CHAPTER 9. THE ROLE OF MODELS

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Models represent systems in the real world. Using them helps us to gain a holistic understanding of problems by identifying relationships (cause and effect), and enabling future predictions (scenarios). Models can simulate the mobility of pollutants and the resulting changes in the state of water quality. They can help us to understand the impacts of pollutants on human health and ecosystems. Models can also be used to determine the effectiveness and cost of remedial actions. The aim of modelling can be research or management oriented. This chapter is devoted to discussing the application of mathematical models in agricultural water quality management.

9.1 Why are water quality models useful?

As a first step towards effective water quality management, it is necessary to know the current status of water quality and the spatial and temporal distribution patterns of contaminant emissions or loads and concentrations in water environments. For example, if pollutant loads in a given water body are high, identifying where, when and from whom the pollutant originated is necessary to ensure an appropriate response.

Although direct measurements of water quality status can be obtained through monitoring, the question of origin cannot be easily answered by simply relying on water quality monitoring data. Agriculture pollution typically comes from diffuse sources and pathways

(Mayorga *et al.*, 2010). Compared to point source emissions, diffuse source emissions into surface waters (also called non-point source emissions) are more difficult to measure.

The term diffuse pollution is sometimes thought to imply that the contribution to loads is sourced evenly across all parts of an agricultural landscape. However, this is rarely the case. The pollution emission rate from agricultural land depends on a number of local site properties, such as climate, topography, soil properties, land use, and management practices etc. (Chapin *et al.*, 2011), which can vary significantly over space and time. In addition, the proportion of load that is exported from a given farm or landscape is transported by different pathways driven by water fluxes. Moreover, pollutants stored in bottom surface water sediments can be released from the sediment, increasing the pollutant concentration in water bodies. It is thus hard for a water quality monitoring network, even in developed countries, to have enough station density to identify the main sources in diffuse pollution. Furthermore, the magnitude and timing of emission rates can be highly variable, and are often driven by extreme climate events, such as storms. The high cost of water quality analysis may prevent sampling with enough frequency to capture temporal variability. For all of these reasons, we require water quality modelling tools to help us to explain what we observe.

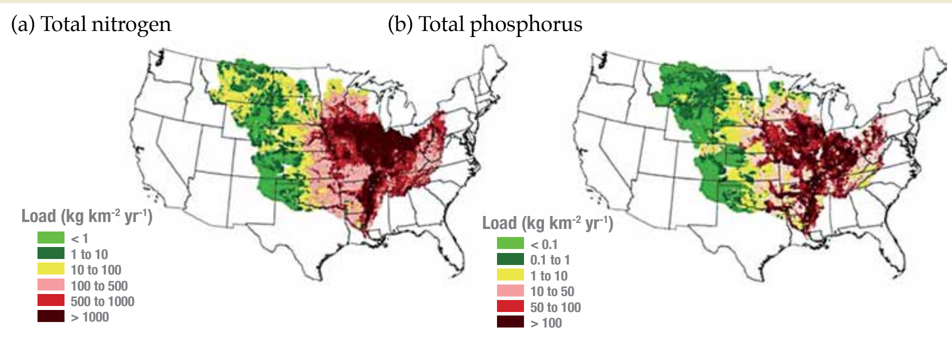
Broadly speaking, water quality models incorporate knowledge about a variety of physical, chemical and biological processes that control the transport, transformation and retention of pollutants. Well-built models can represent pressures, states and impacts at appropriate spatial and temporal scales, and, by linking causes and effects, they offer a way to assess water quality status and identify critical sources of agricultural pollution.

While models could be used to probe the current water quality situation, many water quality models are developed as predictive tools (Argent, 2004). These models can anticipate the effects on water quality as a result of changes in population density, socio-economic development, climate and land use. For example, water quality variation is forced by climate. By introducing climate forcing data, the model can be used to assess the impacts of climate change on water quality. As another example, many water quality models take land use and management practices as input parameters. By varying these input parameters, the models can tell what the water environment quality would be like after land use patterns change or new land management measures are taken. Thanks to their predictive capacity, models are recognized as valuable tools for the development of water quality regulatory programmes and policies. Because the costs of mitigation measures are often considerable and expended well in advance of the materialization of benefits, modelling can be a cost-effective way of to ensure that policies, strategies and actions are on the right track.

BOX 9.1 Using models to understand the role of agriculture in nutrient delivery: the case of the Gulf of Mexico

The Mississippi River and the Atchafalaya River flow through the main agricultural region in the USA. These rivers drain 3.1 million square kilometres in total. The nutrient delivery resulting from intensive agricultural activities in the Mississippi-Atchafalaya River Basin has long been perceived as a culprit for the hypoxia in the Northern Gulf of Mexico. Hypoxia is oxygen depletion in water due to the fast growth of algae blooms stimulated by an over-enrichment of nutrients. In a study by United States Geological Survey scientists (Alexander *et al.*, 2009), the SPARROW (SPAtially Referenced Regressions On Watershed attributes) model was used to estimate the load of nutrients (nitrogen and phosphorus) and contributions of different sources across the river basins, including ungauged areas.

