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REVIEW PAPER

A simple framework for selection of water quality models

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Abstract Water quality modeling is no longer just the preserve of *specialists* who seek to describe water quality processes but also for use by *non specialists* in everyday water quality management issues. With so many models already developed, it becomes prudent to adapt them to a situation than to develop a completely new model that would probably do the same simulations. The question is: which is the most appropriate model to apply to a situation? The *specialist* can always draw on past experiences to make a decision. However, this is not the case for the *non specialist*. A lot of different criteria can be used to decide which model to use for a particular situation based on some important factors. The objectives of modeling exercises differ and each water body is unique so there cannot be hard and fast rules on which is the best criteria for selecting the appropriate model. Furthermore, there is usually hardly any time on the project work plan allocated for model selection. Therefore there is need for a simple procedure to select the appropriate model. The objective of this paper was to develop a simple framework for selecting water quality models to aid the *non specialist*. The framework was then applied to a case study in order to evaluate its usefulness. The results from the case study show that after a thorough literature review, models can be evaluated against chosen criteria and the most appropriate model singled out. It was concluded that the framework is only effective if the research objective is adequately defined and the models are reviewed thoroughly, but it saves time for the actual modeling exercise.

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1 Introduction

According to Velten (2009) generally a mathematical model can be described as a simplified mathematical description of a complex system which helps to solve a problem. In water quality modelling terms, computer based mathematical description of complex water body systems have been developed. Mathematical modeling has become the standard procedure especially in characterizing and investigating water quality management problems in water bodies (Bath et al. 1997; Chapra 1997; Fitzpatrick et al. 2001; Imhoff 2003). Computer based mathematical modeling has been applied successfully in the management of water quality problems in water supply reservoirs. Mathematical models can be used to interpret and describe processes affecting the reservoir hydrodynamics and major ecological components. They can also be used to predict the response of the system to specified inputs under given conditions or constraints by replicating the physical behaviour of a system on a computer (McCartney 2007; Lang et al. 2010). A simulation model allows the testing of alternative scenarios before implementing them as compared to evaluations after costly implementations (Fitzpatrick et al. 2001; McCartney 2007). This makes water quality modeling a very cost effective management tool.

The use of a model for management purposes depends on systems to be modeled and on legislation in place in the country of use. Cox (2003) states that a great deal of work and time would be saved if an existing model suitable for the purposes of the study is chosen based on the data requirements and the appropriateness to deal with the water quality management problem at hand. Although a large body of literature exists that describes individual models and processes, there is very little guidance on suitability of particular modeling systems for specific applications and situations (Cox 2003; Saloranta 2006; Boorman et al. 2007). This could be attributed to the uniqueness of each and every water body and the complexity of processes that govern their water quality dynamics. A natural selection process would be to try out the possible models and determine which would give the most acceptable and reliable results. However, management decision making cannot wait for such a long process, the model user must decide on a model quickly and start working towards the management objective. The little guidance that is there in model selection assumes the model user has prior experience and expertise (e.g. Fitzpatrick et al. 2001; Boorman et al. 2007). Fitzpatrick et al. (2001) assessed and evaluated water quality models in the development of a computer based "Model Selection Tool", and characterized models in terms of such attributes as media of concern, analysis level(s), methods, temporal representation, dimensional capability, source/release types, sources, assessment extent, applicability to water body types, type of chemicals, critical processes, model uses, resource requirements, model use features, model support, and model availability. These characterizations were developed in order to identify distinguishing features that could be used as decision criteria useful for selecting models within each model class (Fitzpatrick et al. 2001; Imhoff 2003). The use of tools such as the "Model Selection Tool" by Fitzpatrick et al. (2001) raises the question of availability and resource requirements in terms of the cost of acquiring the tool as well as time spent in applying the tool for selecting the model. Boorman et al. (2007), on the other hand, suggests a criteria only suitable for a team of water management experts and states that modelling should be left to the experts. This is all very well in an environment where expertise abound but in the developing world, experts are scarce or non existent. Saloranta (2006) applied the benchmark criteria developed for the European Union Water Framework Directive, which is based on a set of fourteen questions that evaluate the different model characteristics. This approach seems user friendly even for the novice model user, except that, the scoring system still present a challenge of requiring some familiarity with the models. As observed by Boorman et al. (2007), many models available in practice may equally be suitable for an application but the water manager requires an auditable process to prove that the appropriate model has been selected. A simple selection procedure would be helpful in guiding the novice model user as well as provide the auditable process and hence save time that would otherwise be wasted by trying out different models. This paper developed a simple water quality model selection framework. In order to evaluate its effectiveness, the framework was applied to a case study.

