A review of modelling tools for implementation of the EU Water Framework Directive in handling diffuse water pollution

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ABSTRACT

A numerical catchment-scale model capable of simulating diffuse water pollution is necessary in sustainable environmental management for better implementation of the EU Water Framework Directive. This paper provides critical reviews of most popular and free models for diffuse water modelling, with detailed sources and application potential. Based upon these reviews, further work of selecting and testing the HSPF model was carried out, with a case study in the Upper Bann Catchment, Northern Ireland. The calibrated and validated HSPF model can well represent the characteristics of surface water quantity and quality. Climate change scenario evaluation in five years showed that when the annual mean temperature increase 3℃ the mean yearly total runoff volume will decrease by 11.1% and the mean daily river flow 11.4%. If 20% crop and pasture land is converted into forest land in the study area, the mean river concentration of nitrate, nitrite, NH_4 and PO_4 in five years will decrease by 19.4%, 33.3%, 31.3% and 31.3% respectively. When applying filter strip method in 80% crop and pasture land in the area, the reduction of the mean concentration of nitrate, nitrite, NH_4 and PO_4 in five years will be 15.3%, 33.3%, 31.3%, and 5.6% respectively. This

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study shows that HSPF is a suitable model in handling diffuse source water pollution, which can be introduced into the Programme of Measures in the River Basin Management Plans for better implementation of the EU WFD.

Keywords**:** Diffuse water pollution; water quality modelling; Catchment; EU Water Framework Directive; Climate change.

Software availability

Software name/source: all reviewed software are mentioned in the text.

1. Introduction

Water pollution, a global problem, is not only an environmental issue but also an economic and human health problem. As a part of a substantial restructuring of EU water policy and legislation, the EU Water Framework Directive (WFD) was agreed by the European Parliament and Council in September 2000 and came into force on 22nd December 2000 (EC, 2000). The EU WFD sets a framework for comprehensive management of water resources in the European Community, within a common approach and with common objectives, principles and basic measures. The fundamental objectives of the Water Framework Directive are to maintain a “high status” of inland surface waters, estuarine and coastal waters and groundwater where it exists, prevent any deterioration in the existing status of waters and achieve at least a “good status” in relation to all waters by 2015 (Heinz et al., 2007; Krause et al., 2007). Member States will have to ensure that a coordinated approach for water management is adopted for the achievement of the objectives of the WFD and for implementation of acting programmes for the purposes (Borowski et al., 2007; De-Kok et al., 2009).

Diffuse water pollution (DWP) has been realised as a major threat for water quality and the biggest remaining problem of water pollution in many countries (Campbell et al., 2004; Gaddis et al., 2007; Orr et al., 2007; Hessea et al., 2008). DWP is also the main threat for meeting the requirement of the EU WFD (DoE and DARD UK, 2003; Ferrier et al., 2004; Torrecilla et al., 2005; Silgram et al., 2008). The serious problem for implementation of the EU WFD is lack of pragmatic methods and tools to fulfil new tasks from the EU WFD for most EU Member States (Mostert, 2003; Giupponi, 2005; Heinz et al., 2007). The scientific measures or tools that can actually be used or developed for implementation of the EU WFD, especially in handling DWP, are still largely unknown to the EU Member States (UK EA, 2005; Krause et al., 2007).

Not all water quality problems require a water quality modelling effort. Numerical water modelling, however, is necessary for the sustainable DWP management at catchment scale. Compared to point pollution, DWP is more complex and difficult to control due to its numerous and dispersed sources, and the difficulties in tracing its pathways (Wang and Yang, 2008). Suitable numerical DWP models not only provide quantitative description of water quantity and quality to the temporal and spatial details and the contaminant fate and transport in the DWP phases of source – pathway – target, varying greatly with different natural and landuse conditions; but also are capable of evaluating the impacts of the management plans on water processes in which the extension and extrapolation of measured data are needed (Van-Ast et al., 2005; Galbiati et al., 2006; Even et al., 2007). The quality and complexity of the DWP models will directly affect the reliability of modelling results. The good DWP models should consider these factors: weather-driven processes and meteorological conditions (e.g. precipitation, air temperature, solar radiation, and wind speed) obviously influencing the water quantity and quality; various diffuse source parameters including pesticides, nutrients, sediments from eroded or overgrazed lands, and microorganisms; complicated soil-water interfaces for water flow and solute fluxes considering natural and human activities (Krause et al., 2007; Collins and McGonigle, 2008). Human activities related to land uses, such as farming, urbanisation and waste water disposals can produce great impact on the status of waters by modifying soil property and structure, changing nutrient chemical process in soil and bringing in pollution loads. In reality a catchment contains not only pervious agricultural land but also impervious urban land; it is important that the DWP models are capable of evaluating the effectiveness of proposed strategies to reduce the loading of agricultural or other contaminants into water course under the climate change – an inevitable global problem that we have to face. Therefore, the factors of application scale, contaminant simulation capability, nutrient cycling processes in soil, climate change response, pervious and impervious shallow geology, land use supporting, etc., should be considered in choosing a numerical catchment water modelling tool for better implementation of the EU WFD in handling DWP. Some modelling comparison literatures can be found, for example Nasr et al. (2007) studied phosphorus export modelling at catchment scale; majority of work was done about specific modelling effort from various, diverse models for various DWP issues from agricultural nutrient loading, coastal water quality assessment (Yuan et al., 2007; Krause et al., 2008), to detailed contribution from root system and large scale transboundary modelling (Diogo et al., 2008; Sohier et al., 2009).

This paper aims to 1) critically review the popular water models in selecting a proper numerical tool for better implementation of the EU WFD in modelling DWP; 2) assess a selected model – Hydrological Simulation Program – FORTRAN (HSPF) by applying it in water quantity and nutrient quality modelling; 3) present a case study with HSPF model in the Upper Bann Catchment, Northern Ireland; and 4) evaluate the impact of DWP management strategies on water quality.

2. Critical review for model selection

The choice of the numerical model depends on the objectives of the study. For better implementation of the EU WFD in the DWP field, water modelling should be able to: 1) get reliable water quantity and quality simulation results; 2) be applied at catchment/watershed scale or larger scale; 3) calculate the complex nutrient biochemical process in different soil types; 4) take into account both diffuse and point source pollutions; 5) model the DWP process from both agriculture and urban land uses; and 6) evaluate the impact of climate change scenarios on water and its quality.

It was the 1970's and early 1980's when people realised increasing water pollution problems. The DWP issue has been a headache since then and scientists have been developing and updating mathematical models to characterise the pollutant loadings and water quality impacts, and more and more water simulation models have been available. Models below are the most notable, well known, operational and free models.

2.1. Model description

Chemicals, Runoff, and Erosion from Agricultural Management Systems (CREAMS) (Knisel, 1980), a field scale model, was developed by the US Department of Agriculture (USDA) - Agricultural Research Service (ARS) for the analysis of agricultural best management practices (BMP) for pollution control. The model can be obtained from the website http://www.wiz.uni-kassel.de/model_db/mdb/creams.html. This model uses separate hydrology, erosion, and chemistry sub-models connected together to calculate runoff volume, peak flow, infiltration, evapotranspiration, soil water content, and percolation on a daily basis; simulate plant nutrients and pesticides; and determine storm load, average concentrations of sediment-associated and dissolved chemicals in the runoff, sediment, and percolation through the root zone (Leonard and Knisel, 1984). User defined management activities, such as aerial spraying, soil incorporation of pesticides, animal waste management, and agricultural best management practices (minimum tillage, terracing, etc.), can be simulated by CREAMS. Groundwater Loading Effects of Agricultural Management Systems (GLEAMS) was developed by the USDA - ARS (Leonard et al., 1987) based on CREAMS. GLEAMS, consisting of three major components namely hydrology, erosion/sediment yield, and pesticides, can be treated as the vadose zone component of the CREAMS model. The soil is divided into various layers, with a minimum of 3 and a maximum of 12 layers of variable thickness are used for water and pesticide routing (Knisel et al., 1989). The limitations of CREAMS/GLEAMS include: 1) the maximum size of the simulated area is limited to a small field plot; 2) they are limited in data management and handling; 3) they can not simulate instream processes; 4) they have limited simulation capability for snow accumulation, melt, and resulting runoff, and hydrologic impacts of frozen ground conditions (Kauppi, 1982; Knisel et al., 1983).

Storm Water Management Model (SWMM) was developed for US EPA as a single-event model specifically for the analysis of combined sewer overflows (CSO) (Metcalf and Eddy Inc. et al., 1971; Roesner et al., 1988). The model is available at http://www.epa.gov/ednnrmrl/models/swmm/index.htm. SWMM consists of several modules, namely Runoff, Transport and Extran, designed to simulate both continuous and single event quantity and quality processes in the urban hydrologic cycle. Storm sewers, combined sewers, and natural drainage systems can be simulated. Storage, Treatment, Overflow, Runoff Model (STORM) was developed by the Corps of Engineers Hydrologic Engineering Center of US for the application of the San Francisco master plan for CSO pollution abatement (HEC, 1977). STORM contains simplified hydrologic and water quality routines for continuous simulation in urban areas, and can be used to calculate hourly runoff volumes and depths, snowmelt, dry-weather flows, suspended solids, settleable solids, BOD, total coliforms, ortho-phosphate, and nitrogen. The weaknesses of SWMM and STORM include that they both are urban models; the quality simulation of SWMM is weak in the representation of the true physical, chemical and biological processes that occur in the nature; SWMM has weak groundwater simulation capability; STORM uses the quality routines embodied in SWMM with very few modifications; although STORM has less data requirements its hydrologic routines are too simple for complicated water simulation (Donigan and Huber, 1991; Shoemaker et al., 2005).

