WATER QUALITY MODELLING IN MESOSCALE AND LARGE RIVER BASINS

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Contents

Summary

Water quality problems turn up as a result of both intensive land use and intensive water use by people. Depending on the objectives of model application and on the availability of measured data, water quality models of different complexity are used: from conceptual models based on statistical and empirical relationships to process-based and physically-based models derived from physical and physicochemical laws, also including some equations based on empirical knowledge. The dynamic process-based modelling has many advantages compared to statistical water quality modelling. The

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ability to provide projections for scenario conditions based on preliminary calibration and validation is one of the most important features. Only dynamical process-based and physically-based models are discussed in this paper. In the introduction different types of water quality models are described, and their levels of complexity and representation of spatial structure are discussed. Section 2 provides an overview of water quality models used for environmental assessment in catchments and river basins. Section 3 contains a short description of SWIM - the ecohydrological process-based model for mesoscale and large river basins, and Section 4 includes selected SWIM applications. Despite all the uncertainties involved in water quality modelling with limited input data, water quality models are very important tools to support water managers and policy makers. It would be impossible to evaluate the effectiveness of land management measures, changes in land use and climate change on water quality without using modelling tools. The dynamic catchment models driven by climate conditions and land use provide functional and useful tools for creating river basin management plans and for evaluation of possible impacts of changing climate.

1. Introduction

Water quality problems turn up as a result of both intensive land use and intensive water use by people. Point and diffuse sources of pollution are usually distinguished. The point sources are represented by easily identifiable inputs where polluted water is discharged to a river, lake or sea from a pipe or drain. Usually industrial wastes and municipal wastewaters, either after or without treatment, are discharged to rivers and the sea this way. Diffuse source pollution is caused by rainfall or snowmelt moving through the soil and carrying away nutrients and pollutants, and finally depositing them into rivers, lakes, and coastal waters. Diffuse pollution is closely linked to land use. Since 1950s, modern intensive agricultural practices often use high levels of mineral and organic fertilizers and manure. A bulk of fertilizers is usually introduced in soil by planting. This leads to high nutrient (nitrogen and phosphorus) surpluses in soil that are transferred to rivers and lakes with water flows. Agricultural systems represent a major source of nutrients, sediments and pesticides into river systems nowadays, many of which show increased levels of pollution in latest decades.

Starting with modelling conservative substances in the 1970s, water quality models for catchments are becoming more and more complex by taking into consideration landscape and river processes as well as transport and transformation processes for reactive substances. Different substances are considered in water quality models: from nutrients (nitrogen, N, and phosphorus, P) and sediments to pesticides, heavy metals and bacteria. Most often conventional substances, such as nitrogen, phosphorus and sediments are modelled.

Depending on the objectives of model application and on the availability of measured data, water quality models of different complexity are used nowadays: from conceptual models based on statistical and empirical relationships to process-based and physically-based models derived from physical and physicochemical laws, also including some equations based on empirical knowledge. The dynamic process-based modelling has many advantages compared to statistical water quality modelling. The ability to provide projections for scenario conditions based on preliminary calibration and validation is

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one of the most important features.

Here only dynamical process-based and physically-based models will be discussed. In the introduction different types of water quality models are described, and their levels of complexity and representation of spatial structure are discussed. Section 2 provides an overview of water quality models used for environmental assessment in catchments and river basins. Section 3 contains a short description of SWIM - the ecohydrological process-based model for mesoscale and large river basins, and Section 4 includes selected SWIM applications.

1.1. Dynamical water quality models

A basic component of a dynamical river basin model is a hydrological submodel. Other model components describing biogeochemical cycles (carbon, nitrogen and phosphorus) and vegetation are coupled with the hydrological submodel. This is necessary in order to include important interactions and feedbacks between the processes, like water transpiration of plants, water and nutrient drivers and stress factors for plant growth, nutrient transport with water, etc. As a rule, vertical and lateral fluxes of water and nutrients in catchments are modelled separately. Climate is usually not modeled, and climate-related parameters are used as external drivers. Land use, including agriculture areas, is also mostly considered as stable. Changes in climate and land use may be treated as external scenarios for such models. The spatial and temporal resolution of the model depends on data availability and the aim of the study.

1.2. Types of dynamical water quality models

Many different classifications of the catchment and river basin models exist. Most often, the differentiating principle is the modelling approach connected with the scale of model application. Usually physically-based and simplified conceptual models, lumped and distributed models, and deterministic and stochastic models, are distinguished. Intermediate or mixed types, like a model based on physical laws with some empirical and statistical equations, a deterministic model including some statistical relationships, and a semi-distributed model are possible.