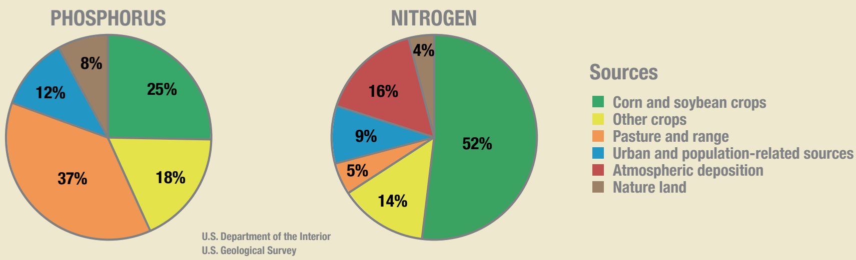
Figure 9.1 I Nutrients delivered to the Gulf of Mexico



Source: National Research Council, 2011.

The SPARROW modelling results showed that agricultural sources contribute more than 70% of the nutrient loads delivered to the Gulf of Mexico. While corn and soybean cultivation contributes 52% of total nitrogen load, manure on pasture and rangeland is the largest source of phosphorus and accounts for 37% of the total phosphorus load.

Figure 9.2 I Sources of nutrients delivered to the Gulf of Mexico



Source: ibid.

BOX 9.2 Water quality models to support policies: the case of the Total Maximum Daily Load (TMDL) programme, USA

To protect water quality from pollution, the United States Environmental Protection Agency (USEPA) launched the Total Maximum Daily Load (TMDL) programme. A TMDL is "the maximum amount of a pollutant that a waterbody can receive and still safely meet water quality standards" (USEPA, 2018). Implementing the TMDL programme involves identifying pollutants, estimating the assimilating capacity of the receiving water body and the current levels of pollution from all sources, determining maximum allowable loads and allocating them to different polluters. The determination of maximum allowable loads and load allocation often requires modelling tools with predictive skill (USEPA, 2004).

In a TMDL case study on nutrients and sediments, the Soil and Water Assessment Tool (SWAT) model was used to evaluate the effects of load reduction under various allocation schemes until a scheme was identified that ensures that the predicted 30-day average concentrations of pollutants at the watershed outlet meet water quality requirements. According to the SWAT simulation results, in some months, nutrients and sediment loads from 29 large, concentrated animal feeding operations (CAFOs) in the study river basin need to be reduced by up to 70%-80% (USEPA, 2004).

9.2 Types, capabilities and limitations of water quality models

Discovering the mechanism and factors impacting water quality and building a water quality model to describe those related processes in mathematical language represents a highly challenging task. It often requires research, which may have considerable costs. Fortunately, practitioners usually do not have to start from scratch. Today, dozens of models with different strengths and limitations are used in the field of water quality. These models operate at different scales (Borah and Bera, 2004; Wang *et al.*, 2013) to support researchers, planners and policy-makers in designing cost-effective measures for addressing water pollution in agriculture. Table 9.1 lists a number of commonly used models with water quality simulation capacity.

Water quality models vary substantially in their complexity and capability, and can be classified in a number of ways. For example, models can be classified on a scale of increasing complexity or scientific rigor.

Input-output models are relatively simple. A typical application of an input-output model is to keep track of nutrient balance. 'Simple' input-output balances can be done

Table 9.1 | Selected models for water quality simulation

Model	Description
MONERIS (Modelling Nutrient Emissions in Rivers Systems)	Designed to calculate emissions of nitrogen and phosphorus to surface waters via different pathways as well as the in-stream retention and transport in the surface water network; moderate demand of input data at river sub-basin level, free of charge, open software license concept (Behrendt *et al.*, 2000; Venohr *et al.* 2011)
GLEAMS (Groundwater Loading Effects of Agricultural Management Systems)	A field scale model developed to evaluate the impact of management practices on pesticide and nutrient leaching (Knisel, 1993)
PELMO (PEsticide Leaching Model)	A 1D model simulating the vertical movement of pesticides in soil by chromatographic leaching (Klein, 1995)
SHETRAN	A 3D finite difference model designed to simulate flow, and sediment and contaminant transfer (Ewen *et al.*, 2000)
QUAL2E & QUAL2K	1D river and stream water quality model that simulates daily water quality parameters, including biological oxygen demand, nitrogen, phosphorus, coliforms and pH (Brown and Barnwell 1987; Chapra *et al.*, 2003; Park and Lee, 2002)
SWAT (Soil and Water Assessment Tool)	Integrated river basin-scale model developed to quantify the impact of land management practices in large, complex watersheds with subroutines designed to simulate transport and fate of nutrients and pesticides (Arnold *et al.*, 1998; Srinivasan *et al.*, 1998)
AGNPS (AGricultural Non-Point Source Pollution Model)	A model developed to estimate pollutant loads from agricultural watersheds; the model can simulate surface water runoff, nutrients, sediment, chemical oxygen demand, and pesticides from point and nonpoint sources of agricultural pollution (Young *et al.*, 1989).
HSPF (Hydrological Simulation Program – Fortran)	An integrated river basin model that simulates runoff and water quality (e.g. nutrients, pesticide, sediment) from various, including agricultural, sources (Donigian, 1995)
L-THIA (Long Term Hydrologic Impact Analysis)	A tool used to evaluate long-term average of runoff and amount of several non-point source pollutants according to land use and soil combinations (Ma, 2004)
WEPP (Water Erosion Prediction Project)	A model that simulates runoff, erosion, and sediment delivery at field or small watershed scale (Flanagan *et al.*, 2007).
BATHTUB	A steady-state water quality model designed to simulate eutrophication conditions in lakes and reservoirs (Walker, 1987; Walker, 1996)