Areal Nonpoint Source Watershed Environment Response Simulation (ANSWERS) was developed by the Agricultural Engineering Department of Purdue University (Beasley and Huggins, 1981). It is available from http://cobweb.ecn.purdue.edu/~aggrass/models/ answers/. The ANSWERS model is capable of predicting the hydrologic and erosion response of agricultural watersheds. Since it is a distributed parameter model, its application requires that the watershed to be subdivided into a grid of square elements. The modular program structure of

ANSWERS allows easier modification and customising of existing program code. However, there are limitations for ANSWERS: 1) although it has a PC version for small watershed application, a mainframe computer is required for a simulation run of ANSWERS on a large watershed; 2) this storm event model requires complex input data preparation; 3) the water quality constituents modelled are limited to nitrogen and phosphorous, and snowmelt processes or pesticides cannot be simulated; 4) nitrogen and phosphorus are simulated using correlation relationships between chemical concentrations, sediment yield and runoff volume, and no transformation of nitrogen and phosphorus is considered (Donigan and Huber, 1991).

Unified Transport Model for Toxic Materials (UTM-TOX) was developed by Oak Ridge National Laboratory for the U.S. EPA Office of Pesticides and Toxic Substances, Washington, D.C. (Patterson et al., 1983). UTM-TOX includes atmospheric transport, terrestrial ecology and hydrology and Wisconsin hydrologic transport model to establish chemical mass balances, make chemical budgets and to estimate chemical concentrations in the environment. The limitations of this model are that it 1) ignores the interaction between chemicals and sediment in streams; 2) is quite complex and requires significant user expertise; 3) concentrates on pesticides and toxic substances only.

Pesticide Root Zone Model (PRZM) was developed at the U.S. EPA Environmental Research Laboratory in Athens, Georgia (Carsel et al., 1984), which is available at http:// www.epa.gov/ceampubl/gwater/przm3/index.htm. PRZM can be used to simulate chemical movement in unsaturated zone within and immediately below the plant root zone using of its hydrology and chemical transport modules. The most recent version of PRZM is included in an integrated root/vadose/groundwater model called RUSTIC (Risk of Unsaturated/Saturated Transport and Transformation of Chemical Concentrations) for the prediction of pesticide fate and transport through the crop root zone, and saturated zone to drinking water wells (Dean et al., 1989). PRZM can not handle lateral flow because of its 1D capability in the vertical direction; PRZM only simulates downward water movement and does not account for diffusive movement due to soil water gradients; the model only simulates organic chemicals, for example pesticides.

Agricultural Nonpoint Source Pollution Model (AGNPS) was developed by USDA - ARS (Young et al., 1986) and is available from http://www.wsi.nrcs.usda.gov/products/w2q/h&h/tools_models/agnps/index.html. It is a distributed parameter model, and can be used to estimate nutrients and sediments in runoff, and to compare the effects of various pollution control practices in watershed management. AGNPS can also handle point source pollutions. The methods used for the prediction of nitrogen and phosphorus yields from the watershed are also used in CREAMS. The methods for nitrogen and phosphorus concentration calculations are similar to ANSWERS. The limitations of AGNPS include: 1) the model does not handle pesticides; 2) the pollutant transport component needs further field testing; 3) nutrient transformation and instream processes are not within model capabilities; 4) it is used only to simulate single event; 5) it is an empirical model; 6) channels are assumed to have a triangular shape (Donigan and Huber, 1991; Shoemaker et al., 2005).

Enhanced Stream Water Quality (QUAL2E) model, a comprehensive and versatile 1D stream water quality steady model, was developed based on Streeter-Phelps model (Streeter and Phelps, 1925) to simulate nutrient dynamics, algal production, and dissolved oxygen with the impact of benthic and carbonaceous demand in streams (Brown and Barnwell, 1987). The model is available at http://www.epa.gov/athens/wwqtsc/html /qual2k.html. Fifteen water quality variables are modelled in QUAL2E. The model is intended as a waste load allocation and water quality planning tool for developing total maximum daily loads (TMDL). It can also be used in conjunction with field sampling for identifying the magnitude and quality characteristics of nonpoint sources. The limitations of QUAL2E include: 1) 1D channel that cannot handle tidal impact; 2) steady flow is not able to model variable flow condition; 3) the model is unsuitable for rivers that experience temporal variations in streamflow or where the major discharges fluctuate significantly over a diurnal or shorter time period (Birgand, 2004).

Simulator for Water Resources in Rural Basins (SWRRB) was developed by modifying CREAMS for evaluating basin scale water quality by daily simulation of weather, hydrology, crop growth, sedimentation, nitrogen, phosphorous and pesticide movement (Williams et al., 1985). It's available at http://rhino.cee.odu.edu/model/swrrbwq.php. The model considers both soluble pollutants and sediment attached pollutants. The nitrogen and phosphorus calculations are performed using relationships between chemical concentration, sediment yield and runoff volume. However in SWRRB, there is very minimal model documentation; the snow accumulation processes are ignored in the hydrology component; no comprehensive instream simulation is available for pesticides calculation; nutrient transformations along with pesticide daughter products are not accounted for in the model (Arnold et al., 1989).

Soil Water and Analysis Tools (SWAT), a physical-based model, was developed by USDA-ARS in the early 1990s for the prediction of the long-term impact of rural and agricultural management practices (such as detailed agricultural land planting, tillage, irrigation, fertilisation, grazing, and harvesting procedures) on water, sediment and agricultural chemical yields in large, complex watersheds with varying soils, land use, and management conditions (Arnold et al., 1998). It can be downloaded free from http://www.brc.tamus.edu/swat/. SWAT incorporates features of several ARS models and is a direct outgrowth of the SWRRB and CREAMS model. Since SWAT is a physically based model, watersheds with no monitoring data can be modelled; the relative impact of alternative input data (such as changes in management practices, climate, vegetation) on water quality or other variables of interest can be quantified using readily available inputs. While SWAT can be used to study more specialised processes such as bacteria transport, the minimum data required to make a run are commonly available from government agencies. In addition, the continuous time SWAT model enables users to study long-term impacts. However, SWAT has some limitations: 1) not for simulating sub-daily events such as a single storm event and diurnal changes of dissolved oxygen in a water body; 2) only route one pesticide each time through the stream network; 3) can not specify actual areas to apply fertilisers; 4) a large watershed can be divided into hundreds of hydrologic response units (HRU) resulting in many hundreds of input files, which are difficult to manage and modify without a solid interface; 5) the parameters of the equations are not directly measured by using data; 6) it has the difficulty in simulating snowmelt; 7) it does not simulate detailed event based flood and sediment routing; 8) it has difficulties in modelling floodplain erosion and snowmelt erosion during the spring and winter months (Peterson and Hamlett 1998; Benaman et al., 2005; Shoemaker et al., 2005). Although efforts have been made to incorporate more process-based equations, some of the basic processes modelled by SWAT still have room for improvement.

The SHETRAN system was developed by the Water Resources Systems Research Laboratory (WRSRL) based on the SHE (Système Hydrologique Européen) through the international collaboration between groups in the UK, Denmark, and France (Ewen, 1995). SHETRAN is a 3D, surface/subsurface, physically-based, spatially-distributed and finite-difference model for water flow, multifraction sediment transport and multiple, reactive solute transport in river basins. It gives a detailed description in time and space of the flow and transport in the basin, which can be visualised using animated graphical computer displays. SHETRAN represents physical processes using physical laws applied on a 3D finite-difference mesh to model the hourly flow and transport for periods of up to a few decades. Since SHETRAN is a new model, its limitations need to be discussed in future worldwide applications.

Hydrological Simulation Program – FORTRAN was developed by US Environmental Protection Agency (USEPA) to represent contributions of sediment, nutrients, pesticides, conservatives and faecal coliforms from agricultural areas; and to continuously simulate water quantity and quality processes on pervious and impervious land surfaces and in streams and well-mixed impoundments (Barnwell and Johanson, 1981). Details are available at http://www.epa.gov/ceampubl/swater/hspf/index.htm. By supporting conventional and toxic organic pollutants from both point sources and diffuse sources, HSPF is one of few comprehensive watershed hydrology and water quality models that allow the integrated simulation of land and soil contaminant runoff processes with instream hydraulic, water temperature, sediment transport, nutrients, and sediment-chemical interactions (Gallagher and Doherty, 2007; Ribarova et al., 2008). The runoff flow rate, sediment load (sand, silt, and clay), nutrient and pesticide concentrations, and historical time series of water quantity and quality at any point in a watershed can be calculated using this model (Tzoraki and Nikolaidis, 2007; Choi and Deal, 2008). The runoff quality capabilities include both simple relationships (e.g. empirical buildup/washoff and constant concentrations) and detailed soil process options (e.g. leaching, sorption, soil attenuation, and soil nutrient transformations). HSPF includes organic chemical transfer and reaction processes of hydrolysis, oxidation, photolysis, biodegradation, a volatilization, and sorption. The instream nutrient processes include DO, BOD, nitrogen and phosphorus reactions, pH, phytoplankton, zooplankton, and benthic algae (Tzoraki and Nikolaidis, 2007). Any time step from 1 minute to 1 day can be used, and any period from a few minutes to hundreds of years may be simulated. HSPF is generally used to assess the effects of land-use change, reservoir operations, point or diffuse source treatment alternatives, flow diversions, etc (Choi and Deal, 2008; Cho et al., 2009). The limitations of HSPF include 1) it relies on many empirical relationships to represent physical processes; 2) its lump simulation processes for each land use type at the sub-watershed does not consider the spatial distribution of one land parcel relative to another in the watershed; 3) it approaches a distributed model when smaller sub-watersheds are used that may result in increased model complexity and simulation time; 4) it requires extensive calibration; 5) it requires a high level of expertise for application; 6) the model is limited to well-mixed rivers and reservoirs and 1D flow (Shoemaker et al., 2005).

