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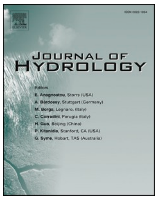

Review papers

Evaluation of the performance and complexity of water quality models for peatlands

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ABSTRACT

Rewetting is accepted as an effective technique in restoring degraded peatlands. However, it may adversely impact water quality, particularly in nutrient-rich peatlands. The aim of this study was to review water quality models applied to peatlands, with a focus on evaluating the performance (such as stability and accuracy) and complexity of the models. In a systematic review of published studies from 01/01/2003 to 10/12/2023, out of 3618 published studies on peatlands and nutrient modelling, only 23 studies applied water quality models to predict the evolution and distribution of nutrients of peatlands by using 16 different water quality models. Out of the 23 studies, only 1 predicted the nutrient concentration and transport of a rewetted peatland. Among the 16 models evaluated, only the mixed mire water and heat (MMHW) model was capable of considering the inherent heterogeneity in peatland characteristics. The HYDRUS 1D/2D model is effective at predicting nitrogen species, despite encountering challenges in some studies due to the complex nature of the peat environment. To enhance the predictive power of water quality models, it is important to consider all the processes that can affect the concentration of nutrients in peatlands such as oxidation of carbon, the nitrogen cycle, decay/production rate for nutrients, adsorption/desorption of nutrients in the soil, and the advection of nutrients due to the influence of ground water and surface water. To date, no peatland-specific water quality model has been developed to simultaneously predict DOC, nitrogen and phosphorus in peatland ecosystems.

1. Introduction

Peatlands are estimated to cover about 3 % of the earth's terrestrial land area but store up to 30 % of the total soil carbon (Cirulis et al., 2022; Escobar et al., 2022). Pristine peatlands play a major role in climate change dynamics (O'Connell et al., 2021) and provide important ecosystem services such as the provision of habitats for biodiversity (Minayeva et al., 2017; Renou-Wilson et al., 2019), carbon sequestration and water purification (Andersen et al., 2017; Tanneberger et al., 2021). It is estimated that 50 % of European peatlands have been degraded due to drainage (Andersen et al., 2017; Tanneberger et al., 2021). Although restoration of degraded peatlands by rewetting is considered to be an effective tool to recover their hydrological and ecological conditions (Menberu et al., 2017; Laine et al., 2019), it may pose a risk to water quality, particularly in the initial stages of restoration of nutrient-rich peatlands (Harpenslager et al., 2015; Koskinen et al., 2017; Healy et al., 2023). Modelling of the potential impacts of rewetting on water quality is therefore of great importance when designing a re-wetting scheme.

Although much research has been conducted on peatland dynamics, there is a dearth of research on models to predict the water quality of peatlands, especially for rewetted peatlands. Hydrological models help gain a better understanding of hydrological phenomena and how changes in the physical characteristics of a watershed may affect the hydrological cycle (USEPA, 2017). Conversely, water quality models are mathematical representations of pollutant/nutrient fate and transport within a water body or from land-based sources to a water body (Cho et al., 2020). The majority of the water quality models depend on hydrological models, as the modelling results of ground/surface water flow of hydrological models are used as inputs in water quality models. Water quality modelling is capable of predicting future water quality dynamics resulting from different management practices (Loucks & Van Beek, 2017) on rewetted peatlands. Therefore, they are potentially a valuable tool for those involved in the management of peatlands.

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Hydrological models may be classified as either empirical (metric), conceptual, or physical (process-based) models (Wheater et al., 2008; Devia et al., 2015; USEPA, 2017). Empirical models, sometimes referred to as data-driven models or observation-oriented models, use non-linear statistical relationships between inputs and outputs which extract information from the existing data and ignore the specific processes of hydrological systems (Kokkonen et al., 2001). Conceptual models, also known as grey-box models, use simplified mathematical equations to conceptualise the hydrological processes (Jaiswal et al., 2020) and interpret outputs by connecting simplified components in the hydrological processes (USEPA, 2017; Singh, 2018). Physical models, or process-based or mechanistic models, are based on the underlying physics of the specific hydrological processes (Sitterson et al., 2018). They use "state" variables which are measurable and are functions of both time and space (Devia et al., 2015; Singh, 2018). They require complex information about the hydrological system and, due to the large number of parameters and the fine-scale spatial discretisation, their parameterisation requires a very large amount of data (Cirulis et al., 2022).

Hydrological models can also be categorized based on how they represent the catchment spatially. These models consider the variability in geology, soil, vegetation and topography, and how they affect flow of water and nutrients in the catchment. Spatially, hydrological models can be divided into lumped models, semi-distributed models, and distributed models (USEPA, 2017; Singh, 2018; Sitterson et al., 2018). Lumped models do not consider spatial variability and consider the catchment as a single homogenous unit (Wheater et al., 2008; Singh, 2018). Semi-distributed models are variations of lumped models, with features of distributed models, in which the input parameters are allowed to vary in space partially by dividing the catchment into several sub-catchments. Distributed models are the most complex because they consider the spatial variability in catchment input parameters (USEPA, 2017; Sitterson et al., 2018). Distributed models divide the model domain into smaller computational elements or cells with each individual element/cell having distinct assigned input parameters (Rinsema, 2014). Distributed models predict the hydrological processes at all computational cells (Singh, 2018). Due to the complexity of distributed models, a large amount of input data is required, and the model can produce the highest accuracy of model results (Singh, 2018).

Rewetting of peatlands increases the water table level (Lundin et al., 2017; Sutikno et al., 2018) and, depending on the topography and nutrient status, may lead to flooding, overland flow, as well as transport of nutrients. The transport of nutrients can be predicted by appropriate water quality models, which can aid in decision making as to which rewetting technique (drain blocking, bunds, etc.) has the least impact on water quality (Loucks & Van Beek, 2017). Water quality models can be classified according to the governing equation (i.e., physically based, conceptual, or empirical), type of solute or dispersed phase (such as nutrients, dissolved organic carbon (DOC), sediments, salts, etc.), area of application (catchment, groundwater, river system, coaster waters, integrated), and spatial analysis (lumped, semi-distributed, or distributed) (Tsakiris & Alexakis, 2012). In addition, nonlinear and empirical models generated using artificial intelligence (AI) techniques have been used in water quality modelling and monitoring (Wu et al., 2014; Khullar & Singh, 2021). These include models based on artificial neural network (ANN), adaptive neuro-fuzzy inference systems (ANFIS), and support vector machines (SVM) (Khullar & Singh, 2021).

Many peatlands comprise a two-layer structure system, with upper and lower layers varying significantly in both structure and functions (Ingram, 1978). The upper thin ($<$0.5 m) layer ("acrotelm") experiences seasonal fluctuations in water saturation, allowing for rapid water movement and litter decomposition. Below this lies the thick ($\gg$1 m) layer ("catotelm") which remains permanently saturated and has significantly slower water flow and peat decomposition rates (several orders of magnitude) compared to the acrotelm (Belyea & Baird, 2006; Ingram, 1978). Peatlands are therefore considered to be 'complex adaptive systems' (CAS), where internal dynamics (autogenic) and external (allogenic) processes control their eco-hydrological interactions (Mozafari et al., 2023). Belyea & Baird (2006) identified four distinctive features of peatlands as characteristic of CAS: spatial heterogeneity, localized flows, self-organizing structure, and nonlinearity. Further to the concept of the diplotelmic (two-layered) peatland model, Morris et al. (2011) proposed the concept of 'hot spots' and 'cold spots' in which the horizontal heterogeneity of peatland is represented. Morris et al. (2011) defined 'hot spots' as zones within the peatland with higher rates of ecological, hydrological and biogeochemical processes compared to the rest of the peatland (i.e 'cold spots', zones that experience slower rate of ecological, hydrological and biogeochemical processes). Successful implementation of models in peatlands requires the model to be spatially detailed, enabling larger scale patterns to develop from the interactions among smaller scale units and external constraints, and forces should be explicitly represented, allowing historical effects to become integrated into the system's physical structure (Belyea & Baird, 2006). Therefore, any hydrological and water quality models selected for the purpose of modelling peat dynamics must consider these key features. Although some models have been used to model both peatland hydrology and water quality, these models may not be specifically designed for peatlands. In addition, the resolution at which these models are applied may be too coarse if applied to peatland catchments, and ecohydrological feedback that operate at smaller scales may be ignored (Baird et al., 2011). It is therefore imperative that existing water quality models are evaluated to ascertain their appropriateness in peatland water quality modelling applications.