A physically based hydrological or water quality model describes the natural system using mainly basic mathematical representations of physical laws on the flow of mass, momentum and energy. As a rule, a physically-based model has to be fully distributed, and has to account for spatial variations in all variables. However, the model quality is not guaranteed by the inclusion of physical laws in it. According to Beven (1996), even if physical laws included in the model are proven to represent a good mathematical description for a soil column under laboratory conditions where soil has been well mixed, this may not automatically be the case at the scale of grid elements used in distributed hydrological models: hundreds of meters or even kilometers. Besides, quite often the so-called physically-based models do include some empirical and statistical equations, especially for geochemical and vegetation growth processes.

On the other hand, the simplified conceptual hydrological models suffer from a lack of description of important physical processes, e.g. representation of soil column and water

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movement through soil layers. As a result, it is difficult or even impossible to integrate biogeochemical processes in such models, which are necessary for describing water quality relationships. This indicates that using the models of intermediate complexity for environmental and water quality assessment may be more promising.

The continuous dynamic models based on mathematical descriptions of physical, biogeochemical and hydrochemical processes by combining significant elements of both physical and conceptual semi-empirical nature, and including a reasonable spatial disaggregation scheme (e.g. in subbasins and Hydrologic Response Units, HRUs) can be called *process-based* ecohydrological (or water quality) river basin models. Such deterministic models may also include some stochastic elements. The models SWAT (Arnold *et al*., 1993 & 1998), HSPF (Bicknell et al., 1997), SWIM (Krysanova *et al*., 1998) and DWSM (Borah et al., 2004) belong to the process-based modelling tools for river basins. Numerous studies published during the last decades have demonstrated that such models are able to adequately represent hydrological, biogeochemical and vegetation growth processes at the catchment scale.

1.3. Levels of model complexity

The question about the level of model complexity is very important for the model developers and model users. How detailed should the parameterization of processes in a hydrological, ecohydrological or water quality model be in order to capture the modelled processes best?

Some modellers believe that the more details are included in the model, the better, and that more complex models guarantee a better representation of real processes. However, the experience of using complex process-based models has lead to the conclusion that the model complexity should not be a self-purpose, and should be generally defined as a compromising solution. The following rule has to be followed by the model developers: if a complex natural phenomenon or process can be described mathematically in a simplified form and parameterized using available parameters and data, this should be preferable to one with a higher level of details and with more and (partly) unknown parameters. In the latter case, the parameterizing the model may be problematic, and controlling model behaviour may become difficult or impossible. In other words, one should include only submodels that are essential and necessary, parameters that can be estimated, and interrelations that can be understood and validated in simulation experiments. Besides, the level of complexity in representation of different components in a model must be comparable, and integrating a detailed patch-scale submodel designed for experimental sites into a river basin model of intermediate complexity cannot be straightforward.

Model overparameterization is dangerous. It can easily lead to losing control over the model's behaviour, and to the inability of verifying important processes. Besides, the modellers should keep in mind that the global optimum parameter set usually does not exist in such models. Instead, there are several parameter sets leading to similar results. This is usually called the problem of equifinality, suggesting that there are many representations of a river basin that are almost equally valid in terms of their ability to reproduce studied processes, due to limitations of both the model structure and input

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data (Beven, 2001). Therefore, the modelling results should never be interpreted as exact predictions, but within the uncertainty ranges related to uncertain model parameters and input data, as indicators of possible trends, as qualitative differences, etc.

1.4. Representation of spatial structure

The way of representing spatial structure in a river basin model is also very important. Lumped models considering the catchment as one homogeneous unit are still used for hydrological modelling of small homogeneous watersheds, but they are generally not appropriate for integrated ecohydrological and water quality modelling in the medium-scale catchments and river basins. Spatially distributed or semi-distributed models are usually required for representation of biogeochemical processes in view of land surface heterogeneity, and in particular for land use change impact studies at the catchment scale.

The simplest way to overcome the lumped structure of a model is to subdivide a catchment into subcatchments or subbasins. This enables taking into account differences in topography, soil types or land use in parts of the catchment, and considering spatial variations in model variables and parameters. The two-level disaggregation can be implemented by (1) first simulating all the processes in the subbasins as homogeneous units, and (2) aggregating the outputs for the whole catchment by describing lateral transport of water, nutrients and pollutants in some reasonable way.

Further subdivision of the land surface delineated by subbasins is either possible into regular grid cells, or into irregular units using the principle of similarity. In the case of regular grid cells (method 1), computing time can become a problem, especially for larger basins and finer spatial resolution. In the case of irregular units the subbasin map, land use and soil maps are usually overlaid to create the so-called Hydrologic Response Units (HRUs), which can also be combined into the hydrotope classes (HRUs having the same land use and soil and located in the same subbasin). Then either every HRU is modelled separately (method 2), or every hydrotope class is modelled once in a time step (method 3). In the latter case the single units included in the hydrotope class and their position in the subcatchment are not distinguished. It is worth mentioning that spatial disaggregation of original maps in the catchment model coupled to GIS is normally based on finer regular grid cells defined by a Digital Elevation Model, even if irregular polygons (HRUs) or hydrotope classes are considered. The last two methods of spatial disaggregation take landscape heterogeneity into account, and they both (especially method 3) are computationally more efficient than method 1.