2.2. Review summary

Among the models reviewed above, HSPF, SWMM, STORM, and CREAMS have persisted for long period of time, while SWAT and SHETRAN are comparatively new and need more reviewing and assessing work. It may be wise to select an appropriate model for a water management project for diffuse pollution according to the specific catchment or water shed and also the data availability. However an initial model testing would be a good practice for a better application of such management projects. The comparison research of the DWP models has been carried out. For example, Im et al. (2003) compared HSPF and SWAT and drew conclusion that considering differences in annual loads and the trend of monthly loads, HSPF hydrology and water quality simulation components are more accurate than SWAT. Nasr et al. (2007) compared HSPF, SWAT and SHETRAN and found that HSPF has better river flow simulation and SWAT has better result in total phosphorus simulation. Of all models discussed, HSPF has the most complex mechanisms for the simulation of subsurface water quality processes in both the saturated and unsaturated zones. Although SWMM includes subsurface flow routing, the quality of subsurface water can only be approximated using a constant concentration. HSPF is one of the most detailed, operational models of agricultural runoff and erosion by simulating land surface and soil profile chemical/biological processes that determine the fate and transport of pesticides and nutrients; and by considering of all stream flow components (i.e., surface runoff, interflow and baseflow) and their pollutant contributions. HSPF can model runoff from any land category, including both pervious and impervious urban categories. Since its initial release, HSPF has maintained a reputation as perhaps the most useful watershed-scale hydrology/water quality model that is available within the public domain (Donigian and Imhoff, 2002). As a proven and tested continuous simulation watershed model, HSPF has been widely reviewed and applied throughout its development cycle since 1980 (Ng and Marsalek 1989; Rahman and Salbe, 1995; Ross et al., 1997; Brun and Band, 2000; Albek et al., 2004; Shoemaker et al., 2005; Luo et al., 2006; Tzoraki and Nikolaidis, 2007; Choi and Deal, 2008; Cho et al., 2009). Although HSPF has its limitations, so far it comparatively better meets the demands of DWP modelling studies than other models. However, more studies are needed in assessing the suitability of HSPF in implementation of the EU WFD in the DWP field. HSPF was therefore further studies in terms of its functions and capability and employed in a DWP modelling assessment in a case study area, which is presented in the following sections of the paper.

3. Materials for model assessment

3.1. Study area

The Upper Bann Catchment, Northern Ireland is the study area used for this study. The Upper Bann, covering an area of 674 km^2, lies in the southeast of Northern Ireland, UK. It has a mean rainfall of 995 mm/a and a mean potential evapotranspiration 516 mm/a. Average altitude in study area is 110 m and the steepest area is located in the Mourne Mountains to the southeast; it gently undulates throughout the rest of the study area, rising from 11 m at Lough Neagh to a maximum of 672 m in the Mourne Mountains. Upper Bann is a complex rural catchment with a wide range of land uses. Agriculture land accounts for 92.9%, dominated by grassland (76.3%), arable land (10.2%), and woodland (6.5%). Details of the study area are presented by Wang and Yang (2008). In Northern Ireland, surface water is the dominant source of public water supply with groundwater estimated to provide only 8% of the total public water supply. Despite the small direct contribution to public supply, groundwater still has an important role to play because of its contribution to baseflow of surface water, where most of public supply originates, and widely used as sources of private supply. Therefore, both surface water and groundwater are vital to social and economic development throughout the rural community. The river monitoring showed deterioration in River Bann’s quality. The diffuse contributions from agriculture may be the primary cause of the current water quality problem in case study area. The area contains Upper River Bann which is the largest river that supplies Lough Neagh - predominant inland water situated centrally in the country with total area of 388 km^2. The dramatic nutrient enrichment in Lough Neagh, occurred in the 20th Century, had been the result of increased nutrients coming both from urban and agricultural sources. While the nutrients from urban sources have decreased appreciably since 1986, the diffuse agricultural nutrient inputs to Lough Neagh have continued to increase. The DWP management from in the Upper Bann Catchment is significant for water quality controlling in Lough Neagh.

3.2. Data for modelling

Digital Elevation Model (DEM) data, vector river network data and river chemical quality monitoring data were obtained from Environmental Heritage Service (EHS); land cover data was provided by Centre for Ecology and Hydrology (CEH), while soil data was acquired from the Department of Agriculture and Rural Development (DARD) of Northern Ireland; weather data, such as hourly precipitation, air temperature, wind speed, and dewpoint, were provided by British Atmospheric Data Centre (BADC); Catchment and watersheds boundaries were derived from DEM data. A multi-sphere GIS database, which supports both raster and vector data formats, was built for this study. All data mentioned above and data derived, such as catchment outline, river network, topography in Triangle Irregular Network format, flow direction, flow accumulation, stream segmentation, sub-catchment grid data, catchment polygon data, drainage point of each sub-catchment, were input into this GIS database. All raster data in this study have the resolution of 50 × 50 m.

3.3. HSPF development and interface

With its predecessors dating back to the 1960s, HSPF is a culminating evolution of the Stanford Watershed Model (SWM) (Crawford and Linsley, 1966), watershed-scale Agricultural Runoff Model (ARM) (Donigian et al., 1977), Nonpoint Source Loading Model (NPS) (Donigian and Crawford, 1976) and Sediment and Radionuclides Transport (SERATRA) (Onishi and Wise, 1979). HSPF is currently in version 12.2 (Bicknell et al., 2005). In order to improve the efficiency of using HSPF, WinHSPF was designed as an interactive Windows interface to HSPF, and fully-integrated into a multipurpose environmental analysis system - Better Assessment Science Integrating point and Nonpoint Sources (BASINS) system, developed by United States Environmental Protection Agency (USEPA) based on Geographic Information System (GIS) foundation for performing watershed and water quality-based studies (Lahlou et al., 1998). User control input (UCI) files are used for data exchange among WinHSPF, BASINS and GIS. Within the BASINS system, WinHSPF is intended to be used in conjunction with the interactive program known as "GENeration and analysis of model simulation SCeNarios," (GenScn) to analyse results of model simulation scenarios and their comparison. HSPF was applied through BASINS and WinHSPF software packages.

3.4. Theoretical description of HSPF

HSPF uses the concept of HRU to divide the watershed into homogeneous segments. In each HRU, the soil layer is vertically divided into three layers (storages), i.e., upper-zone, lower-zone and active groundwater. The water flux and evapotranspiration in each HRU are calculated respectively according to the moisture conditions in these three storages. Horizontally, three types of flow components, i.e., surface runoff, interflow, and active groundwater, contribute to the streamflow routed by a nonlinear function. As Fig. 1 illustrates, HSPF has four application modules, i.e., PERLND for pervious land segments, IMPLND for impervious land segments, RCHRES for river reaches and well-mixed reservoirs, and BMP for simulating constituent removal efficiencies associated with implementing management practices (Donigian and Imhoff, 2002; Bicknell et al., 2005). PWATER, key component of module PERLND, was designed to calculate the components of the water budget, and to predict the total runoff from a pervious area. The algorithms used to simulate these land related processes, the product of over 15 years of research and testing, are based on the original research for the LANDS subprogram of the SWM IV (Crawford and Linsley, 1966). PERLND and IMPLND processes are simulated through water budget, and the generation and transport of water quality constituents and sediment. Empirical equations are adopted in HSPF for the calculations of interception, evapotranspiration, overland flow, interflow, infiltration and groundwater loss processes. Sediment production in HSPF is based on detachment and scour from a soil matrix and transport by overland flow in pervious areas, whereas solids buildup and washoff are simulated for impervious areas. HSPF includes modules to simulate nutrients cycling processes (Fig. 2). The nitrogen biochemical process in HSPF includes plant uptake of nitrate and ammonium, return of plant nitrogen to organic nitrogen, denitrification or reduction of nitrate-nitrite, immobilisation of nitrate-nitrite and ammonium, mineralization of organic nitrogen, fixation of atmospheric nitrogen, volatilisation of ammonium, adsorption or desorption of ammonium, and partitioning of two types of organic nitrogen between solution and particulate forms. A PHOS module in FSPF is designed to simulate the behaviour of phosphorus in a pervious land segment by modelling the transport, plant uptake, adsorption, desorption, immobilisation, and mineralization of the various forms of phosphorus. Because phosphorus is readily tied to soil and sediment, it is usually scarce in streams and lakes. In fact, in many cases it is the limiting nutrient in the eutrophication process. Because of its scarcity, accurate simulation is particularly important.

Fig. 1. HSPF application modules and their capabilities

Fig. 2. Schematic representation of nitrogen and phosphorus cycle

The utility modules of HSPF include COPY (copies time series data), MUTSIN (makes the time series data based on the external file available for use by other modules), PLTGEN (writes a sequential external file containing up to 10 time series and related commands for a stand-alone plotting program), DURANL (examines the behaviour of a time series and computes a variety of statistics related to it's excursions above and below certain specified levels), GENER (performs any one of several transformations on one or more input time series), DISPLY (prints time series data in a tabular format and summaries of the data) and REPORT (produces time series output in a very flexible fashion).

4. HSPF modelling

The HSPF modelling work consisted of building a BASINS project, watershed delineation, setting up WinHSPF environment, time series data preparations, surface water quantity and quality simulation, calibration, and validation. The BASINS project of the study area was built on the ArcView 3.1 platform by choosing data projection, importing land use, DEM, hydrography, and soil data. Watershed delineation was carried out using GIS extensions provided by BASINS to automatically divide study area into hydrologically connected segments or subwatersheds for detailed watershed characterisation and modelling. The selection of watershed outlets was based on the locations of water gauge stations and river quality monitoring stations. Four approximately homogenous segments in the study area were created so that lumped parameters can be respectively assigned to each segment to represent its characteristics (Fig. 3).

Fig. 3. Watershed delineation result in the study area

Meteorological time series data were managed using Watershed Data Management Utility program (WDMUtil) of BASINS. Hourly precipitation, daily air temperature, wind speed, dewpoint, solar radiation, and daily evapotranspiration were reformatted, generated, aggregated, disaggregated, and calculated in WDM. A HSPF project was built using the data of watershed boundary, streams, outlets and land use in the BASINS project, and the weather station time series in WDM files (the principal library for storage of time series). Fig. 4 shows the schematic of HSPF watershed in the study area. Topography characteristic and land uses were taken into account in the surface water simulation of each river segment. Land uses in the area include cropland and pasture land, transitional area, mixed urban or built-up land, mixed forest land, deciduous forest land, evergreen forest land, forested wetland, and reservoirs.