The objective of this paper is to review the existing water quality models, focusing on their structure, accuracy and suitability in peatland (especially rewetted peatlands) water quality modelling.

2. Materials and methods

The review process, summarized in Fig. 1, commenced with a systematic search of literature using the PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) (Page et al., 2021) approach as used in Mozafari et al. (2023). The review process was performed in four steps. The first step included the search of string of keywords (*peatland OR bog OR fen OR mire OR (peat AND swamp*)*) within titles, abstracts, and keywords of published work on the Web of Science (WoS) and Scopus databases from January 1, 2003 and December 10, 2023. This step was performed to get the general overview of the work done regarding peatlands over last two decades. The first step returned 59,385 and 25,069 publications from WoS and Scopus, respectively. These publications were screened by limiting the search to only articles published in the English language. This reduced the number of articles to 56,126 and 18,800 from WoS and Scopus, respectively. The second step of further screening included a second string of keywords (in addition to those used in the first step) used within titles, abstracts and keywords of published work: (*peatland OR bog OR fen OR mire OR (peat AND swamp*)) AND (water quality OR nitrogen OR phosphorus* OR carbon* OR ammonium*)*. This step returned 11,798 and 3,395 articles from WoS and Scopus, respectively. The third step added another string of keywords within titles, abstracts and keywords of published works: (*peatland OR bog OR fen OR mire OR (peat AND swamp*)) AND (water quality OR nitrogen OR phosphorus* OR carbon* OR ammonium*) AND (modelling OR model OR simulation)*. This yielded 2,678 and 940 articles from WoS and Scopus, respectively. The fourth step involved manually reviewing the title, abstract and the keywords to select the most relevant and appropriate articles regarding the scope of this paper (i.e., water quality modelling). The fourth step yielded 35 and 29 articles from WoS and Scopus, respectively. These data were combined, and 14 duplicate articles were removed by using Bibliometric package in the R program language, leaving 50 unique published articles. Further screening was performed by limiting the relevant articles to published works that applied water quality models on peatlands only. This produced 23

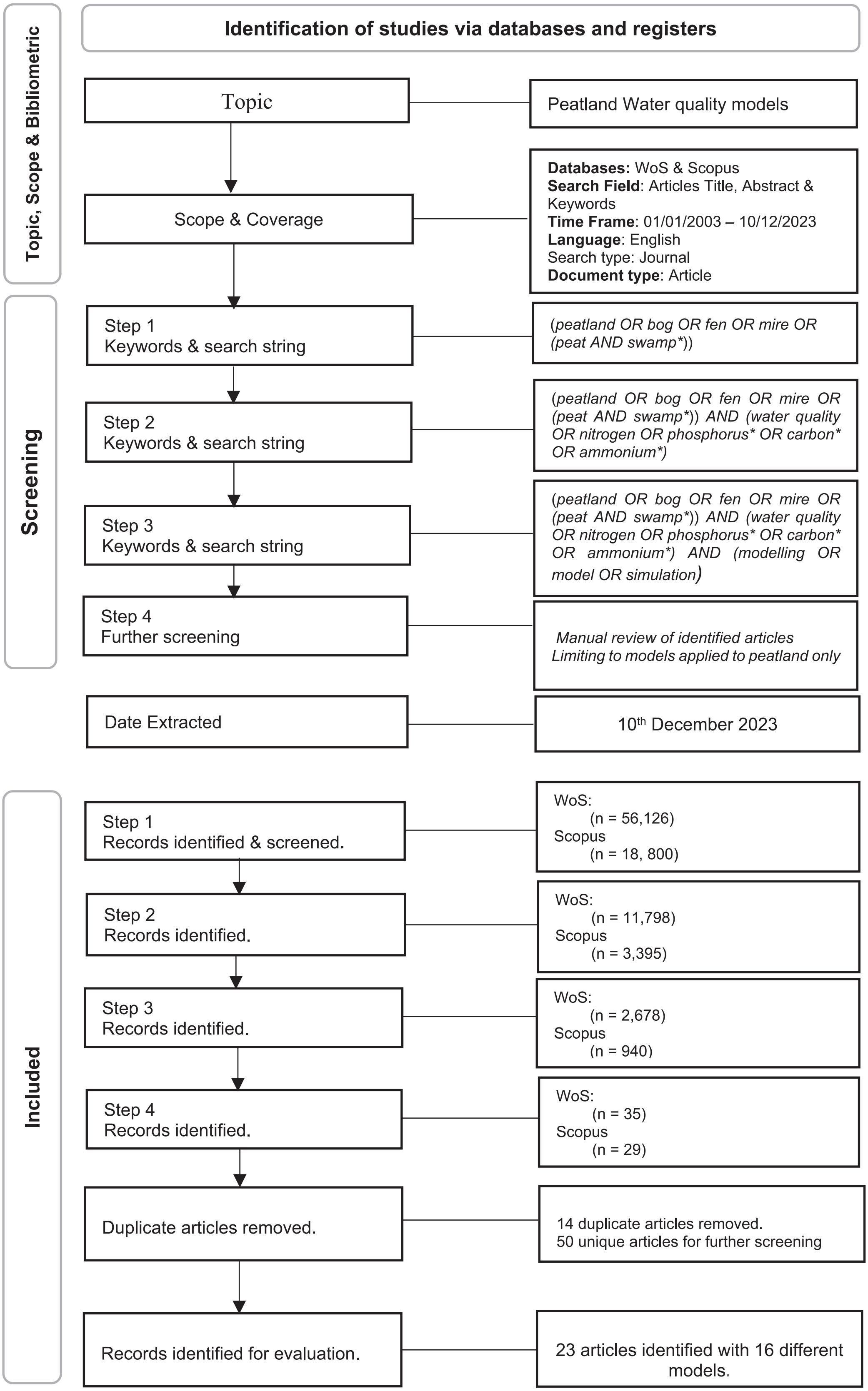

Fig. 1. Summary of the systematic search using the PRISMA approach.

published articles with 16 different water quality models.

2.1. Performance evaluation criteria (PEC) of the computational models

The water quality models are evaluated according to three criteria: (1) performance (2) ability to incorporate the complexity of the peatland, and (3) numerical stability.

2.1.1. Model performance

The most widely used model performance measure (PM) is the statistical performance measure (SPM), which is used to quantify the performance of water quality models in describing the “closeness” of the simulated values to observed data (Moriasi et al., 2015). As no single PM was used across all papers evaluated, in the current paper the following SPMs are used: the coefficient of determination (R^2), root mean square error (*RMSE*), Willmott index of agreement (*d*), Nash-Sutcliffe efficiency (*NSE*), percentage bias (*PBIAS*), and relative error (*RE*). The R^2 describes the degree of collinearity between simulated and observed data. RMSE measures the difference between the predicted and observed values (Moriasi et al., 2015). The index of agreement (*d*) was developed by Willmott (1981) as a standardized measure of the degree of model prediction error (Moriasi et al., 2015). The relative magnitude of the residual variance is determined by NSE (Moriasi et al., 2007). PBIAS is the tendency of the simulated data to be larger or smaller than the observed data (Moriasi et al., 2015). RE is the variance that occurs between the simulated and the observed data expressed in terms of percentages. Table 1 presents the critical values of the performance evaluation criteria.

2.1.2. Ability to incorporate the complexity of the peatland

Processes characterizing peatlands as “complex adaptative systems” must be considered in the application of models in peatlands (Belyea & Baird, 2006). The ability of a model to incorporate the complex characteristics of peat soils was analysed based on how the various models dealt with the spatial heterogeneity of peatlands and how the structure and functions of the acrotelm and catotelm zones of the peat were distinguished from each other.

2.1.3. Numerical stability

Only the models that employ the transport equation (advection/convection–dispersion) to predict nutrient concentration and transport were considered. This is because only the process-based models specifically formulate the particular processes of nutrient transport in peatlands in terms of such as advection, diffusion and dispersion (Khan et al., 2022), by related transport equations. The stability of water quality model depends on the numerical solution method employed in solving the governing transport equations. A numerical solution which does not magnify the errors that appear in the course of numerical solution processes could be considered as stable (Ataie-Ashtiani & Hosseini, 2005).