Model	Description
REMM (Riparian Ecosystem Management Model)	A model designed to simulate hydrology, nutrient dynamics and plant growth for land areas between the edge of fields and a water body (Lowrance *et al.*, 2000)
SPARROW (SPAtially Referenced Regressions On Watershed attributes)	Model developed to identify the source and fate of contaminants in large inland watersheds and water bodies by linking water quality monitoring data with watershed attributes (Alexander *et al.*, 2009; Schwarz *et al.*, 2006)
STEPL (Spreadsheet Tool for Estimating Pollutant Load)	This model uses simple algorithms to estimate nutrient and sediment loads from different land uses and to evaluate the effectiveness of implementing various best management practices (Tetra Tech, 2011).
LSPC (Loading Simulation Program in C++)	A watershed modelling tool that is closely related to HSPF with a simplified stream transport module (Tetra Tech, 2009)
GWLF (Generalized Watershed Loading Function)	A watershed model that simulates runoff, sediment and runoff loading (Haith *et al.*, 1992)
WARMF (Watershed Analysis Risk Management Framework)	A modelling system designed to calculate TMDLs for coliform, total suspended solids (TSS), biochemical oxygen demand (BOD) and nutrients and to guide stakeholders to reach consensus on the implementation of a water quality management plan (Goldstein, 2001)
VFSMOD (Vegetative Filter Strip Modelling System)	This system models field-scale processes associated with filter strips or buffers by routing storm runoff from an adjacent field through vegetative filter strip and calculating outflow, infiltration, and sediment-trapping efficiency (Muñoz-Carpena and Parsons, 2009)
PLOAD	A simple GIS-based model that estimates annual non-point source pollutant loads in watersheds (CH2MHILL, 2001)
MIKE	A commercial system that includes a range of models that simulate hydrological and hydrodynamic phenomena and water quality processes at the river basin scale (Refsgaard and Storm, 1995)
Global NEWS (Global Nutrient Export from Water(S)heds)	An integrated model that determines nitrogen, phosphorus and carbon exports through rivers into coastal areas on a global scale. The model enables future projections of nutrient export and the potential coastal eutrophication risks (Mayorga *et al.*, 2010)
ANSWERS (Areal Nonpoint Source Watershed Environment Response Simulation)	A hydrological and sediment transportation model that describes processes of infiltration, drainage, subsurface export, runoff, soil erosion, and sediment transport (Beasley, 1980)

Model	Description
CASC2D-SED	A simulation model that determines water and sediment runoff temporally and spatially. Overland flow is simulated on a two-dimensional grid and channel flow on a one-dimensional grid (Johnson *et al.*, 2000).
DWSM (Dynamic Watershed Simulation Model)	A model that simulates surface and subsurface runoff, propagation of floodwaves, soil erosion, and export of nutrients, pesticides and nutrients in rural and agricultural watersheds during a rainfall event (Borah *et al.*, 2002)
KINEROS (KINematic runoff and EROSion)	A kinematic and event-oriented model designed to simulate hydrological and sedimentation processes in watersheds (Woolhiser, 1990)
INCA (Integrated Catchement Model)	An integrated watershed model that simulates the transport and fate of nutrients, sediment, carbon, metals and mercury in water environments (Whitehead *et al.*, 1998)
WASP (Water Quality Analysis Simulation Program)	A widely used water quality model allowing for 1, 2 and 3 dimensional simulation of in stream water quality processes (Wool *et al.*, 2001)

on a spreadsheet and can be readily used by qualified consultants and farmers. Such models are easy to implement on farms, where record keeping on land management practices is seen as a basic management activity. Although the nutrient balances revealed by the budget model provide little insight on dynamics and processes, it effectively describes long-term average conditions.

Empirical models attempt to relate water quality variables to input variables without paying attention to the processes behind the correlation. A good example of this type of model is the SPARROW (SPAtially Referenced Regressions On Watershed attributes) model, which correlates pollutant loads and in-stream water quality with spatially referenced watershed attributes. The modelling exercise is data driven and tends to have intensive data requirements. In a study on the Mississippi-Atchafalaya River Basin, monitoring data came from 425 stations (Alexander *et al.*, 2007). This feature may restrict the application of empirical water quality modelling techniques in developing countries, where water quality data are typically scarce.

Process models explicitly describe water quality processes according to physical laws or causal relationships. This type of model may constitute the largest class of water quality models. Indeed, most of the models in Table 9.1 fall into this category. Of course, no sharp dichotomy exists between empirical and process models. Many process models contain empirical elements. In its extreme form, a process-based water quality model consists of a set of equations derived from mass conservation and other laws of chemical and biological kinetics. Process models are typically used to simulate the transport and transformation of pollutants in water bodies. Due to the embedded knowledge in the model, process models may work under conditions in which water quality monitoring data are limited or even in unmonitored regions.