Fig. 4. HSPF watershed schematic of the study area

4.1. Parameter estimation

When a HSPF project was created from BASINS, an UCI file was created to hold and supply parameters to HSPF. The estimation of a large array of parameter values was required to quantitatively represent/depict the watershed hydrological cycle and water quality. Although BASINS can estimate many input parameters using available information in GIS database to improve the efficiency of HSPF applications, these values could be highly inaccurate and should be manually modified if more accurate information is available. Based on these initial parameter values, manual parameter estimation work were carried out using monitoring data and the results of previous researches and experiments in the study area. In order to reduce the uncertainty of water modelling, the recommended value ranges of key parameters provided in HSPF manual were referenced. The important parameters of HSPF include AGWRC, INFILD, INFILT, INTFW, INFEXP, IRC, KVARY, LZETP, LZS, LZSN, PETMAX, and UZSN, etc. (hydrologic component); AFFIX, KSER, JSER, KGER, COVER, JGER, KRER, KSER and SMPF, etc. (sediment component); SQO, POTFW, POTFS, ACQOP, SQOLIM, IOQC, KBOD20, TCBOD, KODSET, SUPSAT, BRNIT, VRPO4, KTAM20, KNO220, TCNIT, KNO320, TCDEN, DENOXT, ALR20, ALDH, ALDL, OXALD, NALDH, PALDH, KAM and KMP, etc. (Nutrients, dissolved oxygen and algae components). The detailed description of HSPF parameters can be found in Bicknell et al. (2005). The initial conditions, such as temperature, amount of soil moisture at the start of the simulation were determined by observation data. In general, parameters in HSPF fall into two categories, fixed parameters and process-related parameters (Al-Abed and Whiteley, 2002). The values of fixed parameter remain constant throughout a simulation period. In this study, the values of fixed parameters (such as soil types, model manipulation switches and the hydraulic characteristics of the drainage network) were mainly established from field measurement work; and were not involved in the calibration process. Since the process related parameters (such as soil water amount, nutrients transport in soil) have no directly measurable physical analogues, their proper values were determined in the calibration and validation processes.

4.2. Calibration, validation and sensitivity analysis

The HSPF Calibration is an iterative process used in establishing the most suitable values for process related parameters. The important water flow and quality parameters were calibrated and validated in the watershed 2 (Fig. 3) for Gamble's Bridge station having monitoring data. These parameters include CEPSC, interception storage capacity; INFILT, infiltration parameter; IRC, interflow recession parameter; INTFW, interflow parameter; UZSN, upper zone nominal storage; LZSN, lower zone nominal storage; LZETP, lower zone evapotranspiration parameter; AGWRC, groundwater recession rate; DEEPFR, fraction of groundwater inflow to deep recharge; BASETP, fraction of remaining ET from baseflow; AGWETP, fraction of remaining ET from active groundwater; KVARY, groundwater recession flow; INFEXP, exponent of infiltration; INFILD, ratio between maximum and mean infiltration capacities; SLSUR, slope of the assumed overland flow plane; KBOD20, BOD decay rate; KNO320, denitrification rate of nitrate; TCNIT, temperature coefficient for the nitrogen oxidation rate; KTAM20, oxidation rate of total ammonia; KNO220, oxidation rate of nitrites; TCDEN, temperature coefficient for the denitrification rate; DENOXT, oxygen concentration threshold above which denitrification ceases; and MALGR, maximal algal growth rate for phytoplankton. Hourly precipitation, hourly air temperature, daily maximum and minimum temperature, solar radiation, evapotranspiration were from weather station "Glenanne_Saws" in the watershed 2. Weather data between 2000 and 2005 were used for river flow quantity and quality simulations. River flow data from 2000 to 2003 were used for river flow calibration. In the calibration process, parameters in HSPF were adjusted by comparing the difference between the simulated and observed river flow data using the GenScn module in BASINS. Flow duration curve and scatter plot methods were used in this process. In order to reduce the parameter uncertainty, only one parameter was adjusted each time. More than 30 runs were carried out before reaching the satisfied simulation results. Table 1 shows the calibrated values with physical explanations of the important parameters in HSPF.

Table 1. Description of the major parameters in HSPF

The calibrated hydrological parameters in HSPF were then validated using river flow data between 2004 and 2005. Then, nutrients, i.e., NO_3, NO_2, NH_4 and PO_4 were simulated, calibrated and validated respectively. River chemical quality monitoring data between year 2000 and 2003 were used for model calibration, while the data from year 2003 to 2005 were used for model validation. The HSPF model well calibrated and validated using monitoring water data can properly describe the characteristics of water quantity and quality processes in this area. Sensitivity analysis can test the overall responsiveness of the model to change of certain input parameters (Oyarzun et al., 2007), thus pointing out the critical parameters that need to be carefully investigated through data gathering and field studies for reliable modelling outputs. Additionally, sensitivity analysis can be used as a way of understanding the general behaviour of a model in evaluating its confidence and in interpreting results during the calibration phase (Kleijnen, 2005). The sensitivity analysis in this study started from carrying out a baseline model run. The value for each parameter in the baseline simulation were worked out by considering the recommended value ranges given in the HSPF manual, available field and laboratory data, and averaged literature values in past modelling studies. Then, the important parameters in the hydrologic, sediment, nutrient and biochemical processes involved in HSPF were selected for sensitivity analysis, which are all process-related parameters. Two sensitivity analysis runs were carried out by using a high (200% of the upper range of the parameter) and a low (50% of the value of the lower range of the parameter) value. Results of 46 model runs in this study were compared to the result of the baseline model run to determine the relative sensitivity of model results to the change of the specific model parameters. The sensitivity analysis highlighted the 10 most important parameters in surface water quality and quantity simulation in this study, namely, INFILT, UZSN, IRC, LZSN, AGWRC, DEEPFR, BASETP, AGWETP, KBOD20, KNO320, KNO220, TCNIT, TCDEN, and DENOXT. The calibration of this study was carried out based on these important parameters.

4.3. Scenario evaluation: climate change

Climate change is one of the most important global environmental problems due to the global warming caused by the increasing concentration of greenhouse gases and others. Most studies predict increasing future temperature. For example, Yanshin (1991) predicted that annual mean temperatures will rise about 2 ℃ by 2025 and 3 ℃ by 2050. In this study, it was assumed that the mean annual temperature will increase 3 ℃ during next 50 years, and other weather features such as solar radiation, wind pattern, and precipitation, will not change. To simulate the river flow based on calibrated and validated model for this scenario, the monitored hourly temperature data in five years were manually modified by adding 3 ℃. Since evaporation, potential evapotranspiration and pan evaporation are greatly influenced by temperature, they were re-calculated using Jensen and Haise (1963) formula and Penman (1948) formula respectively.

4.4. Scenario evaluation: land use change

Generally the crop and pasture land uses have higher nutrient loading rates than other land uses in the diffuse water pollution. The water quality and quantity will be affected by the change of land use in the watershed. In this scenario, it was supposed that decision makers are going to convert 20% crop and pasture land (3104 ha) into forest land; other conditions such as climate, agricultural activities, soil and topography will remain the same. The areas of land uses in the watershed 2 were manually modified in the calibrated and validated HSPF model. The change of land uses had no spatial distribution concept in this study because of the lumped parameter characteristic of the HSPF model.

4.5. Scenario evaluation: BMP

In the DWP management, BMP are effective, practical, structural or non-structural methods which prevent or reduce the movement of sediment, nutrients, pesticides and other pollutants from the land to the water course. In this study, it was assumed that the filter strip method, one of BMP, is to be implemented in 80% crop and pasture land in the study watershed and all other conditions will remain the same. The BMP scenario was set in the “BMP” module of HSPF.

5. Results

5.1. River flow simulation

Flow duration curve is a plot that shows the percentage of chance that flow in a stream is likely to equal or exceed some specified value of interest. For each frequency in the range from 0 to 100 percent in X-axis, the flow that will be exceeded is plotted on the Y-axis. Ideally, simulated and observed flow duration curves should be very similar. Fig. 5 shows that simulated and observed river flow from 2000 to 2003 correlated well in frequency. Fig. 6 is the scatter plot of the simulated flow against the observed flow. The closer the data comes to falling on a 45° angle line, the better the two data sets match. The result of Fig. 6 also shows that the model was well calibrated in study area. The calibrated hydrological parameters of the HSPF model in the study area were then validated using data from 2004 to 2005 (Fig. 7). All results show that HSPF hydrological component was well calibrated. The mean value of runoff components (including surface runoff, interflow, and baseflow) and evaporation for each land use (2000-2005) were calculated from the calibrated HSPF model (Fig. 8). Crop and pasture land has highest interflow whilst mixed urban land has highest surface runoff.

5.2. River quality simulation

Compared with the nutrient simulation results with daily time series data, the river quality monitoring data were limited in number with monthly interval.

Fig. 5. Flow duration curves of simulated and observed river flow (2000-2003)

Fig. 6. Scatter plot of simulated and observed river flow (2000-2003)

Fig. 7. Model validation using simulated and observed river flow data (2004-2005)

Fig. 8. The average value of runoff components and evaporation for each land use (2004-2005)

Therefore simple statistic methods (such as count, percent, mean and standard deviation) instead of complex statistic methods (such as correlation coefficient and coefficient of determination) were used for assessment of the model calibration and validation. The difference between simulated and observed concentrations of nitrate, nitrite, ammonium, and phosphate are 3.8%, 0%, -5.9% and 5.9% respectively. Fig. 9 shows the nitrate simulation result. Based on the calibrated model, quantitative nitrogen and phosphorus cycling processes in the case study area were calculated. For instance, the average NO3 export coefficient for cropland and pasture land, bare land, urban land, mixed forest land, deciduous forest land, evergreen forest land and forested wetland between 2000 and 2005 in study area were 28.7, 7.5, 3.0, 5.7, 5.5, 5.3, and 7.6 kg/ha respectively. Nitrogen TMDL was calculated based on the information of total nitrogen concentration and daily total nitrogen load (Fig. 10). It was supposed that the hypothetic standard was 6 mg/L and the standard minus a 10% margin of safety (MOS) was 5.4 mg/L, the calculated nitrogen TMDL was 68.1 kg.