3. Results and discussion

3.1. Location, scale and type of water quality models

Ninety-six percent of the 23 identified published studies were conducted in Europe and North America (Fig. 2), while the combined peatland area of Europe and North America accounts for an estimated 44.1 % of the global peatland cover (Xu et al., 2018). Although Asia accounts for 38.4 % of the global peatland cover (Xu et al., 2018), there is a dearth of research on peatland water quality modelling in that location. The scale of model application spatially ranges from catchments to laboratory-based simulations, as presented in Table 2. Four of the studies (Jutebring Sterte et al., 2021; Lauren et al., 2021; Whitfield et al., 2010; Xu et al., 2020) were conducted on multiple catchments, two studies (Khan et al., 2022; McCarter et al., 2023) were laboratory-based (miniature peatland) simulations, whilst one study (Yurova et al., 2008) predicted the concentration and fluxes of DOC in mire at laboratory- and catchment-scale. The remaining sixteen studies were conducted on a single catchment.

Although some studies (Harpenslager et al., 2015; Lundin et al., 2017; Zak & Gelbrecht, 2007) have reported observations of high nutrient concentrations in water in the early stages of rewetting or restoration of degraded peatlands, little research has been carried out on the modelling of water quality in rewetted peatlands. Among the identified published studies in this review, only one study (Grygoruk et al., 2015) applied water quality model to a rewetted peatland (fen) in Poland, in which the temporal pattern of potential groundwater and surface water eutrophication was predicted.

Among the 23 published studies, 16 different water quality models were identified. With regards to model type, in terms of the type of governing equations and related assumptions, 15 of the water quality models are process-based models and 1 model is a conceptual model. On the basis of spatial properties, 12 of the water quality models are distributed models, 3 are semi-distributed models, and 1 is a lumped model (Table 2). The most widely used water quality models for predicting the concentration and export of nutrients on peatlands are the Integrated Catchments model (INCA) and HYDRUS 1D/2D (Table 2). INCA is a family of process-based and semi-distributed models comprising an integrated catchment model for carbon (INCA-C) (Futter

Table 1
Performance evaluation criteria using R^2, NSE and PBIAS (adapted from Moriasi et al. (2015)) at catchment-scale (>10 ha) and field-scale (<10 ha) RE (adapted from Ali & Abustan (2014)).

Metric	Range	Output variable	Performance evaluation criteria			
Catchment-scale			Very good	Good	Satisfactory	Not satisfactory
R^2	0.0 to 1.0	Sediment	>0.80	$0.65 < R^2 \leq 0.80$	$0.40 < R^2 \leq 0.65$	$R^2 \leq 0.4$
			>0.7	$0.6 < R^2 \leq 0.70$	$0.30 < R^2 \leq 0.60$	$R^2 \leq 0.3$
		Nutrients				
NSE	$-\infty$ to 1.0	Sediment	>0.8	$0.7 < NSE \leq 0.80$	$0.45 < NSE \leq 0.70$	$NSE \leq 0.45$
		Nutrients	>0.65	$0.5 < NSE \leq 0.65$	$0.35 < NSE \leq 0.50$	$NSE \leq 0.35$
PBIAS (%)	$-\infty$ to ∞	Sediment	$<\pm10$	$\pm10 \leq PBIAS<\pm15$	$\pm15 \leq PBIAS<\pm20$	$PBIAS\geq\pm20$
		Nutrients	$<\pm15$	$\pm15 \leq PBIAS<\pm20$	$\pm20 \leq PBIAS<\pm30$	$PBIAS\geq\pm30$
RMSE[1]	0.0 to ∞	–	≤ 0.09	–	$0.09 < RMSE \leq 0.7$	–
d[1]	0.0 to 1.0	Nutrients	–	$d \geq 0.75$	$0.75 > d \geq 0.6$	$d < 0.6$
RE (%)	0.0 to ∞	All data	≤ 10	$10 < RE \leq 20$	$20 < RE \leq 25$	$RE > 25$
Field-scale						
R^2	0.0 to 1.0	All data	>0.85	$0.75 < R^2 \leq 0.85$	$0.70 < R^2 \leq 0.75$	$R^2 \leq 0.70$

[1] No PEC has been developed for RMSE and *d* due to lack of available data. We therefore adopted the recommendation values of Moriasi et al. (2007) for RMSE and Moriasi et al. (2015) for *d*.

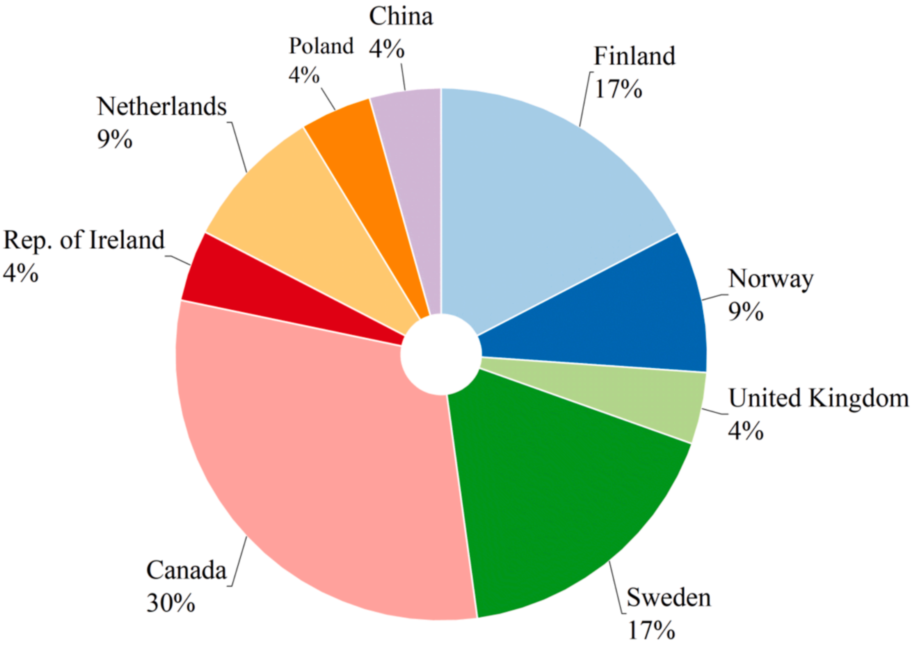

Fig. 2. Global distribution of water quality modelling studies on peatlands using water quality models.

et al., 2007), nitrogen (INCA-N) (Wade et al., 2002) and phosphorus (INCA-P) (Crossman et al., 2021). Its frequent application in water quality simulations may be attributed to its ability to use biogeochemical processes to formulate the production, concentration and export of nutrients in catchments. The HYDRUS 1D/2D model (Šimůnek et al., 2012) was used in four research studies to simulate the concentration and transport of nutrients in peatlands. The HYDRUS 1D/2D model considers ecological processes like evapotranspiration and root zone water uptake, but these mechanisms are solely reliant on hydrology, not biogeochemical processes in the modelling.

3.2. *Simulated water quality parameters*

Fig. 3 shows the linkage between the water quality parameters and the models used in the studies. Dissolved organic carbon was modelled in eight studies on peatlands, followed by ammonium (NH_4^+) (5 studies), nitrate (NO_3^-) (5 studies) and phosphorus (3 studies). At least two studies modelled parameters like sulphur, nitrogen, copper and sediments. The ubiquity of studies modelling the DOC is unsurprising in peat catchments, particularly as its presence has been linked to the occurrence to trihalomethanes in water treatment plants (Ferretto et al., 2021; Kumari & Gupta, 2022). HYDRUS 1D/2D was applied to simulate most of the water quality parameters (7 parameters), followed by INCA group of models (6 parameters), MIKE-SHE (4 parameters), PEATBOG (3 parameters), CTRAN/W (3 parameters) and NutSpaFHy (2 parameters).

3.3. *Identified water quality models*

The sixteen (16) identified water quality models can be grouped into three categories (Table 3): eco-hydrological water quality models, semi eco-hydrological water quality models, and hydrological water quality models, based on how they characterise the nutrient production and how they link the nutrient production to the nutrient transport.

3.3.1. *Eco-hydrological water quality models*

Eight of the identified models, as presented in Table 3, are classified as ecohydrological models, because they link ecological and hydrological processes and consider the interactions between water resources and ecosystems that affect nutrient production, concentration and export (Chen et al., 2019). These models predict concentration and export of nutrients and consider the biogeochemical processes outside and within soil that create the nutrients (Fig. 4). Common features observed among these models are the mathematical formulation of nutrient transformation in the soil as well as the ground and surface water flow, which are modelled using a series of first-order differential equations. Separate independent hydrological models are needed to provide the hydrological properties as inputs to the eco-hydrological water quality models. For example, the INCA models rely on rainfall-runoff modelling toolkits like PERSiST (Precipitation, Evapotranspiration, and Runoff Simulator for Solute Transport) for hydrological input data, as employed in the studies of de Wit et al. (2016) and Xu et al. (2020), or rely on the HBV rainfall-runoff model as applied in the study of Oni et al. (2014).