2 Developing the simple framework for selection of water quality models

In this paper a model was defined according to Cox (2003) as a distinct piece of software with which the user can simulate water quality by inputting relevant system data. The simple framework was developed to select a model from the pool of existing models. The model selection framework was developed based on the following aspects: water quality management objective; selection criteria important to the objective; identification and review of relevant models; and evaluation of reviewed models against the criteria as illustrated in Fig. 1.

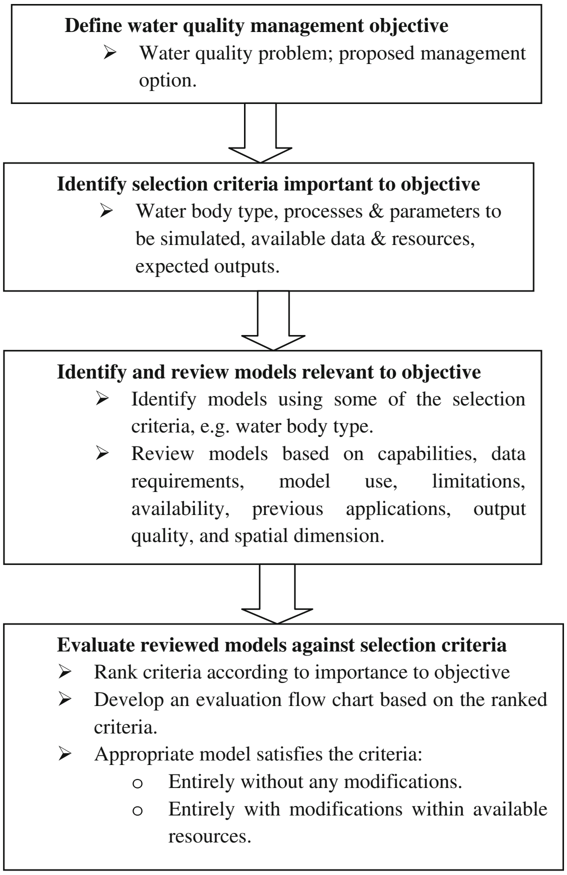

Fig. 1 A simple framework for selection of water quality models

The selection of water quality models is generally guided by the following factors; project goals, use of results, characteristics of the system important to objectives, appropriate level of detail (space and time), important chemical and physical processes, calibration requirements, data requirements and availability, previous applications of model and acceptance in scientific community, ease of use, sensitivity to processes of interest, available time and resources (Fitzpatrick et al. 2001; Engel et al. 2007). The simple framework shown in Fig. 1 encompasses all these factors into three broad categories as elaborated in the following sections.

2.1 Definition of water quality management objective

The water quality management objective is derived from the water quality problem that requires management. The objective is usually defined by stating the water quality problem and how it is proposed to be managed and so dictates the expected results of the modeling exercise. It is therefore the first step in any model selection exercise because the model is a tool which is applied towards achieving the objective. The system that pertains to the problem should also be defined as part of the definition of the water quality management objective (Velten 2009). The objective must be defined clearly and precisely, so that the expected outputs are accurately identifiable. The next step in the model selection framework is to identify selection criteria important to obtaining the expected outputs for the objective.