Fig. 9. Simulated and observed nitrate concentrations at Gamble's Bridge in study area

5.3. Scenario results

The evaluation result of climate change scenario shows that when the annual mean temperature increase 3 ℃ the yearly total runoff volume of five years will decrease by 8%, 12.9%, 10.2%, 13%, 11.2% respectively (Fig. 11), and the mean daily river flow of five years will decrease by 11.4% from 3.5 m^3/s to 3.1 m^3/s.

In the land use change scenario, the mean river concentration of nitrate, nitrite, NH4 and PO4 in five years decreased by 19.4%, 33.3%, 31.3% and 31.3% respectively (Fig. 6.12). In BMP scenario, the reduction of the mean concentration of nitrate, nitrite, NH4 and PO4 in five years were 15.3%, 33.3%, 31.3% and 5.6% respectively.

Fig. 10. A simplified nitrogen TMDL calculation

Fig. 11. The impact of climate change on yearly total runoff volumes

Fig. 12. Variation of nitrate at Gamble's Bridge over 5 years for the land use change scenario

6. Discussions

Being one of few watershed models capable of simulating land processes and receiving water processes simultaneously, HSPF, a free of charge model, can be used for water quantity and quality (from both diffuse and point pollution sources) simulation at catchment/watershed that contains both agricultural and urban land use. The results of HSPF evaluation in this study shows that the calibrated HSPF can derive the quantitative nutrient cycling in each type of land use and soil to help people better understand the DWP mechanism before making water quality management policies in a specific catchment/watershed. HSPF can also be applied for evaluating the impacts of management policies on catchment water processes in the combined conditions of climate change, land use change and BMP. In addition, there is a sound data management component in HSPF that helps users easily manipulate a huge amount of time series data and allows automatic data exchange between data management module and other modules in the HSPF, hence improves the efficiency of modelling. In conclusion, HSPF is a suitable surface water model for supporting the DWP management at catchment scale.

Although there is no high-density groundwater monitoring network in the study area, the observed groundwater nitrate concentration trend, derived from four groundwater monitoring locations in the study area, is in line with the risk assessment result, tending to validate the model. The groundwater monitoring data show that the nitrate concentrations increase slightly from southeast to northwest in the study area. Within 'very high' risk zones, dominant land cover types are arable horticulture (66%) and improved grassland (24%). Arable horticulture and improved grassland in 'high' risk zones are 22% and 66%, respectively. In 'moderate' and 'low' risk zones, the dominant land cover type is improved grassland, while arable land, neutral grass and open dwarf shrub heath occupy relatively small portions of these zones.

In comparison of two types DWP controlling measures, i.e. remedial and preventative measures, the prevention of DWP at a source level – catchment-scale is vital for both sustainable water quality management and implementation of the EU WFD (EHS, 2001; Defra, 2002c; Koo and O'Connell, 2006). Once water is contaminated, it will be very costly to clean-up and can take a long time to be restored, especially for groundwater. Moreover, it is difficult to determine at a regional scale the contribution of diffuse agricultural sources to water pollution. River Basin Management Plan (RBMP), utilising the river basin as the natural unit, is the backbone of the implementation of the EU WFD. It is timely to develop and evaluate suitable models or methods for guiding catchment-scale water resource prevention activities to complement the Programme of Measures in RBMP. HSPF is a suitable model for better implementation of the EU WFD in the field of the surface water DWP management in the UK and worldwide. Further studies are necessary for evaluating HSPF in all EU member states before year 2015.

Each model has its advantages and disadvantages in certain aspects and with specific applications. The selection of HSPF in this study means that HSPF is comparatively more suitable than others at current stage for handling the DWP problems at the catchment scale for better implementation of the EU WFD, rather than means that HSPF is the best one over all other diffuse water pollution models in any aspect. HSPF has its limitations or shortages. For example, HSPF instream model assumes the receiving water body model is well-mixed with width and depth; application of this methodology generally requires a team effort because of its comprehensive but complex nature; for overland flow, model assumes one-directional kinematic-wave flow, etc. With rapid development of diffuse water pollution models, other models (such as SWAT and SHETRAN) might be proven as more suitable for better implementation of the EU WFD in the future after further comparison and evaluation studies in the EU.

Since HSPF and BASINS were particularly designed for water resource studies in the USA, some manual work (such as projection, data collection, and data format converting) is needed to apply them in other countries. In this study, GIS hydrological model was employed to prepare data required in BASINS. Although HSPF and BASINS can be currently used for the implementation of the EU WFD, it may be necessary to develop a new interface and make improvement of the HSPF model based on its free open source code to facilitate its application in European countries in the long run.

7. Conclusion

Based on the review of popular hydrologic models, HSPF was selected for catchment-scale DWP modelling with agricultural diffuse sources. The assessment of HSPF in the Upper Bann Catchment showed that HSPF can well guide the catchment-scale management of water pollution from agricultural diffuse sources, by quantifying nutrient biochemical cycling in different types of soil, and evaluating the impacts of water management plans on surface water under the climate change. HSPF is suitable to be introduced into the Programme of Measures in the RBMPs for better implementation of the EU WFD in the UK. However, further studies are needed to assess the suitability of applying HSFP in all EU member states. In addition, it is necessary to develop a new software interface for HSPF based on its open source code, for its easy applications in the EU member states for the long run.

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Table 1

Parameter	**Meaning**	**Value**	**Unit**
INFILT	Infiltration parameter	8.15 – 19.05	mm/h
UZSN	Upper zone nominal storage	28.8	mm
IRC	Interflow recession parameter	0.65	l/day
LZSN	Lower zone nominal storage	72	mm
AGWRC	Groundwater recession rate	0.992	1/day
DEEPFR	Fraction of groundwater inflow to deep recharge	0.25	-
BASETP	Fraction of remaining ET from baseflow	0.12	-
AGWETP	Fraction of remaining ET from active groundwater	0.1	-
KBOD20	BOD decay rate	0.1	1/h
KNO320	Denitrification rate of nitrate	0.05	1/h
KNO220	Oxidation rate of nitrites	0.05	1/h
TCNIT	Temperature coefficient for the nitrogen oxidation rate	1.01	1/h
TCDEN	Temperature coefficient for the denitrification rate	1.02	1/h
DENOXT	Oxygen concentration threshold above which denitrification ceases	1.6	1/h

Fig. 1

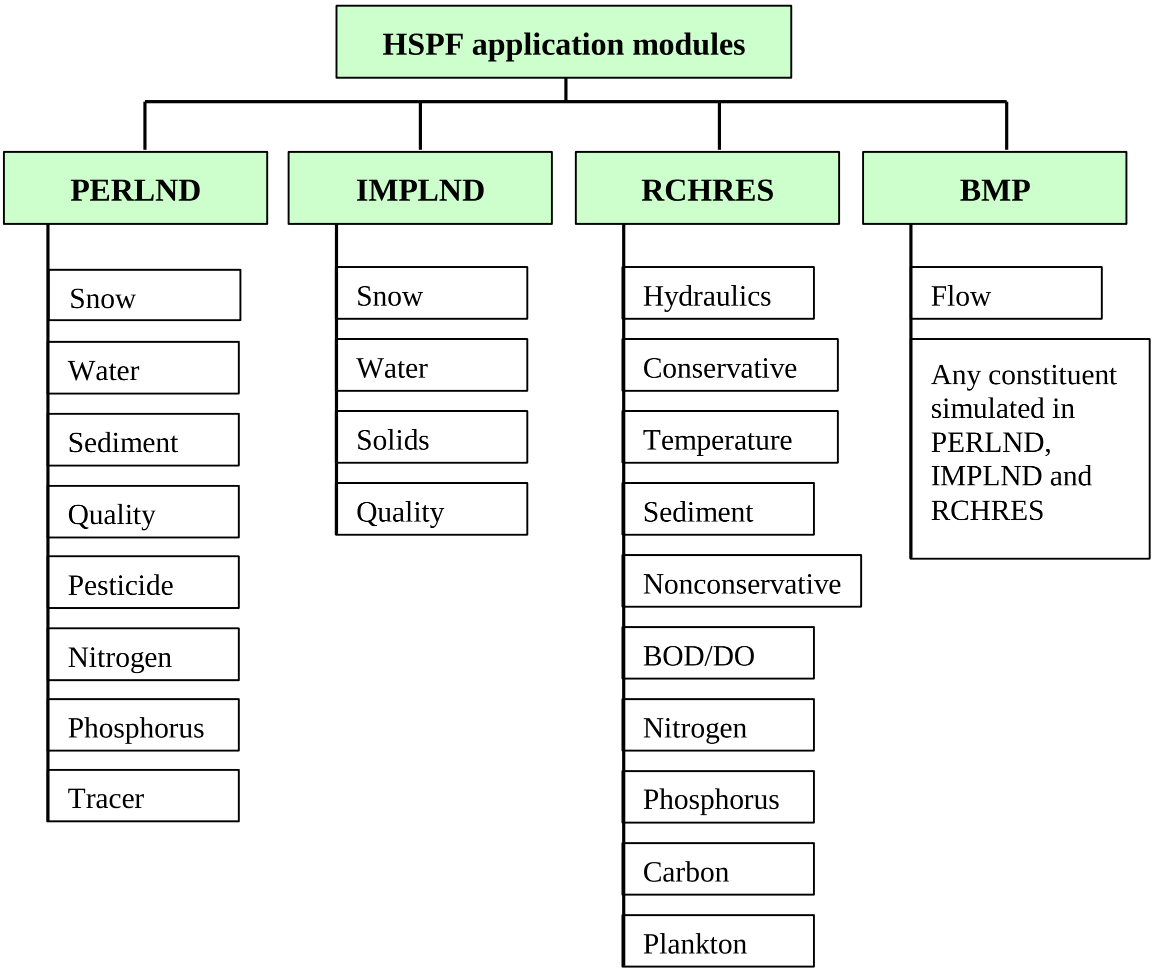

HSPF application modules
PERLND
IMPLND
RCHRES
BMP
Snow
Water
Sediment
Quality
Pesticide
Nitrogen
Phosphorus
Tracer
Snow
Water
Solids
Quality
Hydraulics
Conservative
Temperature
Sediment
Nonconservative
BOD/DO
Nitrogen
Phosphorus
Carbon
Plankton
Flow
Any constituent simulated in PERLND, IMPLND and RCHRES