Other models categorized under eco-hydrological water quality models have internal sub-models to generate the required hydrological inputs to predict the nutrient production, concentrations and export. The PEATBOG model has an environment sub-model that generates daily water table depth (Wu & Blodau, 2013). McGill Wetland Model (MWMmic) depends external hydrological model for hydrological input data to simulate DOC concentration and export bases on biogeochemical processes within the peatland ecosystem (Shao et al., 2022). The Eco-HAT and NutSpaFHY models have internal sub-models that generate the hydrological input for nutrient production and export, as observed in the studies of Wang et al. (2016a), Wang et al. (2016b) and Lauren et al. (2021). The LPJ-GUESS model incorporates a catchment-distributed hydrology to simulate cell-to-cell lateral water movement, which is used in DOC routing within the catchment (Tang et al., 2018). The MAGIC model, based on biogeochemical processes within soil, predicts the acidification of groundwater in catchments (Cosby et al., 2001). This model has a simple hydrology sub-module that predicts the water table level in soil based on precipitation and evapotranspiration (Hinderer et al., 1997).

3.3.2. *Semi eco-hydrological water quality model*

In the category of semi eco-hydrological water quality model, the three models (MIKE-SHE, HYDRUS 1D/2D, and HydroGeoSphere) could be regarded as a particular type of hydrological water quality model that is designed in such a way that it is able to account for ecological processes such as evapotranspiration and root water uptake by plants. These mechanisms do not consider any biogeochemical processes as observed in eco-hydrological water quality models. Solute concentration and

Table 2
Summary of published studies which applied water quality models to peatlands between January 1, 2003 and December 10, 2023.

No.	Model type	Model spatial property	Model name	Location[1]	Area	Peatland type applied/ Catchment	Rewetted peatland	Simulated process (variable)	Reference[2]
1	Conceptual models	Semi-distributed	NutSpaFHy	Finland	31 to 1966 ha	Peatland	No	Nutrient concentration and transport (N & P)	Lauren et al. (2021)[3]
2	Physical/ process-based model	Semi-distributed	INCA-N	Finland	3160 km^2	Peatland	No	Hydrology, Solute transport, Nutrient (DON, NH_4, NO_3 P & sediment concentration)	Rankinen et al. (2023)
3		Semi-distributed	INCA-C	Norway	2.1 km^2	Peatland (ombrotrophic raised bog)	No	Export of DO, DOC concentration and stream discharge	de Wit et al. (2016)
4		Semi-distributed	INCA-C	UK	235 km^2 to 4010 km^2(9 catchments)	Peatland	No	Hydrology, solute transport & DOC	Xu et al. (2020)[3]
5		Semi-distributed	INCA-C	Sweden	50 ha	Peatland (mire)	No	DOC transport, DOC concentration & runoff	Oni et al. (2014)
6		Semi-distributed	INCA-N	Finland	3160 km^2	Peatland forest	No	NO_3-N, & NH_4-N concentration	Rankinen et al. (2006)
7		Distributed model	LPJ-GUESS	Sweden	16 km^2	Peatland	No	DOC transport	Tang et al. (2018)
8		Distributed model	MODFLOW-SURFACT	Canada	2.2 ha	Peatland (Fen)	No	Hydrology and solute transport (Na^+)	Sutton & Price (2022)
9		Distributed model	MODPATH	Poland	3000 ha	Peatland (Fen)	Yes	Nutrient (Phosphate) and solute transport	Grygoruk et al. (2015)
10		Distributed model	HYDRUS2D	The Netherlands	16000 m^2	Peat soil	No	Groundwater flow, heat transport & solute (N, P, Cl) transport	Van Beek et al. (2007)
11		Distributed model	HYDRUS-CWM1	Finland	0.19 m^2	Peatland (peat base pilot wetland)	No	Hydrology, reactive solute transport (Sulfur, Nitrite, Nitrate & Ammonium)	Khan et al. (2022)[4]
12		Distributed model	HYDRUS-1D	Canada	900 cm^2	Peatland (sphagnum)	No	Solute (Ni & Cu) transport	McCarter et al. (2023)[4]
13		Distributed model	HYDRUS2D	The Netherlands	1160 ha	Peatland (sphagnum)	No	Solute (EC) transport	Dekker et al. (2005)
14		Distributed model	PEATBOG	Canada	28 km^2	Peatland (ombrotrophic Bog)	No	NH_4^+, NO_3^-, DOC	Wu & Blodau (2013)
15		Distributed model	PEATBOG	Canada	28 km^2	Peatland (ombrotrophic Bog)	No	NH_4^+, NO_3^-, DOC	Wu & Blodau (2015)
16		Distributed model	Mike SHE	Sweden	0.5 to 69.7 km^2	Peatland (mire)	No	Hydrology & solute transport (Mg, K, Ca, Na)	Jutebring Sterte et al. (2021)[3]
17		Distributed model	Eco-HAT-P	China	108, 900 km^2	Peatland	No	Nutrient (Total Phosphorus transport)	Wang et al. (2016)
18		Distributed model	GEOtop	Ireland	15 km^2	Catchment (Peat)	No	Soil erosion and sediment transport	Zi et al. (2016)
19		Distributed model	HydroGeoSphere	Canada	8.4 km^2	Peatland	No	Hydrology and solute transport (Cl)	Nagare et al. (2022)
20		Distributed model	CTRAN/W	Norway	2.7 ha	Peatland	No	Solute transport (Pb, Cu, Sb)	Okkenhaug et al. (2018)
21		Distributed model	MMWH	Sweden	Lab & field scale	Mire	No	DOC and solute transport	Yurova et al. (2008)
22		Distributed model	MWMmic	Canada	28 km^2	Peatland (ombrotrophic Bog)	No	DOC	Shao et al. (2022)
23		Lumped model	MAGIC	Canada	5.1 km^2 & 9.6 km^2 (2 catchments)	Peatland (Boreal plains	No	Hydrology and solute (S & N) transport	Whitfield et al. (2010)[3]

[1] Location refers to where the model was applied in the published study, but not the origin of the model.
[2] The reference refers to the article in which the model was used, but not the original reference for the model creator.
[3] Studies conducted on multiple catchments.
[4] Laboratory-based simulation (miniature peatland).

transport are formulated either by using advection–dispersion or convection–dispersion (when both heat and solute are considered in governing equation) transport equations (Fig. 4). Compared to eco-hydrological models, all the models in this category have internal sub-models that calculate the hydrological properties of use as inputs required for solute transport. The MIKE-SHE model predicts groundwater and surface water flows using topography, vegetation, soil properties and time-varying climate inputs, and the modelling results of flow are used to facilitate the calculation of solute transport due to advection–dispersion (Jutebring Sterte et al., 2021). Evapotranspiration processes and root water uptake by plants are represented in the groundwater flow equation in the model (MIKE SHE, 2024). Similarly,