Mixed models combine process-oriented and empirical approaches to model the fate and behavior of chemical substances in water bodies and their catchment. An example of this type of model is the MONERIS (MOdelling Nutrient Emission in RIver Systems, Venohr *et al.* 2011). MONERIS is a semi-empirical and process oriented model, which has gained international acceptance as a robust meso- to macro-scale model for nutrient emissions. MONERIS is used to calculate nitrogen, phosphorus and silica emissions into surface waters, in-stream retention, and resulting loads on a river catchment scale. The model distinguishes between sources (atmospheric deposition, fertilizer application, human disposal and industrial discharges); recipients (urban areas, agricultural and other areas); and emission pathways (atmospheric deposition on surface waters, surface runoff, erosion, tile drainage, groundwater, emissions from sealed urban areas and point sources). Compared to other models MONERIS has a moderate demand for input data, has a short computing time, and is applicable to large river basins. An implemented scenario manager can help quantify the effects of potential regionally differentiated measures to reduce nutrient emissions and loads from agricultural and urban sectors in surface waters. Over the past several years, MONERIS results have been used by various national and international river commissions (e.g. Danube, Oder, Elbe, Weser, Sanggan He, São Francisco) to develop river basin management plans and programes and have been the basis for national reporting obligations (e.g. Germany, Austria).

Models can also be grouped by loading models, receiving water models and integrated models. Loading models are designed to estimate pollutants from sources (e.g. crop land, pasture, feedlot, etc.) while receiving water models simulate the transport and fate of pollutants in water bodies (rivers, lakes, reservoirs, wetland, estuaries, and groundwater, etc.). Integrated models combine knowledge from two or more domains into a single framework. An integrated model can be used to address questions such as how reducing the application of fertilizer to conserve water quality will influence crop yields and what is the trade-off between water quality and agricultural productivity. Answering these questions requires simulation of both water quality and crop production process and the interactions between them.

BOX 9.3 Nutrient fluxes and losses in the Danube river basin

The Danube River is the most international river system in the world (Sommerwerk *et al.*, 2010). It drains a catchment area of 809 000 km² across 19 countries. From the Alps, over semi-arid regions to extended lowland plains, the Danube covers a wide range of hydrogeological conditions and shows a wide variation in land-use intensities (e.g. fertilizer application rates, population densities). Management of the Danube is a special challenge since the share of emission contribution and their effects on the water quality is unevenly distributed among the 19 countries – as are the financial resources for the implementation of management plans. Within the framework of the 1st and 2nd Danube River Basin Management Plans (DRBM) MONERIS (Venohr *et al.*, 2011) was applied to quantify the spatial and temporal pattern of nutrient emissions and loads under contract of the International Commission for the Protection of the Danube River (ICPDR) and country representatives (ICPDR 2009, ICPDR 2015).

The moderate data demand and robust model structure allowed the application of MONERIS to the Danube river basin with different data availability and quality from participating countries as well as a complex mixture of management problems and interests. The basin-wide modelled phosphorous (P) and nitrogen (N) emissions for the reference period (2009–2012) indicated that the diffuse sources dominate, making a contribution of 84% (N) and 67% (P). Whereas groundwater is the most important diffuse pathway for N (54%), soil erosion (32%) generates the highest diffuse emissions of P. The agricultural (N: 42%, P: 28%) and urban water management sectors (N: 25%, P: 51%) are responsible for most of the nutrient emissions (ICPDR, 2015). The economic situation of the countries also reflects the spatial distribution of source emissions. While nutrient emission rates from urban sources were relatively low for upstream countries, urban nutrient emissions become more dominant in the downstream countries, indicating the high potential to improve wastewater treatment. In contrast, N emissions from agricultural areas are higher in upstream countries, due to high nitrogen surpluses on agricultural lands. About 32% of the N and 42% of P emissions in the Danube basin are retained in the sediments of lakes, reservoirs, rivers as well as in connected floodplains before being transported to the Black Sea. Although emissions into the Danube's surface waters and groundwater decreased mainly due to waste water treatment measures implemented over the past decade (N: 12%, P. 34 %), a further nutrient load reduction (N: 40%, P: 20%) has been identified by modelling as necessary for improving the water quality of the Black Sea.

Using a set of measures for the short- (realistic) and long-term (vision) development provided by the country representatives, a further decrease of nutrient emissions was modelled. By implementing ambitious measures, a reduction of 20% (N) and 41% (P) seems achievable, although a trend of decreasing nitrogen emissions in the upstream countries and an increasing trend in the downstream countries due to land use intensification was ascertained.

The last two decades have witnessed the development of a number of integrated models. A good example is the Soil and Water Assessment Tool (SWAT) (Arnold, 1998). The SWAT model is the result of combining features of several predecessor models. For example, CREAMS (Chemicals, Runoff, and Erosion from Agricultural Management Systems) (Knisel, 1980) contributed routines for simulating hydrology, erosion and nutrients; EPIC (Erosion-Productivity Impact Calculator) (Williams *et al.*, 1984) provided the original algorithm for crop growth, and the pesticide component came from the GLEAMS (Groundwater Loading Effects on Agricultural Management Systems) model (Leonard *et al.*, 1987). SWAT also includes modules that implement the QUAL2E algorithm for in-stream water quality simulation (see Table 9.1).

It is also possible to classify water quality models in other ways, which may be more relevant to the technical specification of the models.

Steady state vs. dynamic model: Steady state models assume all input and state variables used in water quality simulation are time-invariant, whereas the dynamic models are capable of simulating time-varying water quality phenomena.