Fig. 2

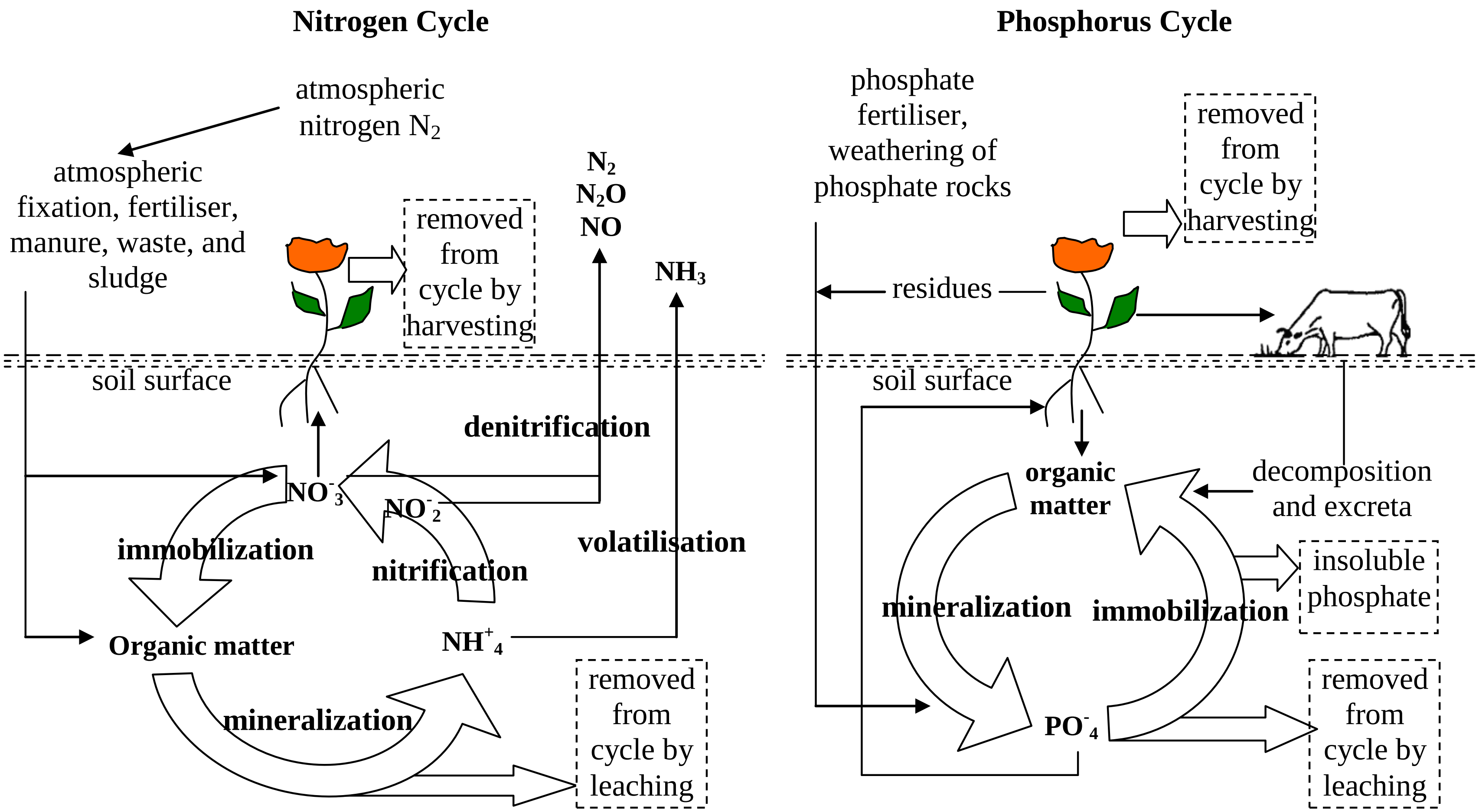

Nitrogen Cycle
atmospheric nitrogen N_2
atmospheric fixation, fertiliser, manure, waste, and sludge
removed from cycle by harvesting
N_2
N_2O
NO
NH_3
soil surface
denitrification
NO^-_3
NO^-_2
immobilization
nitrification
volatilisation
Organic matter
NH^+_4
mineralization
removed from cycle by leaching
Phosphorus Cycle
phosphate fertiliser, weathering of phosphate rocks
removed from cycle by harvesting
residues
soil surface
organic matter
decomposition and excreta
insoluble phosphate
mineralization
immobilization
PO^-_4
removed from cycle by leaching