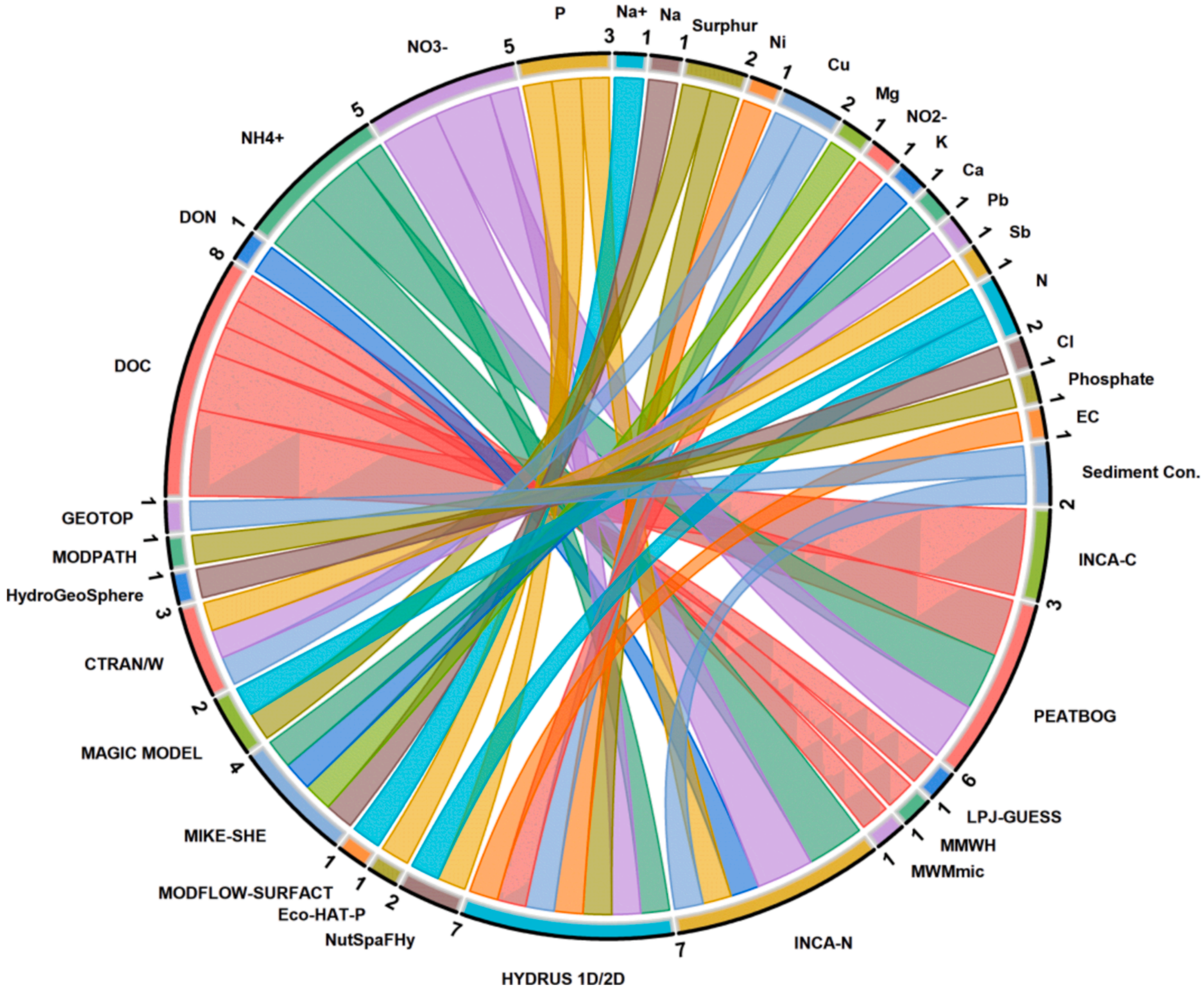

Fig. 3. The computational models (bottom of the circle) and the corresponding water quality parameters (top of the circle) that they can predict. The number at the end of an arc beside the name of a corresponding water quality parameter represents the number of studies that predicted such parameter. The number at the end of an arc beside the name of a computational model represents the cumulative number of published studies that used the model.

HydroGeoSphere (Therrien & Sudicky, 2010) also applies advection–dispersion to simulate solute transport and considers the process of evapotranspiration. HydroGeoSphere is a 3D coupled water and solute transport model that is capable of modelling ground freeze–thaw processes (Nagare et al., 2022). The HYDRUS 1D/2D model program is a finite element model for predicting the movement of water, heat transfer, and transport of multiple solutes in variably saturated media (Van Beek et al., 2007) by using convection–dispersion equation (CDE) for simulation of solute transport (Khan et al., 2022). The HYDRUS 1D/2D model also includes a nutrient uptake model that accounts for the passive nutrient uptake rate by plants roots.

3.3.3. Hydrological water quality models

The hydrological water quality models (GEOTOP, MMHW, MODFLOW-SURFACT, MODPATH, CTRAN/W) employ either the advection–dispersion or convection–dispersion equation for solute concentration and transport process prediction, except for GEOTOP which couples the continuity equation to a kinematic wave approximation of the Saint-Venant equation to formulate the sediment transport process. Unlike semi eco-hydrological water quality models, hydrological water quality models do not consider the effect of any environmental processes such as evapotranspiration and root water uptake in the groundwater flow process. With the exception of the GEOTOP and MMHW models, the other three models in this category are sub-models of a parent hydrological model that uses groundwater inputs to simulate the process of solute transport. For instance, MODFLOW-SURFACT and MODPATH are sub-modules of the MODFLOW groundwater flow model. Contaminant transport is simulated based on groundwater flow calculated by MODFLOW. In a similar process, CTRAN/W simulates the transport of contaminants based on the flow calculated by the Seep/W groundwater flow model. MODFLOW-SURFACT is capable of simulating flow and contaminant transport in both saturated and unsaturated zones (Panday & Huyakorn, 2008; Sutton & Price, 2022). The MMHW model simulates the concentration and transport of DOC using the convection–dispersion equation. The model incorporates terms that account for the adsorption–desorption, as well as microbial production and mineralization of DOC.

3.4. Performance of identified water quality models

3.4.1. Performance of eco-hydrological water quality models

The performances of most of the eco-hydrological water quality

Table 3
Summary of the backgrounds and application of water quality models.

Categories	Models	Model background and application	Common features
Eco-hydrological water quality models	INCA-C	• Runoff generation/hydrological processes by separate or independent hydrological model (e.g., PERiST and HBV and WSFS). Catchment/terrestrial carbon/nutrient processes (e.g., decomposition of organic matter from litter fall, root breakdown, denitrification and nitrification). In-stream or river processes of DOC/N (e.g., advective fluxes in the soil are modelled as the flow of water multiplied by the concentration of DOC or DIC; advective inflows are equal to the flow from the upstream reach multiplied by the concentration of material in the upstream reach).	Simulation of nutrient concentration is by biogeochemical processes in the soil such as decomposition of organic matter from litter fall. Models can simulate the impact of climate on biogeochemical processes. Mathematical formulation of nutrient transformation in the soil, ground and surface waters are modelled as a series of first-order differential equations. Most of these models depend on independent models for hydrological inputs.
	INCA-N		
	PEATBOG	This model has four sub-models: Environment sub-model (simulates water table depth (WTD), soil temperatures, moisture, O_2 profile). Vegetation sub-model (daily gross primary production, autotrophic respiration, biomass and litter production). Soil organic matter sub-model (daily heterotrophic respiration, sequestration of C and N decomposition). Dissolved C and N sub-model (CO_2, CH_4, N_2O, DIN, DOC, DON concentration and export)	
	MAGIC MODEL	Atmosphere Deposition of ions from the atmosphere (wet plus dry deposition) Litter fall and other organic sources Soil water Biological production, removal and transformation of ions. Internal sources and sinks of ions from weathering or precipitation reactions. Denitrification, nitrification Stream water Discharge volumes and flow routing within the catchment.	
	LPJ-GUESS	• Catchment distributed hydrology incorporated to simulate cell to cell lateral water movement. DOC production (microbial decomposition). Sorption and desorption of DOC. DOC export within the catchment.	
	NutSpaFHy	• Hydrological sub-model simulates WTD, root layer water content. The development and growth stage determines the nutrient uptake by ground vegetation and nutrient lost in litter fall. The nutrient balance module keeps account of total nutrient storage and nutrient concentration in the root layer. Nutrient export module moves N and P in groundwater and in surface runoff to the receiving water body, keeping track of N and P storage and concentration.	
	EcoHAT-P	• Hydrological input from another hydrological model (e.g., SWAT). Nutrient cycle. Plant growth.	
	MWMmic	• Runoff generation/hydrological processes by separate or independent hydrological model (e.g. CLASS3W (Canadian Land Surface Scheme)) Vegetation phenology Autotrophic repiration Peat decomposition DOC flux	
Semi eco-hydrological water quality models	MIKE-SHE	• Simulate groundwater flow using 3D Darcy flow equation. Water quality module simulates solute transport using advection–dispersion equation. The model can simulate the effect of climate, vegetation and landscape on hydrological and water quality processes.	They can predict solute transport using advection–dispersion equation or convection–dispersion equation. Models can account for some ecological processes such as evapotranspiration and root water uptake in GW flow processes.
	HYDRUS 1D/2D	• Uses Richards equation to predict saturated–unsaturated water flow. Convection-dispersion equation for heat and solute transport. The flow equation incorporates a "sink" term to account for water uptake by plant roots.	
	HydroGeoSphere	• Modified form of Richards' equation is used to describe three-dimensional transient subsurface flow in a variably saturated porous medium. Uses advection–dispersion equation to simulate solute transport. Accounts for evapotranspiration.	
	GEOTOP	• Kinematic wave approximation of the Saint-Venant equation is used to simulate overland flow. Overland flow equation is coupled to continuity equation to simulate sediment transport.	• Solute transport simulated using advection–dispersion or convection–dispersion equations. Solute concentration is simulated based on changes in groundwater level, soil dispersivity and molecular