2.2 Identification of selection criteria important to the objective

After specifying the objective of the modeling exercise, important factors to be considered become more apparent. The following questions regarding the system to be modelled must be addressed adequately in order to come up with reliable selection criteria:

1. What type of a water body is under investigation (i.e. reservoir, river, estuary, coastal)?
2. Which parts of the water body are relevant to the objective (i.e. sediments, water, aquatic life, etc.)?
3. What processes must be simulated (i.e. mechanistic, empirical)?
4. What are the expected outputs (i.e. deterministic, stochastic)?
5. What parameters are important to the objective (i.e. temperature, dissolved oxygen, etc.)?
6. What are the available resources (i.e. financial, time, modeling skills)?
7. What data is available (i.e. monthly, weekly, daily, hourly and of what parameters)?
8. Who is going to use the outputs (i.e. senior management, reservoir operators, and treatment works operators)?

These questions are addressed by referring to literature. A thorough review of literature is required in order to understand the system to be modelled and identify the parts of the system relevant to the objective. Information on available resources, available data and the use of the outputs can usually be obtained from the parties initiating the modeling exercise.

After identifying the selection criteria important to the objective, some of the criteria are used in identifying the relevant models that would apply to the objective. Models are shortlisted using answers to questions 1–4 above. The relevant available models can then be reviewed and evaluated for appropriateness.

2.3 Review of available relevant models

Water quality models have been developed for all the water bodies that are of interest to the scientific world especially with reference to ecology and water pollution. Some models are specific to particular water body types and others are specific to processes and are therefore applicable to different water body types. Some models have been developed based on empirical data obtained from certain regions of the world and hence their applicability to water bodies in other parts of the world is questionable. Confidence in model results is based on quality of data used to construct the model; capabilities of the model user and proven ability of models to simulate observed phenomena (Fitzpatrick et al. 2001; Imhoff 2003). Chapra (1997) and Cox (2003) stress the importance of matching model complexity with data availability. This means that review of the relevant models should look at the data requirements of the models and compare that with actual data available. It is also important that the model uses an appropriate level of detail and accuracy (simulation capabilities) to achieve the objectives of the study so as to enhance confidence in the model results. As outlined by Fitzpatrick et al. (2001) and Engel et al. (2007), the quality of model results, previous applications and availability, and support from the developers, are also points to note when reviewing the models. Furthermore, according to Cox (2003), it should be noted that all models are based on some assumptions and have limitations that need to be understood for meaningful interpretation of simulations obtained. This factor needs to be taken into account when the models are being evaluated for applicability to the management objective.

2.4 Evaluation of reviewed models

The reviewed models must all be evaluated against the criteria in order to select the appropriate model. Evaluating all reviewed models completes the auditable process to prove that the selected model was the appropriate one. This approach differs from the one taken by Saloranta (2006) where four models were preselected and only two were evaluated against the criteria. The evaluation procedure is outlined in the flow chart in Fig. 2. The criteria are ranked and arranged in the flow chart according to its importance to the objective. That is the criteria that determine the outcome of the modeling exercise should be at the top as these are tied to the management objective under investigation. Therefore models that fail to satisfy these criteria will not be considered further.

The model which can satisfy the criteria outlined in the flow chart with or without modifications would be the appropriate one. If the results obtained from the selection framework are not satisfactory or inconclusive, the model user can quickly review some more models or revisit their objective definition and make sure it is adequately and clearly formulated. Parsons et al. (1998) and Saloranta (2006), also based their evaluations on literature review of the models and not technical assessments. Technical assessments require time, among other resources, which as stated previously is not usually available for this exercise. The model user can also select a model that satisfies most of the criteria and which allows for modifications to satisfy the management objective (see also Saloranta 2006). In the event of two or more appropriate models then the criteria on available resources should be used to select the model that requires the least amount of resources to achieve the objective. The case study in the following section evaluates the usefulness of the framework.

3 The case study: Vaal Dam

3.1 Study area

The Vaal Dam is the second largest dam by area and fourth largest by volume in South Africa. It has a catchment area covering 38,505 km^2, and a capacity to hold 2,575 million cubic metres of water. This dam has a surface area of 321 km^2 and an average depth of 22.5 m (Rand Water ND). Even though the Vaal Dam is only the fourth largest dam in South Africa in terms of volume, it is the most important dam as the primary supplier of water to the economic heartland of South Africa. The reservoir is fed from two major rivers; the Vaal River and the Wilge River. The extent of the Vaal Dam reservoir is shown in Fig. 3.