Fig. 3

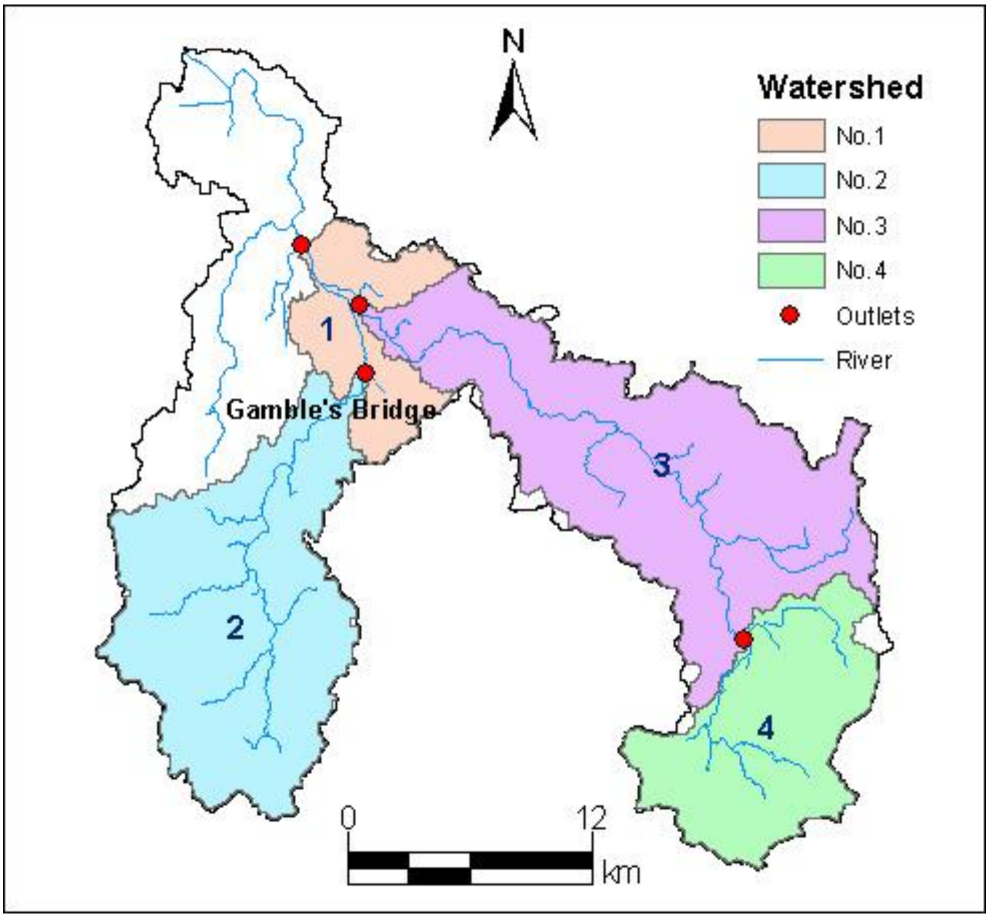

N
Watershed
No.1
No.2
No.3
No.4
Outlets
River
1
2
3
4
Gamble's Bridge
0
12
km

Fig. 4

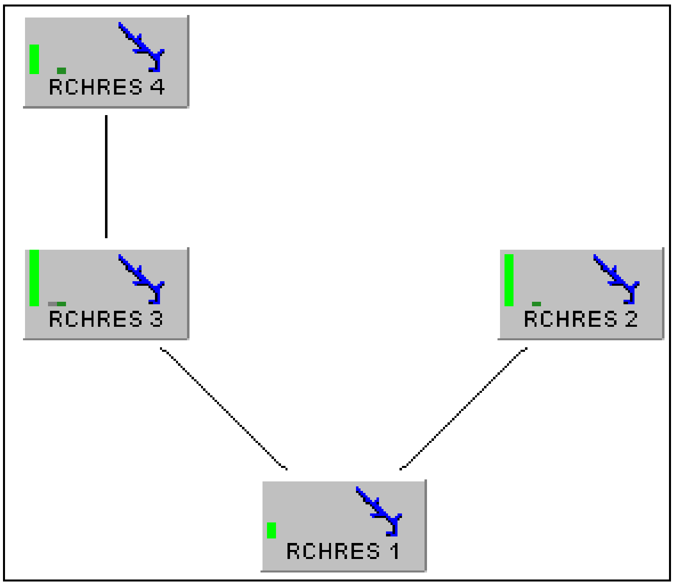

RCHRES 4
RCHRES 3
RCHRES 2
RCHRES 1

Fig. 5

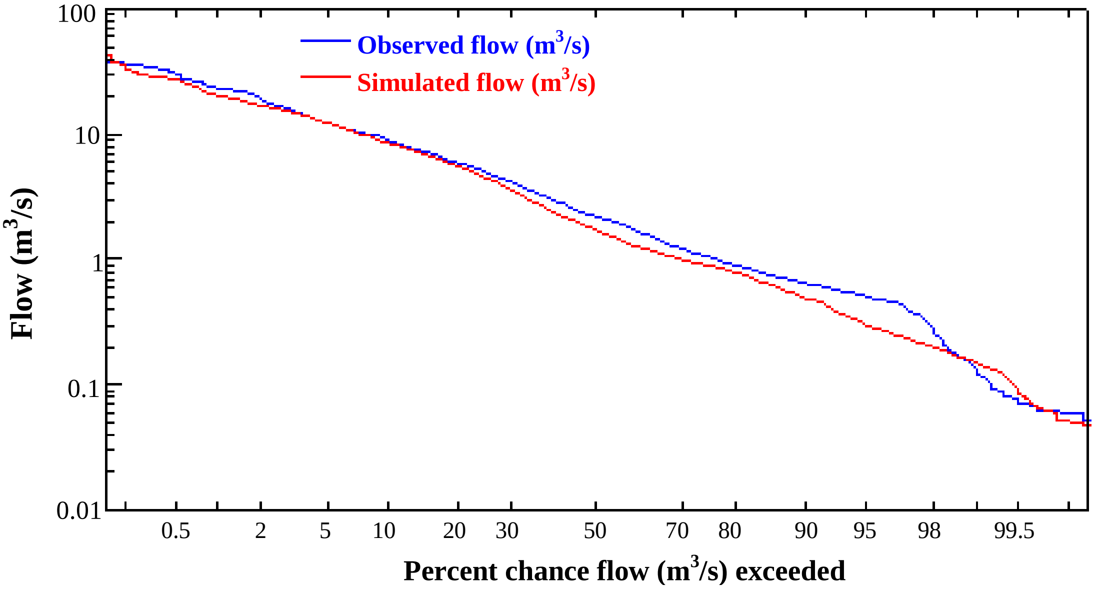

Observed flow (m^3/s)
Simulated flow (m^3/s)
Flow (m^3/s)
100
10
1
0.1
0.01
0.5
2
5
10
20
30
50
70
80
90
95
98
99.5
Percent chance flow (m^3/s) exceeded

Fig. 6

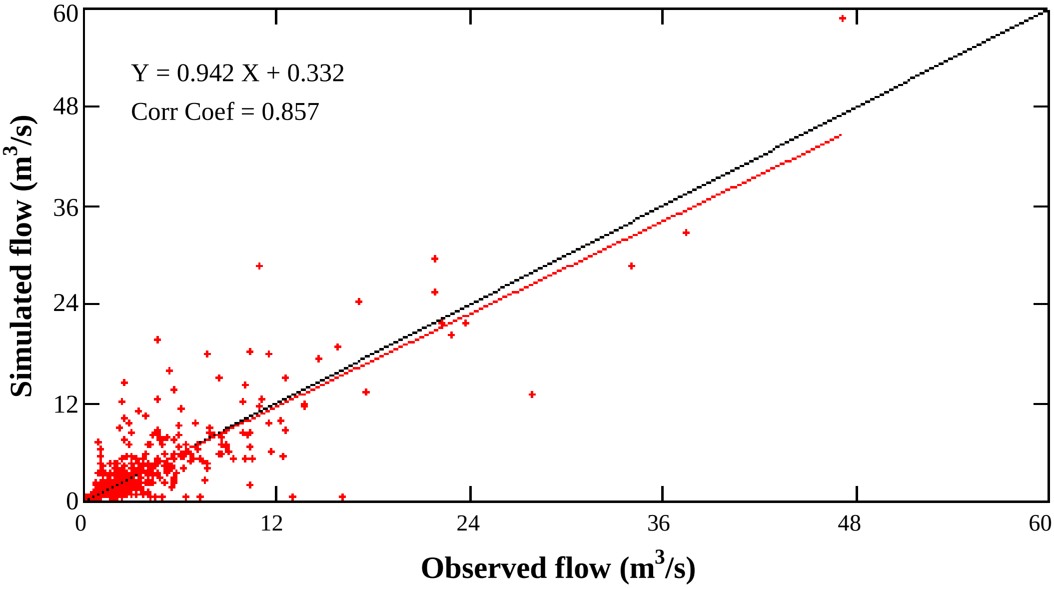

Y = 0.942 X + 0.332
Corr Coef = 0.857
Simulated flow (m^3/s)
60
48
36
24
12
0
0
12
24
36
48
60
Observed flow (m^3/s)

Fig. 7

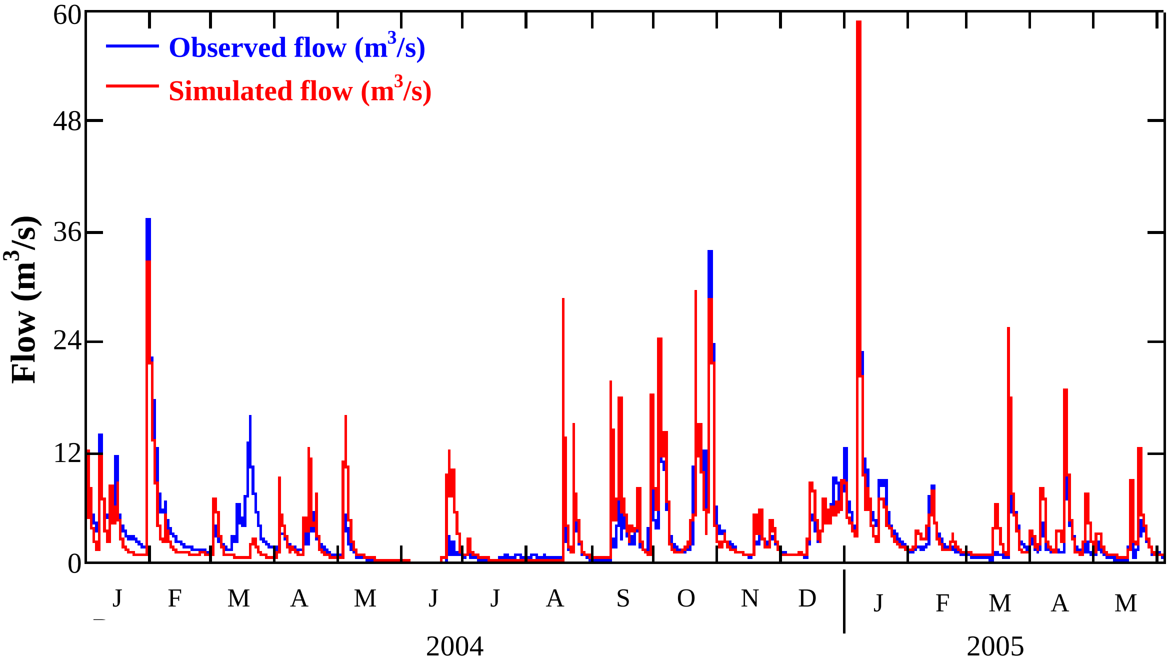

60
48
36
24
12
0
Flow (m³/s)
Observed flow (m³/s)
Simulated flow (m³/s)
J
F
M
A
M
J
J
A
S
O
N
D
J
F
M
A
M
2004
2005

Fig. 8

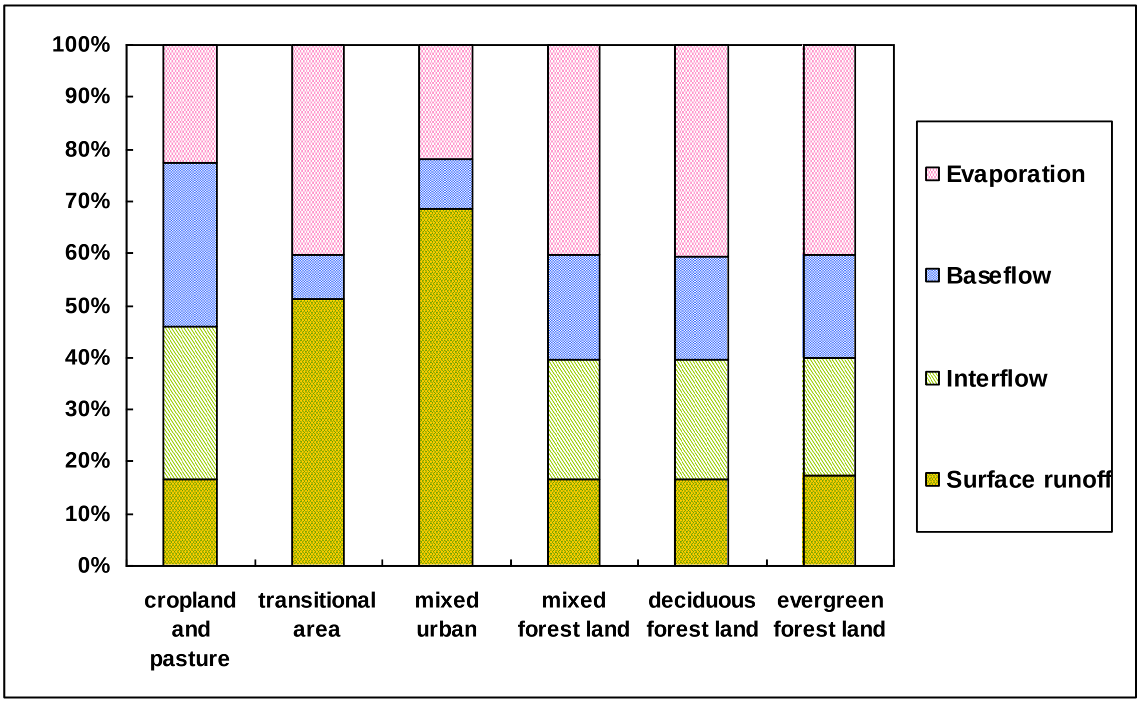

100%
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
cropland and pasture
transitional area
mixed urban
mixed forest land
deciduous forest land
evergreen forest land
Evaporation
Baseflow
Interflow
Surface runoff