(*continued on next page*)

Table 3 (*continued*)

Categories	Models	Model background and application	Common features
Hydrological water quality models	CTRAN/W	- Groundwater flow is simulated by a different model, Seep/W. CTRAN/W simulates the transport of contaminants (based on the flow calculated by Seep/W) using advection–dispersion equation.	diffusion. Models depend on other models for simulated groundwater flow
	MMWH	Sorption Predicts the adsorption of soluble organic matter to, and its desorption from solid organic matter. Sorption plays a key role in controlling the DOC concentration in pore water. Microbial DOC transformation by microorganism. Hydrology Prediction of DOC concentration in pore water using the convection–dispersion equation.	
	MODFLOW-SURFACT	- Groundwater flow is predicted by MODFLOW MODFLOW-SURFACT simulates the transport of contaminants (based on the flow calculated by MODFLOW) using advection–dispersion equation.	
	MODPATH	- Groundwater flow is predicted by MODFLOW. MODPATH predicts the transport of contaminants (based on the flow calculated by MODFLOW) using advection–dispersion equation.	

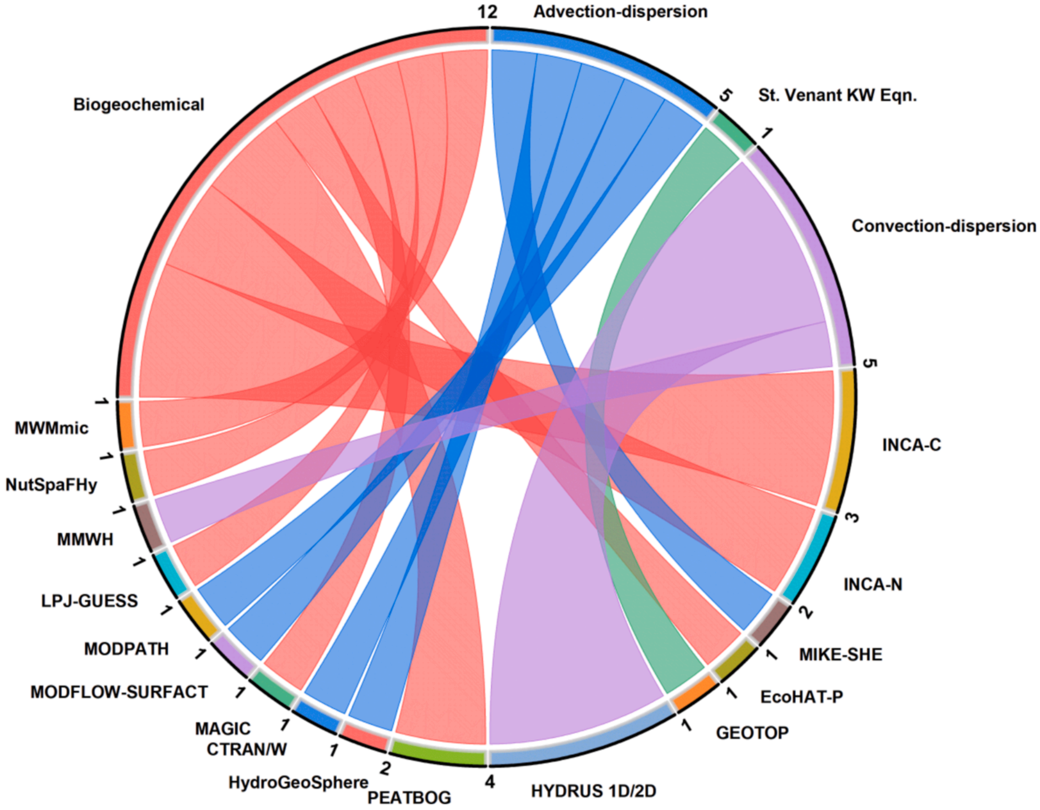

Fig. 4. Computational models (bottom of the circle) and the modelling methods (top of the circle) they employ for predicting the concentration and transport of nutrients. The number at the end of an arc beside the name of a computational model indicates the number of studies that applied that computational model. The number at the end of an arc beside the name of a modelling method indicates the number of studies that used that modelling method.

models were above satisfactory (Table 4). The apparent contradiction between the ability of INCA-N to model nitrogen species in the studies of Rankinen et al. (2006) (where the results were satisfactory) and Rankinen et al. (2023) (where the results were not satisfactory), which were conducted on the same catchment but during different periods, may suggest there existed processes such as nitrogen uptake of aquatic plants during the growing season which are not accounted for in the INCA-N model. This fact was confirmed by Jarvie et al. (2002), who concluded that this missing process in INCA model is the reason for occasional inaccurate estimation of NO_3^- as observed in their research study.

The performance of INCA-C model in simulating DOC in all three studies (de Wit et al., 2016; Oni et al., 2014; Xu et al., 2020) was satisfactory or above satisfactory. All the study sites were well monitored and pristine peatlands. This suggests the performance of water quality models may be affected by anthropogenic activities, especially if these activities are not considered in the modelling processes. Proper consideration of these processes in water quality modelling for peatlands could improve the model performance in predicting the nutrient concentrations and transport processes in peatlands.

Table 4
Summary of the results of performance evaluation of the water quality models.

No.	Category	Model	Nutrient	Measure	Performance	Reference
1		INCA-C	DOC	R^2 (0.85)	Very good	de Wit et al. (2016)
2		INCA-C	DOC	R^2 (0.38 – 0.69)[1]	Good	Xu et al. (2020)
3			NO_3^-	PBIAS (3.38)	Very good	
			NH_4^+	PBIAS (60.3)	Not satisfactory	
			ON	R^2 (0.1)	Not satisfactory	Rankinen et al. (2023)
		INCA-N	Susp. Sed	R^2 (0.07)	Not satisfactory	
			TP	PBIAS (64.5)	Not satisfactory	
4			NH_4^+	NSE (0.472)	Satisfactory	Rankinen et al. (2006)
		INCA-N	NO_3^-	NSE (0.809)	Very good	
5		INCA-C	DOC	NSE (0.49)	Satisfactory	Oni et al. (2014)
6		EcoHAT-P	P	R^2 (0.661)	Good	Wang et al. (2016a), Wang et al. (2016b)
7		NutSpaFHy	N	RMSE (0.076)	Very good	Lauren et al. (2021)
			P	RMSE (0.037)	Very good	
			NH_4^+	RE (−4.90 %)	Very good	
	Eco-hydrological water quality model[2]		NO_3^-	RE (3.94 %)	Very good	
			SO_4^{2-}	RE (−0.83 %)	Very good	
		MAGIC MODEL	Ca	RE (0.05 %)	Very good	
8			Na	RE (0.15 %)	Very good	Whitfield et al. (2010)
			K	RE (0.73 %)	Very good	
			Mg	RE (0.18 %)	Very good	
9		PEATBOG	(NH_4^+, NO_3^-)	R^2 (0.88)	Very good	Wu & Blodau (2015)
			DOC	R^2 (0.77)	Very good	
10			Mg	R^2 (0.9)	Very good	
			K	R^2 (0.86)	Very good	
		MIKE SHE	Ca	R^2 (0.75)	Very good	Jutebring Sterte et al. (2021)
			Na	R^2 (0.79)	Very good	
11		HYDRUS 1D/2D	($NO_3^- + NO_2^-$)	R^2 (0.43)	Not satisfactory	Khan et al. (2022)
	Semi eco-hydrological water quality model[3]		NH_4^+	R^2 (0.25)	Not satisfactory	
12		HYDRUS 1D/2D	Cl	R^2 (0.74)	Good	Van Beek et al. (2007)
13		HYDRUS 1D/2D	EC	R^2 (0.64)	Good	Dekker et al. (2005)
14		[5]MODPATH	PO_4^-	R^2 (0.86)	Very good	Grygoruk et al. (2015)
15		GEOTOP	Sediment	R^2 (0.79)	Good	Zi et al. (2016)
16	Hydrological water quality model[4]	[6]MODFLOW-SURFACT	Na	RMSE (0.07)	Very good	Sutton & Price (2022)
17		MMHW	DOC	*d* (0.7)	Good	Yurova et al. (2008)

[1] The study was conducted on multiple catchments and the performances were measured for each catchments and R^2 values obtained lies between the range indicated.