1D, 2D and 3D model or lumped vs. distributed model: The simulation of transport and transformation of pollutants can be carried out in one dimension (1D), two dimensions (2D) and three dimensions (3D). 1D simulation would suffice if the water quality in each longitudinal division is assumed to be homogeneous, while 2D and 3D simulations are required when the water quality variability in other dimensions cannot be ignored, such as on large lakes and estuaries. The terms 'lumped' and 'distributed' are mostly used to classify a loading model. In a lumped model, the study area is regarded as a single entity. By contrast, in a distributed model, there is a partition (usually a grid of cells) in the study region; input variables and model parameters are allowed to vary across the study area.

Continuous model vs. event model: Continuous simulation is used to generate estimates/predictions over a relatively long-term period. Continuous models can be run on a daily, monthly or even yearly basis. Event-based water quality simulation is primarily used to address pollution related to storm events. Such models typically run at hourly or even smaller time steps.

Given the large number of models/modelling techniques that have been developed for water quality simulation, choosing an appropriate model to use is by no means a simple task. When there are options, answering the following questions may help the practitioner decide:

- Can the output from the model satisfy the needs of the study (in terms of reported outcome variables, spatial and temporal resolution etc.)?
- Are the required input data available?
- Are the computational costs affordable?

It is worth noting that computational efficiency may be an important factor in the decision, especially when model calibration and uncertainty analysis are carried out. Models can merely provide a simplified representation of reality. Any modelling activity involves uncertainty (see Box 9.4). Quantifying and analyzing such uncertainty should be an integral part of model-based water quality studies. A number of calibration and uncertainty analysis techniques have been developed and these typically require a large number of model runs.

Finally, while this chapter hopefully provides some support for practitioners choosing an appropriate model to use for their water quality modelling work, there are reviews and comparison studies that provide discussions on this topic from a more technical perspective. (e.g., Borah *et al.*, 2003 and 2004; Kronvang *et al.*, 2009; Malagó *et al.*, 2015; and Wang *et al.*, 2013) Interested readers are encouraged to consult the literature for further information.

BOX 9.4 | **A caveat on uncertainty in water quality simulation using process-based deterministic models**

Process-based deterministic models are widely used for water quality simulation. Uncertainty may arise concerning the model input data and values of model parameters that are used for the simulation. When water quality monitoring data or other observations related to model output variables are available, the parametric uncertainty can be reduced through calibration. A model can be calibrated by selecting parameters that maximize model fit to observed data given certain criteria (e.g. Kling-Gupta efficiency coefficients or the Nash–Sutcliffe model efficiency coefficient). Although this approach is still extensively used in water quality modelling practices, more sophisticated calibration methods for deterministic simulation have been developed (e.g. Beven and Binley, 1992; Kennedy and O'Hagan, 2001; Refsgaard *et al.*, 2007; Efstratiadis and Koutsoyiannis, 2010). These approaches enable predictions or predictive intervals to indicate the parametric uncertainty resulting from model calibration. ➤

➤ Since parameters in process-based models often have physical meaning, a knowledge of parameters from literature or other studies can be used to improve the estimates of these parameters. This idea is particularly useful with regard to modelling unmonitored or poorly monitored regions. A recent well-known endeavour is the International Association of Hydrological Sciences' initiative on predictions in ungauged Basins (Hrachowitz *et al.*, 2013), which investigated the transferability of model parameter values at river basin scale according to watershed attributes.

Uncertainty may also originate from the structure of the model. No matter how sophisticated, a model can only provide an approximate representation of the real world. As Box (1987) observed, "essentially, all models are wrong, but some are useful." A method to cope with model structural uncertainty is model averaging (Hoeting *et al.*, 1999). When alternative models are available, instead of trying to select the 'best' one, a modeller can combine or average the results from multiple models. By synthesizing predictions from multiple models, model averaging helps to improve the accuracy and reliability of the prediction. For example, for a study of the Patuxent estuary, Maryland, USA (Boomer *et al.*, 2013), six models were used to predict water, nitrogen, and phosphorus discharges into the estuary. After comparing the results with observed data, it was found that the predictions constructed by combining simulation results from the six models outperform predictions from any single model.

9.3. Linking the outcome of water quality modelling to water policy

Water quality modelling reports the pollutant loadings from different sources and the resulting concentrations in water environments. When the outcome is used to inform water policy, it is often necessary to carry out further analysis to reveal the implications of different policies on water related ecosystem services.

Effectively linking water quality modelling and water policy requires being knowledgeable about relevant areas, such as water quality standards. Such standards define the water quality goal of a water body according to its designated use and are key elements in water quality management. Agriculture is an important source of nutrient pollution. The limits of nutrients in drinking water have been well established through epidemiological studies (WHO, 2006). However, developing water quality criteria to protect aquatic ecological systems from pollution remains challenging. In some countries, such as China, maximum concentrations of nutrients in ambient water environments are set, and the water quality standard is enforced uniformly nationwide. This type of water quality standard has the advantage of easing implementation, but it apparently neglects the variability in ecological water quality requirements. In 1998, the United States Environmental Protection Agency (USEPA) initiated an effort to develop numeric region-specific nutrient criteria. As of July 2017, the endeavor was still in progress due to the complexity of determining water quality requirements in ecological systems (US EPA, 2017). In Europe, many water bodies are still affected by pollutants and only 53% were found in 2015 to exhibit a good ecological status. In 2000, the European Environment Agency (EEA) established the European Water Framework Directive (WFD) for European Union member states to achieve the good qualitative and quantitative status of all water bodies in the EU by 2027. To achieve this goal, environmental quality standards and threshold values have to be complied for 41 chemical pollutants across the EU. If these values are exceeded, the contaminant sources have to be examined and measures implemented to restore the good status.