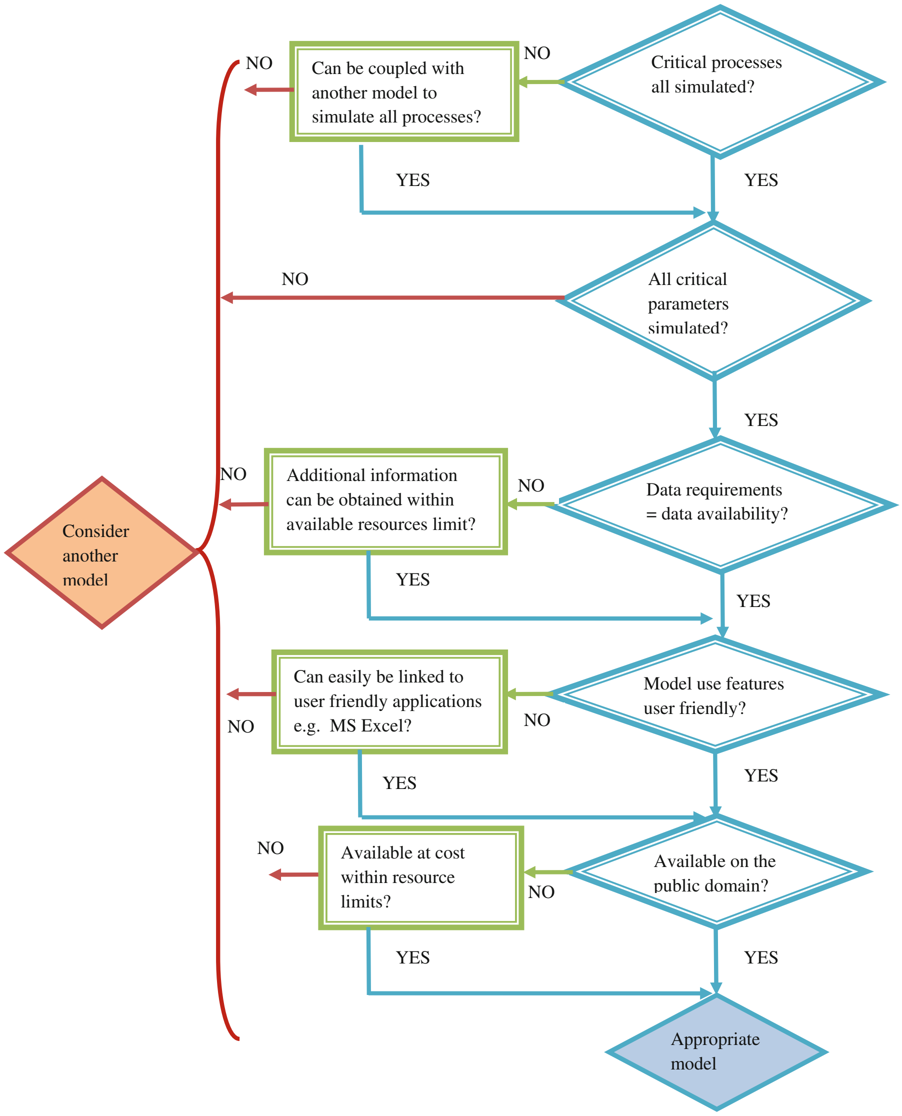

Fig. 2 Water quality model evaluation flow chart

Vaal Dam reservoir is used for urban potable water supply in most parts of the Gauteng province of South Africa. Rand Water Board is the bulk supplier of potable water in the province. Rand Water Board abstracts 80 % of the water it treats for potable use from Vaal Dam reservoir through twelve multi-level intake openings on the intake tower to a canal and three intake openings in the dam wall to a pipeline (Ceronio et al. 2000). The presence of blue–green algae (cyanobacteria) in the raw water abstracted from the Vaal Dam, impacts on the treatment processes required to produce potable water (Ceronio et al. 2000; Gyedu-Ababio 2004). The concentration of cyanobacteria in the water body varies temporally and spatially hence by modeling; one can predict its possible concentration in the water column. In doing this, the abstraction points can then be optimally located to minimize the impact of cyanobacteria on the treatment processes required to produce potable water. Therefore, the water quality management objective is managing cyanobacteria in water supply reservoirs by optimizing raw water abstraction.