[2] Two studies (Tang et al., 2018; Wu & Blodau, 2013) did not report on the performances of LPJ-GUESS and PEATBOG, respectively, under in the category of eco-hydrological water quality models.

[2] Shao et al. (2022) did not report on the performance of the performance of MWMmic in simulation DOC flux based on the performance indicators.

[3] Nagare et al. (2022) and McCarter et al. (2023) did not report on the performances of HydroGeoSphere and HYDRUS-1D, respectively, under in the category of semi eco-hydrological water quality models.

[4] Okkenhaug et al. (2018) did not report on the performance of CTRAN/W model in the category of hydrological water quality models.

[5,6] The model performances in these studies are with regards to prediction of water table levels but not nutrient concentration. Futher discussion on this is in section 3.4.3.

3.4.2. *Performance of semi eco-hydrological models*

MIKE-SHE has been used successfully to model Mg, K, Ca and Na in a catchment comprising a mixture of peat mire, silty sediments, sandy sediments and till (Jutebring Sterte et al., 2021). However, unlike nitrogen, these elements are not affected by biogeochemical processes within the peat soils. The model accuracy is impacted by the spatial resolution of the computational grid, with a fine resolution improving its accuracy (Vázquez. et al., 2002; Ali et al., 2007; Rujner et al., 2018). It is robust and insensitive to spatial variation of soil properties when a fine computational grid is employed (Rujner et al., 2018). The computational grid resolutions used in the studies (Ali et al., 2007; Vázquez. et al., 2002) and the technical reference documents of MIKE SHE (2024) range from 1200 m to 50 m in terms of the cell size, which may imply it may be too coarse for the modelling of peatlands.

The HYDRUS 1D/2D model was used to predict the concentration of NH_4^+ and $NO_3^- + NO_2^-$ in unfrozen peatland conditions (on a fields scale i.e. < 10 ha) (Khan et al., 2022), but had poor results: $R^2 = 0.25$ for the prediction of NH_4^+ and $R^2 = 0.43$ for the prediction of $NO_3^- + NO_2^-$. This could be attributed to several factors such as exclusion/underestimation of (1) nitrification or denitrification processes (2) the pH of the peat soil, which plays significant role in nitrogen transformation (Wang et al., 2019), and (3) adsorption/desorption of NH_4^+ by peat soil. These processes have been confirmed to be major contributing factors for variances in nutrient concentration and fluxes (Yurova et al., 2008;Tang et al., 2018).

The ability of HYDRUS 1D/2D in considering the complex nature of peatland soil characteristics was demonstrated by Dekker et al. (2005), where the computational grid resolution was 0.25 m and the model performance in predicting the concentration of nutrient in the form of electrical conductivity (EC) was “good” ($R^2 = 0.64$). In this study, the spatial heterogeneity of peatland characteristics was accounted for by considering the hydraulic properties that vary in the three dimensions in the peat soil. The underlying organic muck layer was distinguished from the surface floating fen in the study (Dekker et al., 2005). This characterisation of peat properties illustrates the ability of HYDRUS 1D/2D model to consider the spatial heterogeneity of peatland.

3.4.3. *Performance of hydrological water quality models*

The performances of MODPATH ($R^2 = 0.86$) (Grygoruk et al., 2015) and MODFLOW-SURFACT (RMSE = 0.07) (Sutton & Price, 2022) were “very good”. Although the performance of these models was considered to be “very good”, there is concern regarding their suitability in peatland application. For example, the MODPATH model and MODFLOW-SURFACT model both need to get inputs from the MODFLOW model regarding the groundwater flow. According to Baird et al. (2011), the MODFLOW model was not designed for conditions such as those observed in the upper layers of peat bogs where the hydraulic conductivity, *K*, may vary vertically and horizontally by more than two orders of magnitude over a short distance. This may cause MODFLOW to become unstable. In a situation when MODFLOW was used for peatland application, a lumped value of *K* was assigned to the upper layers of the peat (Reeve et al., 1999), which may lead to inaccurate outputs of groundwater flow rates and water table, which could subsequently affect the modelling results of water quality.

The Mixed Mire Heat and Water (MMHW) model is specifically designed for mire (peat) to predict the DOC concentration and transport. Soluble organic carbon is represented in mires in two states (DOC and sorbed potentially soluble but currently solid carbon) (Yurova et al., 2008). This model considers how DOC is generated and consumed in a mire ecosystem. These processes are all included in the transport equation employed in this model. Yurova et al. (2008) applied a MMHW model to predict the concentration and transport process of DOC in a boreal stream draining a mire. The model performance at catchment-scale was "good". However, modification to the model needs to be done if the model is intended to be used to predict the concentration of other nutrients (such as NH_4^+, NO_3^-, nitrite and phosphate).

GEOTOP focuses on the mass and energy balance of the hydrological cycle, which can be used to simulate continuum in small catchments (Rigon et al., 2006; Zi et al., 2016). A kinematic wave approximation of Saint-Venant equation is used to simulate the overland flow, which is then coupled with the continuity equation to calculate the sediment concentration. The model performance in simulating suspended sediment concentration in a catchment composed of peaty gley and podzol soils was considered to be "good" (Zi et al., 2016). This model in its current state is not suitable for application in the peatland nutrient simulation, unless major modifications are made to it.

3.5. *Numerical stability of the identified water quality models*

The governing transport equation for predicting the solute transport process within the saturated zone of soil takes the form (Loucks & Van Beek, 2017):

$$\frac{\partial C}{\partial t} = -\left[v_x\frac{\partial C}{\partial x} + v_y\frac{\partial C}{\partial y} + v_z\frac{\partial C}{\partial z}\right] + D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2} + s + f_R \qquad (1)$$

where D_x, D_y and D_z are dispersion coefficient in x, y and z directions (m^2/day); v_x, v_y and v_z are groundwater fluxes in x, y and z directions (m/day); *C is* solute concentration (mg/L) and *t* is time (day). *S* is the source term which can represent discharge or waste-loads or additional inflow mass. f_R is the reaction term that represents physical processes, biochemical processes and chemical reactions. Depending on the context, this transport equation can be referred to as either an advection–dispersion equation or a convection–dispersion equation. Artificial oscillation is one of the causes of instability in numerical solution, especially where a sharp concentration is present in advection dominated processes (Ataie-Ashtiani & Hosseini, 2005). In order to circumvent numerical instability problems, different numerical techniques have been employed in the water quality models to solve the governing equations. Moreover, depending on the water quality parameters of interest, some models have included corresponding extra terms in the transport equation to account for processes such as decay or production rate of nutrients, plants and microbial absorption, desorption and adsorption of nutrients by the soil matrix.

In MIKE SHE, the advection–dispersion transport equation is numerically solved using the QUICKEST (Quadratic Upstream Interpolation for Convection Kinematics with Estimated Streaming Terms) method, which applies upstream differencing for the advection term and central differencing for the dispersion term. It minimizes numerical instability when relatively steep concentration fronts are being simulated (MIKE SHE, 2024). The model also takes the source or the sink term into account, which can reflect the influence of adding solute in a peatland due to, for example, the inflow of water. With regards to other processes such as biochemical and chemical reactions, the MIKE SHE incorporates MIKE ECO lab, a general equation solver for any kinetic reaction process. Despite the robustness and versatility of MIKE SHE, researchers have encountered significant challenges when applying it in a peatland context. Similar to MODFLOW, the configuration of MIKE SHE is not well-suited for the specific conditions observed in the near-surface layer of peatlands. Friedrich et al. (2024) used MIKE SHE to assess rewetting scenarios on a partially restored raised bog, but could not implement the thin acrotelm saturated zone peat layer with a higher horizontal and vertical hydraulic conductivity. To avoid numerical instability, they simplified the model by treating the upper layer as one larger average layer. This is one of the shortcomings of the MIKE SHE in peatland applications, which may result in inaccurate hydrological input data for solute transport modelling.