Ecological modelling tools have been developed as part of the effort to address the water quality needs of aquatic ecosystems. A few of such tools are listed in Table 9.2. In a review by Bartell (2001), AQUATOX, CATS, CASM and ECOWIN were ranked as having the

Table 9.2 | Selected ecological modelling tools

Model	Description
AQUATOX	A modelling system distributed by USEPA and designed to predict the effects of multiple stressors (suspended sediment, nutrients and organic toxicants, etc.);
CATS (Contaminants in Aquatic and Terrestrial Ecosystems)	An integrated ecosystem modelling system developed by the National Institute of Public Health and Environmental Protection (RIVM), Bilthoven, the Netherlands to simulate bioaccumulation and the combined effects of nutrients and toxicants;
CASM (Comprehensive Aquatic Systems Model)	A modelling system that uses bioenergetics to simulate population dynamics of multiple aquatic organism;
SIAM (System Impact Assessment Model)	A model developed by the US Geological Survey (USGS) and consisting of a suite of tools, among which SALMOD (Simulation by Means of an Analytical Lake Model) is an ecological model developed to simulate lake phytoplankton and zooplankton;
ECOWIN	A model that provides an object-oriented approach to modelling aquatic ecological systems;
PhytoBasinRisk	A water quality model that simulates the risk of critical phytoplankton biomass and composition in large river basins. The model is free of charge and is based on an open software license concept.

highest level of realism, and SALMOD in SIAM were considered to have a medium level of realism. Ecological modelling tools include water quality simulation components that can be linked to water quality models to evaluate the effects of water quality change on the habitat suitability of an aquatic community. Ecological models have been successfully used in a number of case studies. However, in general, simulating the transport and fate of toxic chemicals in a biotic system is more challenging than doing so in an abiotic environment. The development of ecological models remains firmly in the realm of research, mostly due to the time intensity of data collection required for calibration. There is also a considerable amount of work to be done in observing, capturing and simulating processes and dynamics in ecosystems. Ecological modelling will constitute a main topic in future research and efforts to strengthen agricultural water quality management.

9.4 References

Alexander, R.B., Smith, R.A., Schwarz, G.E., Boyer, E.W., Nolan, J.V. & Brakebill, J.W. 2007. Differences in phosphorus and nitrogen delivery to the Gulf of Mexico from the Mississippi River Basin. *Environmental Science & Technology*, 42(3):822-830.

Alexander, R.B., Woodside, M.D., & Hamilton, P.A. 2009. *SPARROW modelling: enhancing understanding of the nation's water quality*. Washington, DC, US Department of the Interior, US Geological Survey.

Argent, R.M. 2004. An overview of model integration for environmental applications – components, frameworks and semantics. *Environmental Modelling & Software*, 19(3):219-234.

Arnold, J.G., Srinivasan, R., Muttiah, R.S. & Williams, J.R. 1998. Large area hydrologic modelling and assessment part I: model development. *Journal of the American Water Resources Association*, 34(1):73-89

Bartell, S.M. 2001. Ecosystem models – aquatic. In Ginzburg L R, Ferson S, Pastorok R A, Bartell S M (eds.) *Ecological modelling in risk assessment: chemical effects on populations, ecosystems, and landscapes.* CRC Press, Boca Raton, USA, pp. 107-126.

Beasley, D.B., Huggins, L.F. & Monke, A. 1980. ANSWERS: a model for watershed planning. Transactions of the ASAE, 23(4):938-0944.

Behrendt, H.; Huber, P.; Kornmilch, M.; Opitz, D.; Schmoll, O.; Scholz, G.; Uebe, R. 2000. Nutrient Emissions into River Basins, 1st ed.; UBA-Texte; Federal Environment Agency (Umweltbundesamt): Berlin, Germany,

Beven, K., & Binley, A. 1992. The future of distributed models: model calibration and uncertainty prediction. *Hydrological processes*, 6(3):279-298.

Boomer, K.M.B., Weller, D.E., Jordan, T.E., Linker, L., Liu, Z.J., Reilly, J., Shenk, G. & Voinov, A.A. 2013. Using multiple watershed models to predict water, nitrogen, and phosphorus discharges to the Patuxent Estuary. *Journal of the American Water Resources Association*, 49:15–39.

Borah, D. K., Xia, R., Bera, M. (2002) DWSM - a dynamic watershed simulation model. Mathematical models of small watershed hydrology and applications, in Mathematical models of small watershed hydrology and applications, edited by V. P. Singh and D. Frevert, Water Resources Publications, LLC., Highlands Ranch, USA, pp.113-166.

Borah, D.K. & Bera, M. 2003. Watershed-scale hydrologic and nonpoint source pollution models: review of mathematical bases. *Transactions of the ASAE*, 46(6):1553-1566.

Borah, D.K. & Bera, M. 2004. Watershed-scale hydrologic and nonpoint source pollution models: review of applications. *Transactions of the ASAE*, 47(3):789-803.

Box, G.E.P. & Draper, N.R. 1987. *Empirical model building and response surfaces*. p. 424. John Wiley & Sons, New York, USA.