When all the main vertical and lateral flows between regular grid cells or irregular units are considered in the model, and the model accounts for spatial variations in all variables, it is called a fully distributed model. There are also other ways to take spatial variability into account, and reduce the level of complexity in comparison with the fully distributed model. This can be done by considering lateral transport processes for some aggregated units only, between subbasins for example. If the model subdivides the catchment into relatively homogeneous subcatchments only, or if it considers HRUs or hydrotope classes to simulate hydrological and biogeochemical processes in soil but the

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lateral flows of water and nutrients are aggregated at the subbasins level and then routed, the model is called semi-distributed.

The spatial and temporal resolution of the model should be appropriate for its use, and also depends on data availability. The scale of application, spatial resolution and objective of the study are connected. A fine spatial resolution may be required for a small catchment in order to study water flow components and their pathways using tracers. A lumped model may be sufficient for the case where only 'precipitation – runoff' relations are investigated in a homogeneous small or medium-size catchment. A coarser resolution could be applied for a mesoscale or large river basins for water resources assessment and climate impact studies.

2. Overview of water quality models for the catchment scale

This Section includes an overview of water quality models used for environmental assessment in catchments and river basins nowadays.

The **HBV-N** model (Arheimer & Brandt, 1998) is a semi-distributed conceptual model developed by extending the well known and widely used HBV model (Bergström, 1992) by water quality components for large-scale assessment of nitrogen load and retention in Sweden. The river basin can be divided into subbasins, and the time step is daily. Nitrogen concentrations are assigned to the water percolating from the unsaturated zone of soil originating from different land use categories (forest, urban and arable land). The arable land may be subdivided into a number of crops and management practices, for which nitrogen lea ching is estimated by using the field-scale model SOIL-N. Nitrogen from point sources, such as rural households, industries, and wastewater treatment plants, is also added. HBV-N simulates residence, transformation and transport of nitrogen in groundwater, rivers and lakes. The model includes a number of free parameters, which are calibrated against observed time-series of water discharge and nitrogen concentrations. The step-wise calibration procedure is possible for large-scale basins.

The **INCA** model (Whitehead et al., 1998) is a semi-distributed deterministic dynamic water quality model designed to investigate the fate and distribution of nitrogen in the catchments. Sources of nitrogen can originate from the terrestrial environment, direct discharges and from atmospheric deposition. The so-called hydrologically effective rainfall (HER) is used to drive the nitrogen fluxes. The model simulates water flows, nitrate nitrogen and ammonium nitrogen, and considers the flow paths operating in both the land phase and in the river. The model operates dynamically with the daily time steps. Six land use classes are distinguished in the model. Dilution, natural decay and biochemical transformation processes are included in the model, as well as the interactions with plant biomass such as nitrogen uptake by vegetation. INCA can be also used to investigate changes in land use.

The **LASCAM** model (LArge-Scale CAtchment Model) (Viney et al., 2000) was developed for large catchments to predict the long-term impacts of land use and climatic changes on stream flow and water quality represented by salt, sediments and nutrients. LASCAM can be classified as a semi-distributed model with a modest resolution. The

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subcatchments, ranging from 1 to 10 km^2, are determined on the basis of spatial variability and data availability. The model was developed for Australian conditions. It simulates the hydrological processes at the subcatchment scale, which are then aggregated. The model is being used as a management tool to evaluate a number of catchment management options for sediment and nutrients inputs to a number of catchments feeding the Swan River near Perth. LASCAM has also been used to assess land use changes in tropical environments (Malaysia).

The **HSPF** model (Hydrologic Simulation Program Fortran) (Bicknell et al., 1997) was developed for simulating watershed hydrology and water quality for both conventional and toxic organic pollutants. The model is driven by meteorological parameters and land surface characteristics such as land use patterns and land management practices. HSPF simulates dissolved oxygen, biochemical oxygen demand (BOD), ammonia, nitrite, nitrate, organic nitrogen, orthophosphate, organic phosphorus, pesticides, conservative substances, fecal coliforms, and sediments. The model can simulate one or many pervious or impervious unit areas discharging to one or many river reaches or reservoirs. Any time step from 1 minute to 1 day can be used. HSPF is generally used to assess the effects of land-use change, reservoir operations, point or nonpoint source treatment alternatives and flow diversions. There have been hundreds of applications of HSPF all over the world. The largest application is the 62,000 square mile tributary area to the Chesapeake Bay in the USA.

