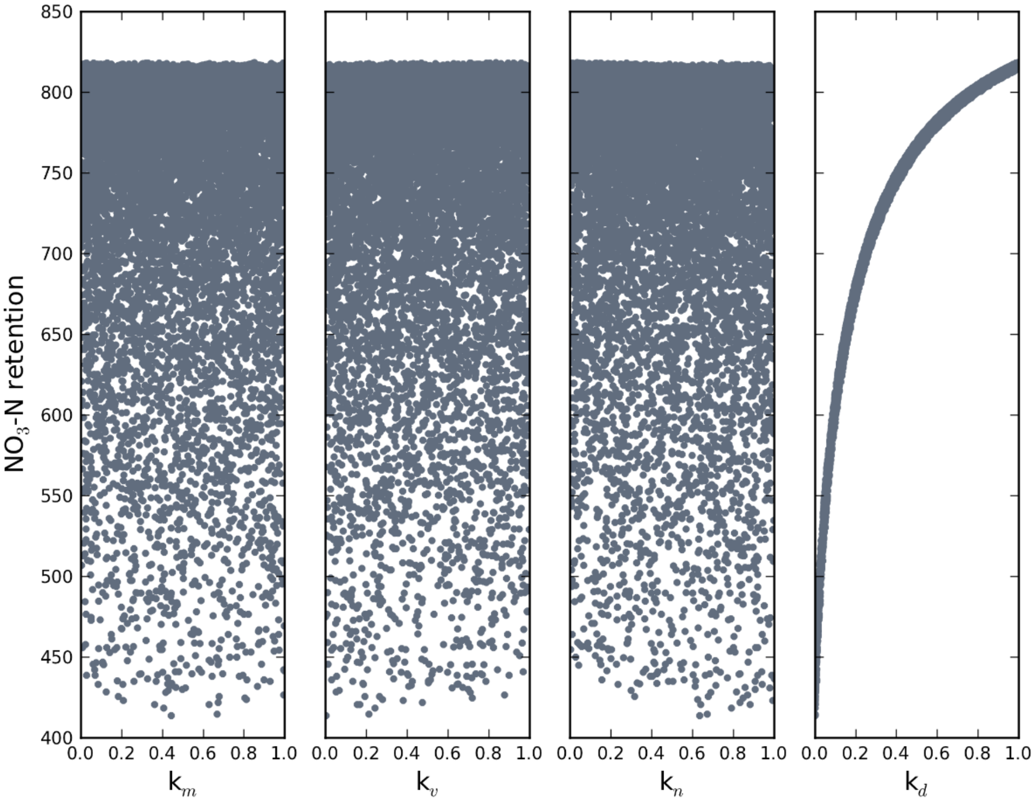


Figure 4 Sensitivity of the retention to the different parameter values

2.4 Conclusion

The wetland module always predicts plausible global denitrifying conditions with any of the randomly chosen parameter sets. However, the first application of the wetland model is still very conceptual and cannot be considered as a definitive statement on the effect of mitigation zones in this region. Moreover, a large prediction uncertainty remains due to model parameter uncertainty, but the sensitivity analysis already highlights the dominant role of the denitrification processes. This is however not really surprising due to the usually high contribution of NO3-N inflow to the inner N balance of the wetlands.

The next step in the current development is to implement the module into the SWAT code. This will allow us to directly simulate the pilot sites at their true locations. Meanwhile, chemical measurements should become available for model testing and verification. Then, we should also be able to calibrate the module parameters and quantify the true effect of the pilot sites on the in-stream N balance.

Chapter 3

Implementation of the new wetland module in SWAT

3.1 Introduction

The first version of the new wetland module was developed as a stand-alone program (Exbrayat et al., 2011). The surrounding idea was to utilise the flexible Python programming language to allow quick adjustments of the model structure. Therefore, besides meteorological forcing, this model had to be driven by some output generated by a SWAT run: daily runoff and losses of different nitrogen species (Organic-N, NO3-N, NH4-N, NO2-N).

