

Surface Water Quality Modelling

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Surface water quality modelling has become an important means of better understanding aquatic and riparian ecosystem processes at all scales, from the micro-scale (e.g., bottom sediment dynamics), to the meso-scale (e.g., algal bloom growth) and the macro-scale (e.g., the role of cascading reservoirs in sediment transport). Increasingly, surface water quality models are being coupled to other models (e.g., hydrological models) to determine catchment area impacts on water quality. These impacts include future climate change and land-use developments. Coupling with water resource dynamics models also provides insight into changes in water supply and demand and flow regulation as they relate to surface water quality. Modelling the quality of surface waters under ice-covered conditions has also gained special attention due to the increased realization that a holistic all-year perspective is required to deepen our understanding of aquatic ecosystem functioning (e.g., the impact of lake ice phenology on spring succession of phytoplankton) (excerpts and adaptations from my Global Water Futures <https://gwf.usask.ca/> (accessed on 16 February 2023) reporting and https://www.mdpi.com/journal/water/special_issues/surface_water (accessed on 16 February 2023) announcement).

Table 1 summarises the contents of the papers [1–10] submitted to this Special Issue into categories of global region, type of water body and model or modelling approach used. From North America, modelling exercises on rivers in Canada have been reported, particularly the Athabasca [9] and South Saskatchewan [1] rivers in western Canada. The Athabasca River is a natural flowing river draining a catchment area that is predominantly forested, whereas the South Saskatchewan River is a prairie river mostly draining agricultural lands and regulated by the Gardiner Dam, which impounds Lake Diefenbaker. Both studies look at the transport and fate of heavy metals (copper, nickel and vanadium) to verify the sources of these metals, with copper stemming mainly from anthropogenic and nickel and vanadium from geogenic sources.

The water quality of a Canadian reservoir, Buffalo Pound Lake, was also modelled [7]. Buffalo Pound Lake receives water from Lake Diefenbaker (mentioned above) and is an important drinking water source for southern Saskatchewan. Managing water transfers from Lake Diefenbaker is an important aspect when modelling the algal-nutrient dynamics in Buffalo Pound Lake.

China is represented in this Special Issue by the modelling applications of surface waters in Guangzhou Province [2] of southern China and the estuary Sanmen Bay in Zhejiang Province of eastern China [3]. Both applications use chemical oxygen demand (COD) as a determinant to assess the impact of urban pollutants on aquaculture facilities. A study of the transport of nutrients, particularly ammonium nitrogen, in overland runoff from the Haihe River basin near Beijing and the Poyang Lake basin, which drains into the Yangtze River in east central China [8], is also available. The Haihe River basin study looks more at reducing diffuse loadings, whereas the Poyang Lake basin study investigated point loadings as mitigation options to control sediment and nutrient loadings in receiving waters.

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Table 1. Summary of the models used, surface waters investigated and study regions of the articles in this Special Issue, *Surface Water Quality Modelling*.

Model	Region						
	Canada	China	Vietnam	India	South Korea	Malawi	Nordic Europe
HEC-RAS	river [1]						
WASP	river [1]			river [5]	river [5]		
WASP (Quasi-2D)	river [9]						
statistical		river [2]					
Delft 3D		estuary [3]					
Machine Learning			river [4]				
conceptual						lake [6]	
CE-QUAL-W2	reservoir [7]						
SPARROW		overland [8]					
various							river [10]

Other river water-quality modelling studies reported from Asia include the Yamuna River in northern India [5], the Ara River in South Korea [5] and the La Buong River in Vietnam [4], listed in the order of wetness ranging, respectively, from dry, moderately wet to wet. Typical water-quality constituents such as biological oxygen demand (BOD) and dissolved oxygen (DO) with different arrays of total or dissolved nutrients were modelled for different seasons (dry/wet, spring/summer/autumn/winter).

One study from Africa (Lake Malombe in Malawi) [6] and another from Nordic Europe (various rivers in Norway, Sweden, Finland, eastern Germany and Poland) [10] are included in this Special Issue. The first study links overarching demographic, socio-economic, climatic and other factors to the lake's ecosystem health. The second study focuses more on river ice processes and reveals the importance of increased water temperatures from urban heat islands and increased salinity due to fertilizer applications in agricultural areas for long-term trends in water parameters.

The Special Issue also provides a spectrum of different model applications, from the more conceptual [6], to empirical approaches [2,4,8] to the more deterministic methodologies [1,3,5,7,9]:

Conceptual modelling:

The conceptual model uses driver, pressure, state, impact, and response (DPSIR) indicators to assess the ecosystem health of Lake Malombe in Malawi [6].

Empirical modelling:

A diagnostic model consisting of visible near-infrared spectroscopy combined with partial least squares discriminant analysis was applied to determine the water quality status of 127 surface water sites [2]. Twelve machine-learning approaches were employed to assess the water quality of the La Buong River in Vietnam [4]. SPARROW, too, is an empirical model relating catchment area characteristics and discharges to nutrient loading in large river basins [8].

Deterministic modelling:

The WASP (Water Quality Analysis Simulation Program), originally developed by the US Environmental Protection Agency, is a popular model applied to rivers and lakes to track water quality changes in surface water bodies [1]. Its modules of HEAT, EUTRO and TOXI allow a diverse set of processes and constituents to be modelled. The discretisation scheme also allows different dimensionality schemes, from one-, two- and three-dimensional schemes but also a quasi-two-dimensional scheme, where one-

dimensional equations are applied across a two-dimensional discretisation network providing flexibility in model setup at lower computational expenditure [9]. Coupling to a hydraulic model such as HEC-RAS gives the WASP modelling system a better description of the hydraulic flow fields [1]. The two-dimensional CE-QUAL-2D and three-dimensional Delft 3D models provide more descriptive power by including changing constituent concentrations in depth, such as in lakes and reservoirs [7], plus lateral gradients, such as in estuaries [3], not just longitudinally, which is often the only dimension requirement for modelling rivers [1].

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