RHESSys (Regional Hydro-Ecologic Simulation System) (Band et al., 2001) is a coupled spatially distributed hydroecological model that is designed for representing feedbacks between hydrologic, vegetation, and nutrient cycling processes in forested catchments. RHESSys combines the terrestrial ecosystem process model Biome-BGC with spatially explicit meteorological information, and the TOPMODEL hydrologic routing model. It is aimed at spatial and temporal predictions of carbon, water, and nitrogen dynamics across landscapes. Input information for the model is derived from weather records, satellite imagery, digital terrain models, and soils maps. The model constructs a so-called climatic surface. Based on this and other input surfaces, it simulates time series and maps of various ecosystem properties including snowpack, soil moisture, streamflow, evaporation, and photosynthesis. RHESSys is a tool for understanding the effects of anthropogenic impacts on landscape-level processes, such as stream hydrology and forest productivity.

The **SWAT** model (Soil and Water Assessment Tool) (Arnold et al., 1993 & 1998) is a continuous-time semi-distributed process-based river basin model operating on a daily time step. It was developed to evaluate the effects of alternative management decisions on water resources, sediments and agricultural pollutants (nutrients, pesticides, bacteria and pathogens) in mesoscale and large river basins. The model is computationally efficient and capable of continuous simulation over long time periods. A watershed is divided into multiple subbasins and HRUs based on homogeneous land use, management and soil characteristics, but HRUs are not identified spatially within a subbasin. There are numerous SWAT applications worldwide for hydrological assessment (water discharge, groundwater dynamics, soil water, snow dynamics and water management), water quality assessment (land use and land management change, best management practices in agriculture) and climate change impact reported in the

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literature. Many studies demonstrated the robustness of SWAT in simulating sediment and nutrient concentrations, and loads. There are also several publications reporting climate change impacts on streamflow, water yield, groundwater recharge and pollutant transport. An overview of SWAT applications and SWAT comparisons with other process-based models can be found in Gassman *et al*. (2007).

During the last decade, a number of SWAT model versions were developed, adapted to applications outside the USA for specific purposes and using different data formats. Among them is the **SWIM** model (Krysanova *et al*., 1998 & 2000) based on SWAT-93 and MATSALU (Krysanova et al., 1989) tools. SWIM was developed for climate and land use change assessment in Germany and Europe. It is a continuous-time spatially distributed model, integrating hydrological processes, vegetation growth (agricultural crops and natural vegetation), nutrient cycling (nitrogen, phosphorus and carbon), and sediment transport at the river basin scale. Many processes are represented identically in SWIM and SWAT, though there are some differences. One of the most important features of SWIM is a more advanced spatial disaggregation scheme, namely: HRUs are spatially identified in the model code, and there is a version of SWIM, where such features as distance from HRU to the subbasin outlet can be considered. However, SWIM does not include modules for pesticides, bacteria, reservoirs and lake water quality, which are included in SWAT. Recently, several model extensions were added to SWIM: for wetland processes (Hattermann et al., 2006), carbon dynamics (Post et al., 2007), and forest growth (Wattenbach et al., 2005).

This overview of the water quality models is of course not full, but it includes models for river basins with different levels of complexity. The models described above have different strengths and weaknesses, partly described in the cited literature. The data to calibrate and fully test such models are generally not sufficient, especially for the water quality components. A lot of input data and special knowledge about the study area are needed, yet often difficult to get. This is the most serious constraint on the accuracy of modelling results.

The uncertainty is always included in the water quality modelling results. There are different sources of uncertainty, which should be kept in mind during the interpretation of modelling results: in input data, in model parameters, and in the measurements used for the comparison with the model outputs. Therefore, the modelling results should be interpreted within the uncertainty ranges related to uncertain model parameters and input data. This paper includes examples of SWIM validation for mesoscale and large basins, and selected SWIM applications.

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Biographical Sketches

Dr. Valentina Krysanova is a leading scientist at the Potsdam Institute for Climate Impact Research, Research Domain II Climate impacts and vulnerabilities. She holds Diploma (1973) in mathematics and PhD (1981) in biophysics. Her principal research fields are: assessment of impacts of climate and land use change on water availability, water quality and agriculture at the regional scale, and spatially-distributed ecohydrological modeling in river basins. She is the author of more than 80 scientific publications. She has participated as a coordinator in many national and international projects dealing with assessment of water resources, land use change, and climate change impacts. Currently she is coordinating the Elbe Case Study in the EU integrated project NeWater. She is Associated editor of the Regional Environmental Change Journal, and a President-elect of the International Commission on Water Quality (ICWQ) of the International Association of Hydrological Sciences (IAHS).

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