Fig. 3 Vaal Dam reservoir (Google 2013)

3.2 Definition of the water quality management objective

It is imperative that the concentration of cyanobacteria cells in the water column be determined on temporal and spatial scales. However, the distribution of the cyanobacteria cells in the water column is mainly affected by the hydrodynamics of the reservoir, water temperature, climatic conditions, and availability of nutrients and light in the water column. Therefore the questions that the modeling system has to address are:

- How are the cyanobacteria cells distributed in the water column and seasonally?
- Is there a significant temporal and spatial variation in the distribution of the cyanobacteria cells?
- What factors affect the distribution of cyanobacteria cells in the water column?
- How can selective abstraction reduce the concentration of cyanobacteria cells found in the raw water abstracted for treatment?

Expected outputs derived from these questions are: temporal and spatial trends of cyanobacteria cells and related parameters in the water column; selection of abstraction outlets to open, in order to reduce the concentration of cyanobacteria cells found in the raw water abstracted for treatment.

3.3 Model selection criteria for the management objective

The selection criteria for the water quality model for the water supply reservoir are highlighted in Table 1. The objective requirements related to the criteria are also highlighted to show the importance of the criteria to the objective. If there is no link of a criterion to the objective then that criterion is redundant and will not affect the choice of model to be used.

For this water quality management objective, the water body of concern is a water supply reservoir, so that automatically limits the choice to only reservoir water quality models. Based on the critical processes identified in Table 1 and supported by classification of models by Fitzpatrick et al. (2001) the study requires a hydrodynamic model coupled with a water quality model in order to describe the processes related to the distribution of cyanobacteria cells in the water column. Hydrodynamic models are mechanistic models that determine the circulation, transport, stratification and depositional processes within a reservoir. Since transport of pollutant within water body is driven by surface water flow and mixing processes, the knowledge of how the physical features of the water body configuration determine water circulation and water movement is essential in many water quality investigations (Fitzpatrick et al. 2001). To fully satisfy

Table 1 Model selection criteria for the management objective

Criterion	Objective requirements
Water body	Reservoir
Parts of the water body relevant to objective	The water contained in the reservoir
Critical processes	Mechanistic (i.e. eutrophication and hydrodynamic processes)
Expected outputs	Hybrid i.e. partially stochastic and partially deterministic (temporal and spatial trends of cyanobacteria cells and related parameters in the water column; selective abstraction scenarios that would reduce the concentration of cyanobacteria cells found in the raw water abstracted for treatment)
Parameters	Secchi depth, chlorophyll-a, cyanobacteria biomass, water temperature, electrical conductivity (EC), dissolved oxygen (DO), and nutrients (Nitrogen and Phosphorus)
Resource availability	Project time—2 years, minimal funding, very basic modeling skills, Computers based on Windows operating system
Data availability	Monthly water quality, daily meteorological data excluding cloud cover, inflow and outflow data, reservoir cross sections
Output users	Senior management, reservoir operators, and treatment works operators

the management objective, an optimization algorithm is required. The optimization algorithm specifies target cyanobacteria concentration and regulates the selective withdrawal ports to achieve intake water quality concentrations lower than or equal to specified concentration and thus finds a unique operating strategy to achieve that target. This requirement then limits the selection to hydrodynamic reservoir water quality models which can accommodate optimization.

3.4 Review of available models

This review focused on hydrodynamic reservoir water quality models that showed some relevance to the objective of managing cyanobacteria in water supply reservoirs by optimising raw water abstraction as informed by the selection criteria in the preceding section. Models that have been previously applied to the study area stated in literature are also a good place to start. Bath et al. (1997) applied various hydrodynamic models to various water quality management problems in water supply reservoirs in South Africa. The models were matched to reservoirs based on data needs and appropriateness to deal with the water quality problem. The models were used to evaluate reservoir management options such as destratification by bubble plume aeration, selective abstraction, and control of reservoir operating level, freshening options, hypolimnetic releases and changes to reservoir input loading. Examples of these models applied by Bath et al. (1997) which were included in the review were DYSREM, MINLAKE and CE-QUAL-W2. The summary of the review of models is as presented in Table 2. The models reviewed in Table 2 were two dimensional and one dimensional. Three dimensional models were considered to be too complex for the available resources and therefore were not reviewed.