After its successful testing, the wetland module has now been implemented into the SWAT source code itself. Hereafter follows a summary of the changes that were made to the SWAT source code. Then, a short description of the modifications required to be made to the input files is provided to effectively use the new module. Finally, as a quality test, a comparison of the outcome of the original offline Python module with the newly implemented online module is given as well as a short outlook of what could now be achieved with this new capabilities.

3.2 Changes to the source code

As previously discussed in Exbrayat et al. (2011), SWAT defines wetland as a buffer zone between two successive upstream and downstream sub-catchments. This type of inter-catchment structure is called a 'reservoir' in the SWAT model. Each reservoir is associated to an input file (***.res) that contains different wetland's attributes such as: maximum volume, surface area, conductivity of substrate, starting date on which the wetland is operational, etc... (Neitsch et al., 2004).

All equations previously described in Exbrayat et al. (2011) were implemented in the SWAT 2005 source code previously downloaded from SWAT's official website at the Texas A&M University (http://www.brc.tamus.edu/swat/). The new module relies on a switch contained in the ***.res that tells SWAT which version it should use (see section 3). This means that model users have now the choice to simulate each wetland using either the classical or the new approach. Table 1 summarises the location of these modifications. For a better overview, reader are referred to commented lines in the attached source code.

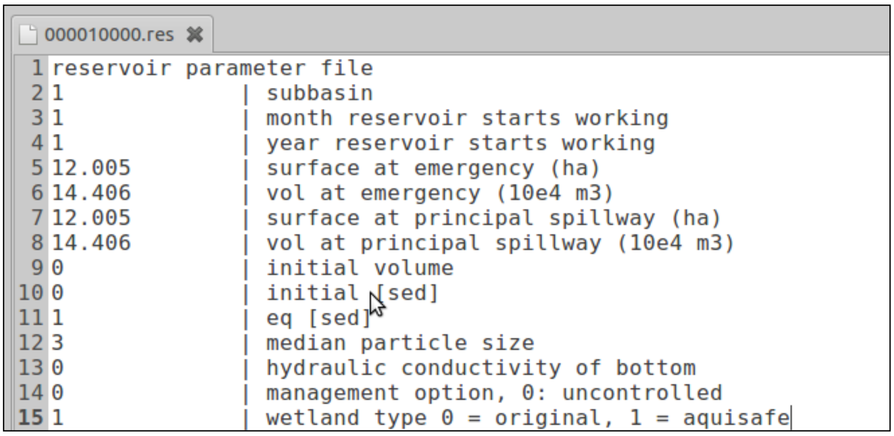
Table 1 Summary of modifications in the source code

File	Modifications overview
readres.f	Read-in wetland shape parameters (volume and surface area) and type
resinit.f	Initialise wetland water content
res.f	Computes wetland's water balance
resnut.f	Computes wetland's nutrient balance

The new model has been compiled successfully using the GNU Fortran compiler on different Linux 64 bits systems. The executable has to be placed in the same folder than the input files.

3.3 Input files

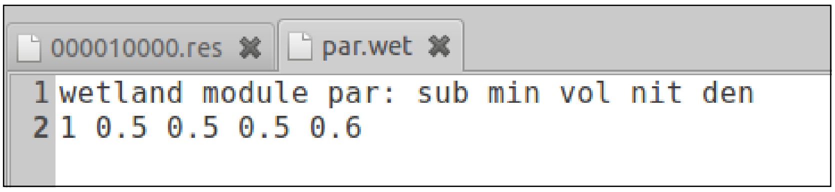
Due to the large amount of input files, the most challenging part of the coding was to implement a straightforward way to tell SWAT when to use the new model version, and when to use the original one. All input files of the SWAT project are contained in the same folder as the one containing the model executable. Each wetland is associated to its own parameter file ***.res and we implemented a switch on line 15 of this file. As illustrated in Figure 1, a value of 0 leads SWAT to use the old wetland routines while value of 1 corresponds to the new wetland ones.



```
 1 reservoir parameter file
 2 1                | subbasin
 3 1                | month reservoir starts working
 4 1                | year reservoir starts working
 5 12.005           | surface at emergency (ha)
 6 14.406           | vol at emergency (10e4 m3)
 7 12.005           | surface at principal spillway (ha)
 8 14.406           | vol at principal spillway (10e4 m3)
 9 0                | initial volume
10 0                | initial [sed]
11 1                | eq [sed]
12 3                | median particle size
13 0                | hydraulic conductivity of bottom
14 0                | management option, 0: uncontrolled
15 1                | wetland type 0 = original, 1 = aquisafe
```