In the HYDRUS 1D/2D model, the solute transport equation considers the convective–dispersive transport in the liquid phase, as well as the diffusion process in the gas phase (Šimůnek et al., 2012). The governing transport equation is numerically solved using the Galerkin finite element method (Šimůnek et al., 2012). Like MIKE SHE, the HYDRUS 1D/2D model also uses the upstream weighing formulation to prevent numerical oscillations in situations where convection transport is dominant. Adsorption-desorption processes are considered in the mathematical formulation of the transport equation. First order decay reactions are included in the solute transport equation to account for nitrification/denitrification processes. Although not originally designed for peatlands, HYDRUS 1D/2D has been adapted for modelling solute transport in such ecosystems, as demonstrated by Khan et al. (2022) and Dekker et al. (2005). While Dekker et al. (2005) did not report any substantial challenges with HYDRUS 1D/2D, Khan et al. (2022) assessed the model's performance under varying climatic conditions (frost and without frost) and noted discrepancies between simulated and observed flow processes. These discrepancies were attributed to the inherent heterogeneity and unique layering structure of peatlands. This highlights the limitations of HYDRUS 1D/2D in accurately representing the CAS characteristic of peatland environments.

The four models, MODPATH, MODFLOW-SURFACT, CTRAN/W and HydroGeoSphere, employ the advection–dispersion solute transport equation while employing the appropriate term in the transport equation to formulate the decay, adsorption and desorption of solutes. The major difference between these four water quality models is the how the solute transport equation is numerically solved and the stability of the numerical scheme. Three of the models (MODPATH, MODFLOW-SURFACT and HydroGeoSphere) apply a finite-difference method to discretise the solute transport equation, while CTRAN/W employs a finite element method. With regards to stability, finite difference/element method has a problem of truncation error. To improve the stability of model, the MODFLOW-SURFACT and HydroGeoSphere models discretized the advection term using mass conservative second-order total variation diminishing (TVD) scheme which applies the upstream weighing formulation to minimize the numerical dispersion (Panday & Huyakorn, 2008; Therrien & Sudicky, 2010). The TVD method applied to the advective term ensures a physically correct solution without oscillation even for totally advective dominant transport process (Panday & Huyakorn, 2008). However, HydroGeoSphere was not purposely designed for peatland applications and therefore has some limitations. For example, due to the inability of HydroGeoSphere to incorporate a heterogeneous peat structure, Autio et al. (2020) modelled the peat as a simple homogeneous layer of uniform thickness. Spatial variability of peat properties, which has been consistently observed in many studies (Li et al., 2019; Baird et al., 2008; Lewis et al., 2012), may be neglected as a result of this simplification. Consequently, this approach may ignore the impact of spatial variability on hydrological and water quality modelling in peatlands.

The CTRAN/W (GEO-SLOPE, 2012) and MODPATH (Hanson et al., 2013) models employ a different approach to deal with numerical instability by having an option to simulate the purely advective solute transport process using a particle tracking method. In this method, the effect of dispersion, adsorption and decay is not considered. Solute dilution, caused by dispersion, is a very significant component of solute transport; ignoring it can lead to inaccurate results, especially if applied in peatlands (GEO-SLOPE, 2012).

The MMHW model also uses the convection–dispersion solute transport equation to predict the concentration of DOC in mire ecosystems. MMHW applies a finite difference method to discretized (vertical discretisation) the model domain and assumes there is no lateral import of DOC from the surrounding areas into the mire (Yurova et al., 2008). This assumption can be a challenge as water flow in shallow aquifer such as peatlands underlain by impermeable layers are predominantly horizontal (Baird et al., 2011). The model includes additional terms in the transport equation to formulate the rate of desorption/adsorption, the microbial production rate of DOC and first order microbial DOC mineralization constant. The governing equations of DOC and SPSOC (sorbed, potentially soluble organic carbon) are numerically solved using the CVODE (a program package written in C programming language for solving ODE) program package (Yurova et al., 2008). CVODE solver includes an algorithm called STALD (STAbility Limit Detection) which in combination with the CVODE solver improves the model stability in advection-dominated advection–dispersion problems (Hindmarsh et al., 2005).

4. Key processes for water quality modelling in peatlands

Hydrological inputs (i.e. water table level/groundwater movement within peat soil) are critical for water quality modelling in peatlands (Table 3), particularly as many processes such as plant community succession, plant/litter productivity, peat decay and accumulation depend on water table level, which regulates the soil water chemistry (Whitfield et al., 2009). Sorption and desorption processes control the nutrient fluxes in peatlands and must also be considered in the formulation of mathematical equations for water quality models. Sorption and desorption of nutrients by the soil matrix control the concentration and transport of DOC (Tang et al., 2018). Indeed, the store of SPSOC in any given year may affect the DOC concentrations and fluxes in the subsequent year (Yurova et al., 2008). Finally, decay/production rate and nutrient mineralization are critical processes that must be considered in water quality models. These processes control microbial decomposition of nutrients, nitrification/denitrification and DOC mineralization within peat soils. Their exclusion or underestimation could lead to inaccurate prediction of nutrient concentration and transport (Khan et al., 2022a; Rankinen et al., 2006).

4.1. Development of a peatland-specific water quality model

Water quality models need to take cognisance of the spatial heterogeneity of peatlands and consider them as complex adaptive systems (Belyea & Baird, 2006). Accordingly, any newly developed water quality model for peatlands should (1) be 2-D process-based and fully distributed (Baird et al., 2011) (2) include a peatland-specific hydrological model (either as an inbuilt sub-module or coupled to an existing hydrological model) that generates input data or is capable of considering the spatial variability of peat characteristics (Macrae et al., 2013; Molenat et al., 2008; Hefting et al., 2004) (3) include a hydrological model for the prediction of the impact of restoration methods (e.g. drain blocking, bunds) on raising the water table level (which affects nutrient concentrations and transport) (Koskinen et al., 2017; Lundin et al., 2017) (4) contain mathematical formulations for solute transport and concentration fluxes based on the advection/convection–dispersion equation, and (Khan et al., 2022) (5) consider processes capable of altering the concentration and transport of DOC and nitrogen-based nutrients (Tang et al., 2018; Yurova et al., 2008).

4.2. Avenues for future research

Advances in artificial intelligence (AI) has made it possible to integrate machine learning (ML) into numerical modelling systems to enhance model outputs (Pandya et al., 2024). Many ML models are nonlinear and function as black boxes (Sitterson et al., 2018), providing limited insight into their predictions. However, combining models, such as hydrological models with water quality models, and incorporating ML for optimization and calibration, may be beneficial in peatlands. An example is the use of Support Vector Machine (SVM) for groundwater quality prediction, which maximizes forecast accuracy and detects overfitting (Pandya et al., 2024). Nordin et al. (2021) reviewed AI-based groundwater quality forecasting, and found SVM, ANN, LWPR (locally weighted projection regression) and RVM (relevance vector machines) to be more accurate and faster compared to a physically-based modular 3-dimensional transport model. Hybrid ML-numerical models hold promise for future peatland water quality research.

Tracer-aided water quality modelling may also be useful when identifying the sources or path of pollutants in peatlands and investigating controls of nutrients in peatlands. Wu et al. (2022) successfully used a tracer-aided model to differentiate the primary influences of hydrological and biogeochemical controls on water quality in riparian peatland. Remote sensing to estimate water quality parameters is a very promising avenue to explore in peatlands. Cherukuru et al. (2021) used an optical remote sensing model to estimate suspended sediments and DOC in coastal waters influenced by a peatland-draining river. This concept could be explored in peatland settings.

5. Conclusions

The selection of an appropriate computational model to predict the impacts of management of peatlands is important. This paper identified 16 different water quality models (15 processed-based and 1 conceptual) and reviewed their efficacy in 23 reported studies. INCA and HYDRUS 1D/2D are the most widely modelled water quality models. Dissolved organic carbon and nitrogen-based nutrients are the most widely modelled water quality parameters. Models such as MIKE SHE, MODPATH, MODFLOW-SURFACT and HydroGeosphere are unable to implement the complex characteristics of peat soil observed at the near surface, which has compelled researchers to resort to simplifications of peatland structure. Similarly, HYDRUS 1D/2D has challenges in considering the inherent heterogeneity of peatlands. Although the MMHW model was designed for peat mire ecosystems, it does not consider horizontal export of nutrients. To date, it has only been used to predict the concentration and transport of DOC.

CRediT authorship contribution statement

Emmanuel Opoku-Agyemang: Writing – original draft, Methodology, Investigation, Formal analysis, Data curation. **Mark G. Healy:** . **Mingming Tong:** Writing – review & editing, Supervision, Project administration, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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