3.5 Evaluation of reviewed models

The following relevant models were reviewed: BATHTB, SELECT, DYSREM, MINLAKE and CE-QUAL-W2. When the attributes of the models as presented in Table 2 were evaluated using the flow chart (Fig. 2), the results were as shown in Table 3.

From Table 3, BATHTUB was limited by the data requirements for the catchment which would stretch the resources of the project but not necessarily add value to the project. SELECT and DYRESM can simulate all critical processes when coupled with another model. The range of water quality parameters that they can simulate when coupled will depend on the model they are coupled with. Coupling would also have implications on the available resources. MINLAKE would simulate all the processes but, it is not clear how one would access it. CE-QUAL-W2 demands some extra data in the form of daily and weekly measurements of some water quality parameters. These additional requirements can be obtained within the available resources and will enhance the reliability of the results. It also has the advantage of being readily available in the public domain and being well supported by the developers.

Table 2 Summary of reviewed models

Review aspect	BATHTUB	SELECT	DYSREM	MINLAKE	CE-QUAL-W2
Simulated processes	Steady-state hydrodynamics, eutrophication water quality—empirical and mechanistic	Withdrawal hydrodynamics, release water quality—mechanistic	Vertical hydrodynamic processes—mechanistic	Vertical hydrodynamic processes—mechanistic	Longitudinal and vertical hydrodynamics, water quality in stratified and non-stratified systems—mechanistic
Simulated parameters	Nutrients, Algae (Chl-a) temperature, DO, transparency	Release temperature, DO, TDS and pH	Density, temperature, salinity can be coupled with CAEDYM water quality model for water quality parameters	Temperature, algae, nutrients, DO, zooplankton, inorganic suspended sediment	Water surface, velocity, temperature, nutrients, multiple algae, zooplankton, periphyton, macrophyte species, DO, pH, alkalinity, multiple CBOD, suspended solids, and organic matter groups
Data requirements	Characteristics of catchments and tributaries contributing runoff, contaminants to water body, inflows and quality of inflows	Release elevation, and discharge at each release point, levels where ports are located, water quality profiles	No calibration required if coupled with CAEDYM water quality model water quality profiles required.	Inflow quality and quantity data, metereological data, morphology of lake, water quality data	Reservoir bathymetry, stream flow, temperature, meteorological data, spatial data on dimensions, volume, morphology, outlet configuration of reservoir basin and its embankment, water quality depth profiles
Spatial Dimension	1D	1D	1D	1D	2D (longitudinal-vertical)
Outputs and quality	Runoff, nutrient load, bathymetry, temperature, oxygen, phosphorus profiles	Water quality parameters, temperature, DO, pH, and specific conductivity	Density, temperature, salinity profiles,	Predicted lake and outflow water quality	Temperature, PO_4, NH_4, NO_3, DO, TP, Chlorophyll-a. profiles
Examples of previous applications	Dye (2006), Nieber (2011)	Baltar and Fontane (2006), Anderson (2011)	Nandalal and Bogard (1995), Bath et al. (1997), Lang et al. (2010)	Herb and Stefan (2005), Batick (2011)	Bath et al. (1997), Gelda and Effler (2007), Huang and Liu (2008), Ma et al. (2008), Batick (2011)
Availability and support	Open source, http://el.erdc.usace.army.mil	Open source, http://el.erdc.usace.army.mil	Available at a cost http://www.cwr.uwa.edu.au	Not easily accessible	Open source, http://www.cee.pdx.edu/w2
Model use	Predictions, scenario testing; implemented in MS DOS format	Predictions, scenario testing; implemented on a spread sheet	Predictions of seasonal, inter-annual variability; uses programming platform	Predictions; user interface not discussed	Predictions, scenario testing; spread sheet based pre-processor and post processor user interface
Limitations	Limited to steady-state evaluations of relations between nutrient loading, transparency, hydrology, and eutrophication responses	Has been only applied to stratified reservoirs (Schneider et al. 2004)	Considers only vertical variations (Imerito 2013)	Its incapability to address anaerobic tendency of the hypolimnion	Best for predominantly longitudinal variations i.e. long and narrow reservoirs (Cole and Wells 2011)