Figure 1 Details of the reservoir input file set to use the new module

If one decides to use the original module version, complementary parameters are required and have to be set on the following line of the ***.res file as in Neitsch et al. (2005). On the other hand, if one decides to use the new module version developed for the Aquisafe application, a new input file par.wet containing wetland specific parameters is required. As illustrated in Figure 2, the first line of this file is used for comments and following lines indicates the subcatchment that discharges into the wetland and its specific mineralisation, volatilisation, nitrification and denitrification rates.



```
1 wetland module par: sub min vol nit den
2 1 0.5 0.5 0.5 0.6
```

Figure 2 Details of the new input file containing process rates

3.4 Results

The first step following the implementation of the module was to compare the output of the previous Python stand-alone module with the output of the module embedded in the complete SWAT model structure. The following Figure 3 and 4 compare the water and NO3-N discharge from the wetland, respectively.

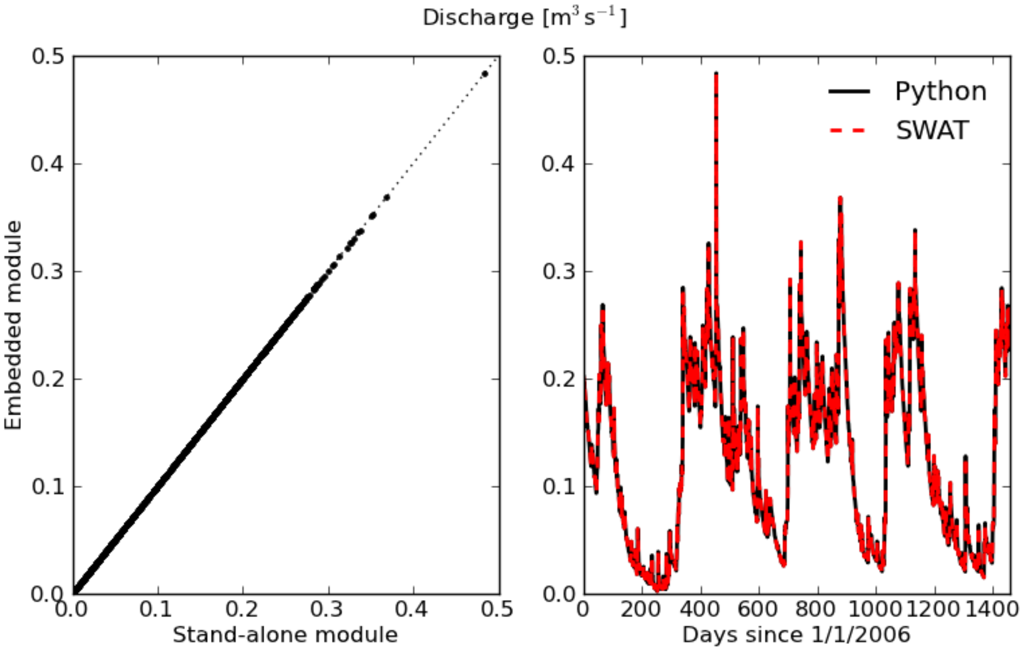


Figure 3 Comparison of water discharge from the wetland simulated by the stand-alone module and the embedded version