Brown, L.C. & Barnwell, T.O. 1987. *The enhanced stream water quality models QUAL2E and QUAL2E-UNCAS: documentation and user manual*. Washington, DC, Office of Research and Development. Environmental Research Laboratory, US Environmental Protection Agency.

Chapin F.S., Matson, P.A. & Vitousek, P. 2011. Principles of terrestrial ecosystem ecology. Springer Science & Business Media.

Chapra, S.C. & Pelletier, G.J. 2003. *QUAL2K – a modelling framework for simulating river and stream water quality: documentation and users' manual*. Medford, USA., Civil and Environmental Engineering Dept., Tufts University.

CH2MHILL. 2001. *PLOAD version 3.0. An ArcViewGIS tool to calculate nonpoint sourcesof pollution in watershed and stormwater projects*. [Cited on 03/06/2016]. http://permanent.access.gpo.gov/lps49376/PLOAD_v3.pdf.

Donigian Jr, A.S., Bicknell, B.R., Imhoff, J.C. & Singh, V.P. 1995. Hydrological Simulation Program-Fortran (HSPF). In Singh, V.P (ed). *Computer models of watershed hydrology, Water Resources Publications*, Highlands Ranch, USA, pp. 395-442.

Efstratiadis, A. & Koutsoyiannis, D. 2010. One decade of multi-objective calibration approaches in hydrological modelling: a review. *Hydrological Sciences Journal–Journal Des Sciences Hydrologiques*, 55(1):58-78.

Ewen, J., Parkin, G., & O'Connell, P.E. 2000. SHETRAN: distributed river basin flow and transport modelling system. *Journal of Hydrologic Engineering*, 5(3):250-258.

Flanagan, D.C., Gilley, J.E. & Franti, T.G. 2007. Water Erosion Prediction Project (WEPP): development history, model capabilities, and future enhancements. *Transactions of the ASABE*, 50(5):1603-1612.

Goldstein, R.A. 2001. *Watershed analysis risk management framework (WARMF): update one*. Topical Report. Palo Alto, USA, EPRI (Electric Power Research Institute).

Haith, D.A., Mandel, R. & Wu, R.S. 1992. GWLF, generalized watershed loading functions, version 2.0, user's manual. Ithaca, USA, Cornell University, Department of Agricultural & Biological Engineering.

Hoeting, J.A., Madigan, D., Raftery, A.E. & Volinsky, C. T. 1999. Bayesian model averaging: a tutorial. *Statistical Science*, 14(4):382-401.

Hrachowitz, M., Savenije, H.H.G., Blöschl, G., McDonnell, J.J., Sivapalan, M., Pomeroy, J.W., Arheimer, B. *et al.* 2013. A decade of predictions in ungauged basins (PUB): a review. *Hydrological Sciences Journal*, 58(6):1-58.

ICPDR (International Commission for the Protection of the Danube River). 2009. Danube River Basin District Management Plan. Part A – Basin-wide overview. Final Version 14 December 2009. ICPDR, Vienna. (also available at http://www.icpdr.org/icpdr-pages/danube_rbm_plan_ready.htm).

ICPDR. 2015. Danube River Basin District Management Plan - Update 2015. Part A – Basin-wide overview. Final Version 2 December 2015. ICPDR, Vienna. (also available at http://www.icpdr.org/main/management-plans-danube-river-basin-published).

Johnson, B.E., Julien, P.Y., Molnar, D.K. & Watson, C.C. 2000. The two dimensional upland erosion model CASC2D-SED. *Journal of the American Water Resources Association*, 36(1):31-42.

Kennedy, M.C. & O'Hagan, A. 2001. Bayesian calibration of computer models. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 63(3):425-464.

Klein, M. 1995. *PELMO: pesticide leaching model, version 2.01. Users Manual*. Frauenhofer-Institut für Umweltchemie und Ökotoxikologie, Schmallenberg, Germany, 91pp.

Knisel, W.G. 1980. *CREAMS, a field scale model for chemicals, runoff and erosion from agricultural management systems*. USDA Conservation Research Report. No. 26.

Knisel, W.G. 1993. *GLEAMS: groundwater loading effects of agricultural management systems. Version 2.10 (No. 5)*. Tifton, USA, University of Georgia Coastal Plain Experiment Station, Biological & Agricultural Engineering.

Kronvang, B., Behrendt, H., Andersen, H.E., Arheimer, B., Barr, A., Borgvang, S.A., Bouraoui, F *et al.* 2009. Ensemble modelling of nutrient loads and nutrient load portioning in 17 European catchments. *Journal of Environmental Monitoring*, 11:572–583.

Leonard, R.A., Knisel, W G. & Still, D.A. 1987. GLEAMS: groundwater loading effects of agricultural management systems. *Transactions of the ASAE*, 30(5):1403-1418.

Lowrance, R., Altier, L.S., Williams, R.G., Inamdar, S.P., Sheridan, J.M., Bosch, D.D. & Thomas, D.L. 2000. REMM: The riparian ecosystem management model. *Journal of Soil and Water Conservation*, 55(1):27-34.

Ma, Y. 2004. L-THIA: a useful hydrologic impact assessment model. *Nature and Science*, 2(1):68-73.

Malagó, A., Venohr, M., Gericke, A., Vigiak, O., Bouraoui, F., Grizzetti, B. & Kovacs, A. 2015. Modelling nutrient pollution in the Danube River Basin: a comparative study of SWAT, MONERIS and GREEN models, JRC Technical Reports, European Commission, Italy.