Fig. 9

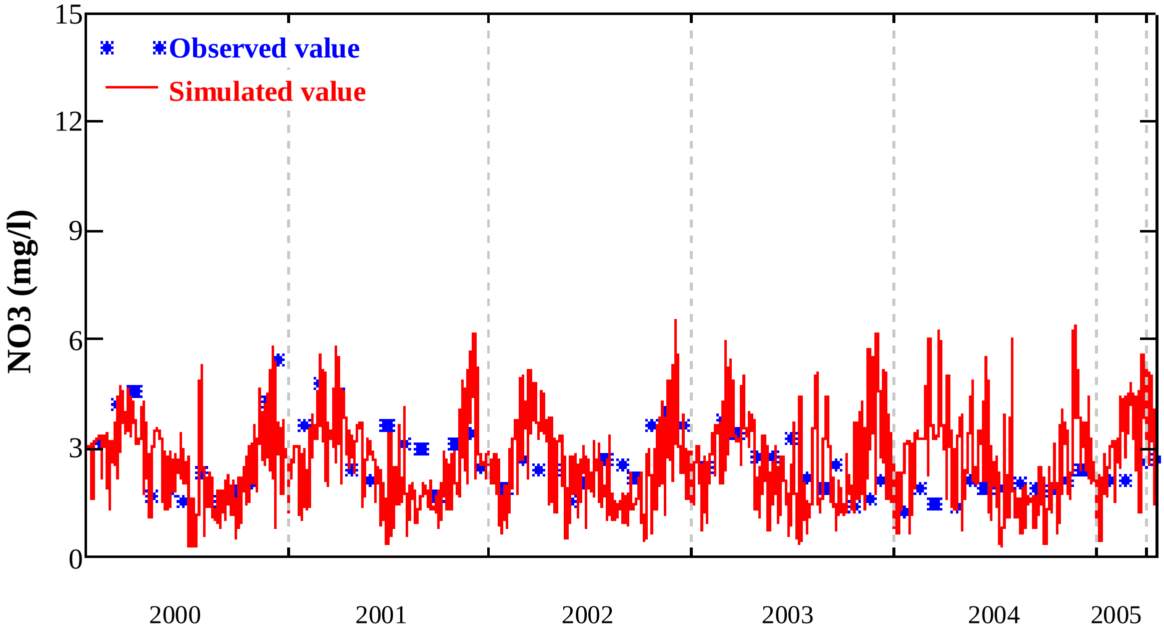

NO3 (mg/l)
15
12
9
6
3
0
Observed value
Simulated value
2000
2001
2002
2003
2004
2005

Fig. 10

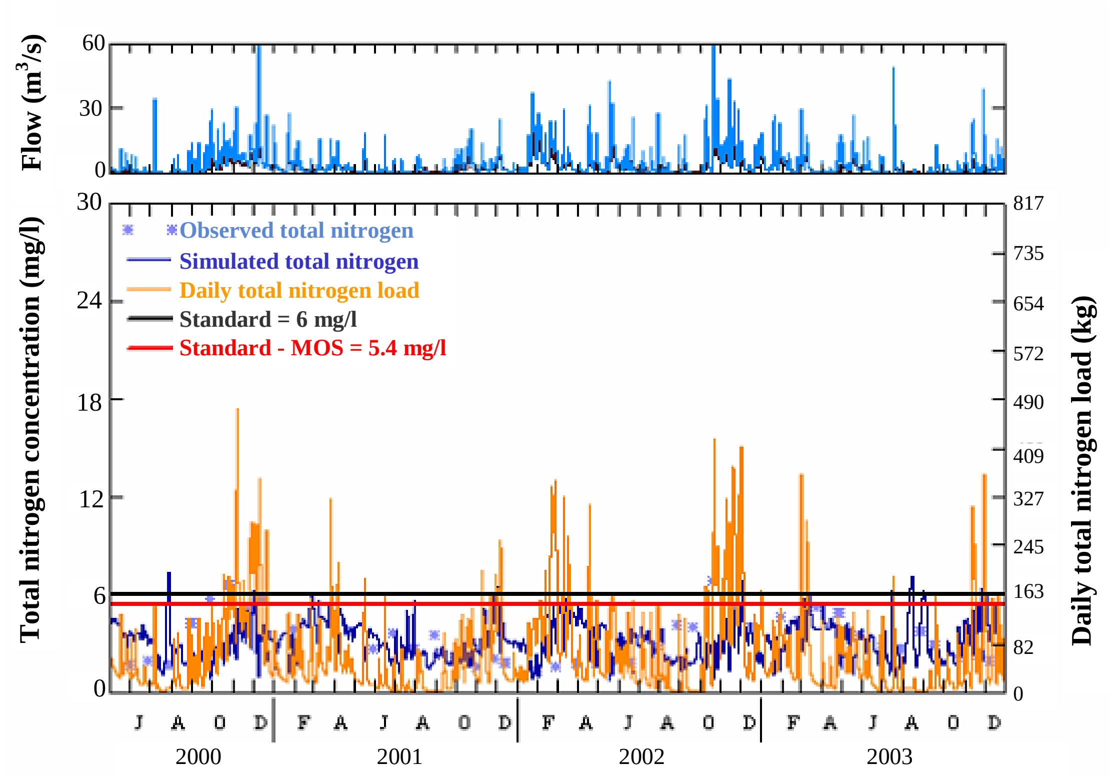

Flow (m^3/s)
60
30
0
Total nitrogen concentration (mg/l)
30
24
18
12
6
0
Daily total nitrogen load (kg)
817
735
654
572
490
409
327
245
163
82
0
Observed total nitrogen
Simulated total nitrogen
Daily total nitrogen load
Standard = 6 mg/l
Standard - MOS = 5.4 mg/l
J A O D F A J A O D F A J A O D F A J A O D
2000
2001
2002
2003

Fig. 11

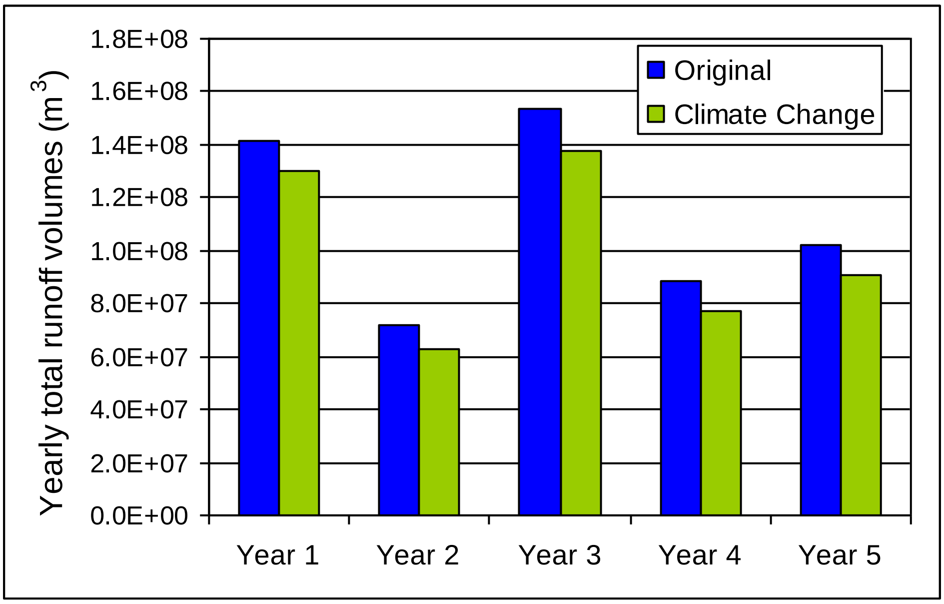
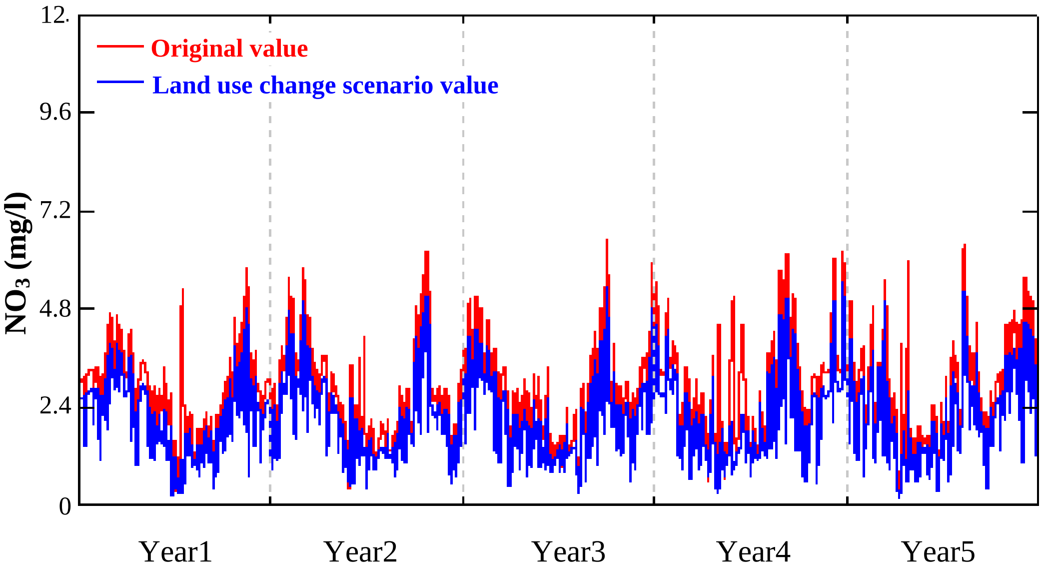

Original
Climate Change
Yearly total runoff volumes (m^3)
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
Year 1
Year 2
Year 3
Year 4
Year 5

Fig. 12


Original value
Land use change scenario value
NO$_3$ (mg/l)
12.
9.6
7.2
4.8
2.4
0
Year1
Year2
Year3
Year4
Year5