Table 3 Model selection results

Criterion	BATHTUB	SELECT	DYSREM	MINLAKE	CE-QUAL-W2
All critical processes simulated	Yes	Yes with coupling	Yes with coupling	Yes	Yes
All parameters simulated	Yes	Depends on coupling	Depends on coupling	Yes	Yes
Data requirements = data availability	No	*	*	Yes	No. Extra data but within resources
Model use	*	*	*	Not clearly described	Yes with MS Excel
Availability and support (manuals etc.)	*	*	*	No	Yes

* Model not evaluated against subsequent criteria if it fails preceding criteria (see Fig. 2)

From the case study, the results show that any one of the five models would be suitable given some modifications. For example, in this case BATHTUB can be selected if it allows for surrogate values for the catchment data requirements without adversely affecting the outcome of the model. SELECT and DYRESM would also be suitable if coupled with other models that would make up for their shortfalls but those models would also then need to be reviewed and evaluated as well. Coupling DYSREM would possibly also impact on the costs of accessing the model from the developers. If the availability issues could be resolved for MINLAKE, it too would be suitable. Given the guidelines provided by the framework for the model selection exercise, the appropriate model for the case study would be CE-QUAL-W2. This is because it satisfies all criteria entirely with some modifications.

4 Discussion and conclusion

Although Boorman et al. (2007) state that modeling for water quality management is specialist work, early researchers and and other non specialists also need to acquire modeling skills. This is because of the fact that mathematical modelling has proven to be a useful tool in water quality management. Although there are now many available models, it is not prudent to “thumb suck” a model to apply in investigating a water quality management problem. This would be risking wasting time on a model that may not deliver the expected outcomes. There is need therefore for some guidance for novice model users on how to select the appropriate water quality model. A simple but effective method of selection is to apply a set of criteria to several models and select the one that satisfies the criteria. The simple framework for selection of water quality models presented in this paper does not require any computer software and so is suitable, where time for the project is very limited and there is no access to sophisticated selection tools. The framework is flexible and criteria depend entirely on the water quality management objective being investigated. The evaluation of the models is based on literature review, which is less time consuming than technical assessments. Technical assessments may also require input of data and one can run the risk of expending resources on data that may not add value to the water quality management objective at hand. The literature review is also guided by the criteria, so that there is no need for a scoring system, rather the question is whether or not the model satisfies criteria and also whether it can be modified to satisfy criteria. This is a simple evaluation which can be done even by someone without any prior experience with the models being reviewed.

The results of applying the framework to the case study show that after a thorough literature review, models can be evaluated and the most appropriate model singled out. Although the simple framework seeks to save time during the selection stage of the modeling exercise, enough time should be allocated to it to allow for the proper definition of the management objective and the thorough review of the models. The effectiveness of this framework therefore depends on the proper definition of the study objectives and the criteria linked to the objectives. If this is not done properly then it affects the short listing of models to review and may result in spending more time doing the selection. A thorough review of the models is also important in order to have an adequate evaluation process. As alluded to in earlier sections of the paper, the criterion related to availability of resources may be used to further refine the evaluation process if one appropriate model cannot be singled out after the initial evaluation. It can therefore be concluded that the framework gives a simple and straight forward guide to selecting a water quality model.

Results from the case study also suggest that developers are not adequately marketing their models and hence they may not be selected just for the simple reason of lack of availability and support. This scenario limits the application of what may have been a useful tool in solving a water quality management problem. It is recommended therefore that developers make available user manual and model description on the public domain even if they intend to charge for the actual software. This will go a long way in providing a wider choice of models.

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