Mayorga, E., Seitzinger, S.P., Harrison, J.A., Dumont, E., Beusen, A.H., Bouwman, A., Fekete, B.M., Kroeze, C. & Van Drecht, G. 2010. Global nutrient export from WaterSheds 2 (NEWS 2): model development and implementation. *Environmental Modelling & Software*, 25(7):837-853.

Muñoz-Carpena, R. & Parsons, J.E. 2014. VFSMOD-W Vegetative Filter Strips Modelling System: Model documentation and user's manual, Version 6.x. Gainsville, USA, University of Florida.

Park, S.S., & Lee, Y.S. 2002. A water quality modelling study of the Nakdong River, Korea. *Ecological Modelling*, 152(1):65-75.

Refsgaard, J.C. & Storm, B. 1995. MIKE SHE. *Computer models of watershed hydrology*. In V. P. Singh, ed. Pp. 809-846. Highlands Ranch, USA, Water Resources Publications.

Refsgaard, J.C., van der Sluijs, J.P., Højberg, A.L., & Vanrolleghem, P.A. 2007. Uncertainty in the environmental modelling process – a framework and guidance. *Environmental Modelling & Software*, 22(11):1543-1556.

Schwarz, G.E., Hoos, A.B., Alexander, R.B. & Smith, R.A. (2006). *The SPARROW surface water-quality model: theory, application and user documentation. US geological survey techniques and methods report, book*, 6(10), p.248, Reston USA

Sommerwerk, N., Bloesch, J., Paunović, M., Baumgartner, C., Venohr, M., Schneider-Jacoby, M., Hein, T. and Tockner, K., 2010. Managing the world's most international river: the Danube River Basin. Marine and Freshwater Research, 61(7), pp.736-748.

Srinivasan, R., Ramanarayanan, T.S., Arnold, J.G. & Bednarz, S.T. 1998. *Large area hydrologic modelling and assessment, part II: model application, Journal of the American Water Resources Association*, 34(1), pp.91-101.

Tetra Tech. 2011. *User's guide spreadsheet tool for the estimation of pollutant load (STEPL), Version 4.1.*, Fairfax, USA.

Tetra Tech. 2009. *Loading simulation program in C++ (LSPC). Version 3.1 User's Manual*. Fairfax, USA.

US EPA (United States Environmental Protection Agency). 2004. *Total maximum daily load (TMDL) for the Wabash River Watershed, Ohio*. Washington DC, USA.

US EPA (United States Environmental Protection Agency). 2017. *State progress toward developing numeric nutrient water quality criteria for nitrogen and phosphorus*. https://www.epa.gov/nutrient-policy-data/state-progress-toward-developing-numeric-nutrient-water-quality-criteria, last access: March 10, 2018.

US EPA (United States Environmental Protection Agency). 2018. Permitting to Meet a Total Maximum Daily Load (TMDL), https://www.epa.gov/npdes/permitting-meet-total-maximum-daily-load-tmdl, last access: April 29, 2018

Venohr, M., U. Hirt, J. Hofmann, D. Opitz, A. Gericke, A. Wetzig, S. Natho, F. Neumann, J. Hürdler, M. Matranga, J. Mahnkopf, M. Gadegast & H. Behrendt. 2011 Modelling of nutrient emissions in river systems – MONERIS methods and background. *International Review of Hydrobiology*, 96:435–483.

Walker, W.W. 1987. *Empirical methods for predicting eutrophication in impoundments. Report 4. Phase III.* Applications Manual, Technical Rep. E-81-9, U.S. Army Engineer Waterways Experiment Station, Vicksburg, USA.

Walker, W.W. 1996. *Simplified procedures for eutrophication assessment and prediction: user manual*. Instruction report. W-96-2. (Updated 1999). Vicksburg, USA, U.S. Army Engineer Waterways Experiment Station.

Wang, Q., Li, S., Jia, P., Qi, C., & Ding, F. 2013. A review of surface water quality models. *The Scientific World Journal*, 2013.

Whitehead, P.G., Wilson, E.J. & Butterfield, D. 1998. A semi-distributed integrated nitrogen model for multiple source assessment in catchments (INCA). Part I – model structure and process equations. *Science of the Total Environment*, 210:547-558.

Williams, J.R., Jones, C.A. & Dyke, P.T. 1984. A modelling approach to determining the relationship between erosion and soil productivity. *Transactions of ASAE*, 27(1):129-144.

Wool, T.A., Ambrose, R.B., Martin, J.L., Comer, E.A. 2001. Water Quality Analysis Simulation Program (WASP) Version 6.0: User’s Manual. U.S. Environmental protection Agency, Athens, USA.

Woolhiser, D.A., Smith, R.E. & Goodrich, D.C. 1990. *KINEROS: a kinematic runoff and erosion model: documentation and user manual.* Washington, DC, US Department of Agriculture, Agricultural Research Service.

WHO (World Health Organization). 2006. *Guidelines for drinking-water quality: First addendum to Volume 1, Recommendations (Vol. 1)*. Geneva.

Young, R.A., Onstad, C.A., Bosch, D.D., & Anderson, W.P. 1989. AGNPS: a nonpoint-source pollution model for evaluating agricultural watersheds. *Journal of Soil and Water Conservation*, 44(2):168-173.