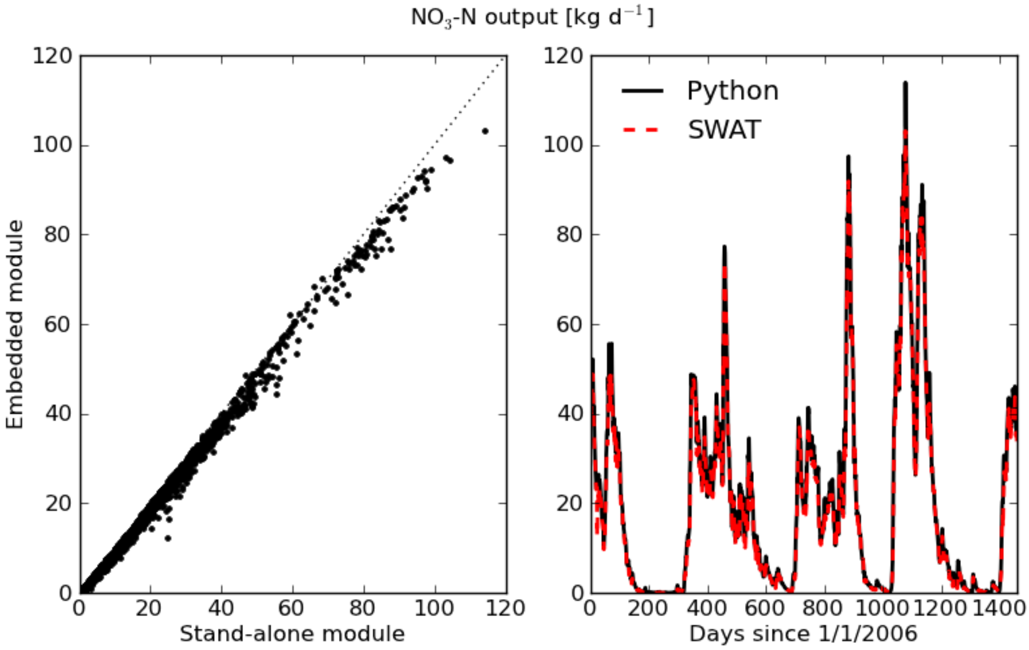


Figure 4 Comparison of NO3-N output from the wetland simulated by the stand-alone module and the embedded version

The water discharge simulated by the two versions of the module is identical (left panel in Figure 3) and the time series present a perfect match (left panel in Figure 3). However, some slight differences in the simulated NO3-N discharge are observed in the left panel of Figure 4. These are probably due to the precision at which Python and Fortran calculate float operations, especially when transforming nutrient stores to concentrations to compute turnover processes. However, as illustrated in the right panel of Figure 4, these discrepancies are really minor if we consider the time series and have a negligible effect on the total nutrient balance of the wetland.

3.5 Conclusion

The new wetland module version was successfully implemented in the SWAT 2005 model structure and performs comparatively to the previous stand-alone version. However, whilst the Python module could only recycle the output of SWAT, the output of the embedded module are routed downstream which allows studying spatial effects of upstream wetland on downstream nutrient losses.

When observation data become available, one will be able to easily calibrate the stand-alone module before propagating the optimised parameters in the embedded module in order to see spatial effects of mitigation measures.

Chapter 4

Conclusions and outlook

We successfully developed a new SWAT add-on that can be used simulate the effectiveness of constructed wetlands on solute N fluxes on the landscape scale. Prior to SWAT implementation the module was intensively tested as a stand-alone version. A full sensitivity and uncertainty analyses based on Monte Carlo simulations was realized to identify most sensitive and constrained parameters.

The model proofed to provide plausible results. A full test with real world data was not possible due to a lack of data that were not available at the time of the end of this project. We therefor recommend to test the new module with either literature data or look for sites where the relevant and needed data are available. We assume that the four parameters of the SWAT wetland module need to be calibrated in the course of the model set up. However, it should be tested whether a reduced number of calibrated parameters would result in similar results.

Nevertheless, given the results of the plausibility check we consider the SWAT wetland module as a reliable tool to answer “what – if” questions with regard to the overall questions raised by the Aquisafe project on which management practices could results in a reduction of N loads in the Ic catchment.

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