Water quality improvement by good system design using modelling approaches: A review article

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Abstract

Water quality assessment has increasingly become a vital part to meet the water needs for domestic, industrial and irrigation purposes. Water quality assessment is a multi-criteria decision-making approach subjected to qualitative and quantitative uncertainties. Certainly, many methods and models are available to identify and evaluate the water quality. In the last five decades, groundwater modelling has developed several simulations and optimization models to identify water quality issues such as contamination reduction and irrigation water management. New generation planners are facing challenges regarding aquifer storage, groundwater quality, geogenic and anthropogenic contamination, and long-term water sustainability. Improper datasets and variable parameters make groundwater modelling typically time-consuming and also hinder elaborative analysis and calibration. This study is presented to evaluate several available modelling approaches to identify their ability and inability as well. The study has presented an analysis of simulation modelling, optimization modelling, spatiotemporal modelling, a brief analysis of the surrogate models and inter comparison design models for groundwater quality measurement. The review is found to be informative and also highlighting key gaps and advantages of the models. Key findings are suggesting that inter comparison modelling is advantageous to evaluate more than one parameter at the same time and it is also feasible for consistent output over a period of time.
Water quality improvement by good system design using modelling approaches: A review article

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Key Points:

- For the given period of time, simulation modelling is enabled to generate feasible results.
- Spatiotemporal models are only efficient when using with correct set of data.
- Inter-comparison modelling approach is most competent for groundwater quality management.
Abstract
Water quality assessment has increasingly become a vital part to meet the water needs for domestic, industrial and irrigation purposes. Water quality assessment is a multi-criteria decision-making approach subjected to qualitative and quantitative uncertainties. Certainly, many methods and models are available to identify and evaluate the water quality. In the last five decades, groundwater modelling has developed several simulations and optimization models to identify water quality issues such as contamination reduction and irrigation water management. New generation planners are facing challenges regarding aquifer storage, groundwater quality, geogenic and anthropogenic contamination, and long-term water sustainability. Improper datasets and variable parameters make groundwater modelling typically time-consuming and also hinder elaborate analysis and calibration. This study is presented to evaluate several available modelling approaches to identify their ability and inability as well. The study has presented an analysis of simulation modelling, optimization modelling, spatiotemporal modelling, a brief analysis of the surrogate models and inter-comparison design models for groundwater quality measurement. The review is found to be informative and also highlighting key gaps and advantages of the models. Key findings are suggesting that inter-comparison modelling is advantageous to evaluate more than one parameter at the same time and it is also feasible for consistent output over a period of time.

1 Introduction
Groundwater management is an challenging issue considering the increasing demand of the irrigation system, industrial and domestic application and reducing water resources (Singh, A 2013). Contamination in the groundwater possess challenges to its quantification and application. Although there are several strategies to remove physical and chemical contamination, groundwater confronts significant challenges related to subsurface contamination. Current approaches to manage groundwater contamination uses mathematical models to identify groundwater flow and contamination based on physical process, which include simulation and optimization approaches for effective groundwater quality management (Singh, A 2013). The Models used for the groundwater contamination are based on the data obtained from the site assessment. (Chadalavada, Datta & Naidu 2012). This article reviews several models based on its application for water quality management. The review can be used to choose appropriate model for certain conditions and decision making.

2 Water Quality Models and Methods
2.1 Simulation model for groundwater management:
Traditional approach of the simulation model is to analyze the water quality over a period of time. Water and wastewater flows are considered constant over the distinct time period intervals. Each water bodies are segmented or divided into volume elements and assumed to be in steady-state condition over a time period of the simulation. Quality of groundwater resources can be managed by field experiments but considering the field conditions and ecohydrological conditions, it is expensive and time consuming (Singh, R, Helmers & Qi 2006). According to Mylopoulos et al. (2007), groundwater flow models are used to identify the possible human impacts on groundwater dynamics. Traditional approach of the simulation model is to analyze the water quality over a period of time. Water and wastewater flows are considered constant over the distinct time period intervals. Each water bodies are segmented or divided into volume elements and assumed to be in steady-state condition over a time period of the simulation (Loucks & Van Beek 2017). Furthermore, Simulation models help to identify the “what if” conditions. Simulation techniques are used significantly by the researchers to analyze groundwater quality across different parts of the world. This simulation models are based on the finite-difference or finite-element technique (Kulkarni 2018). It plays a vital role for the field water balance and can be used to estimate the consequences of the irrigation scheduling on the water balance. For any effective and reliable groundwater quality analysis would need evidence-based data, but evaluation of these models are impacted by the weak observation from arid and semiarid region...
Hydrological measurement always provide one point data which can be uncertain sometimes thus, it is often difficult to perform effective simulation for the groundwater quality (Kasahara & Hill 2006).

Furthermore, according to Momblanch et al. (2015), SIMGES is another simulation model used to identify optimal water resource allocation. It helps to maintain water quality by determining flow network which consist of storage, transport, diverting, consumption and return as well. All these factors are focused on the reality of the model and should be calibrated according to different characteristics. Moreover, GESCAL by Paredes-Arquiola et al. (2010) can be used to analyze the water quality and quantity in Spain. The model allows the water quality analysis for water, reservoirs and the demand discharges. Water quantity can be considered as continuous stirred tank while using this model. It helps to simulate dissolved oxygen, biological oxygen demand, Total Nitrogen, ammonium, nitrates, organic phosphorus, heavy metals, organic compounds and temperature of the water.

There are several benefits of integrating SIMGES and GESCAL at the same platform. It is convenient to perform different scenario by using these models because the results are easily transferred, and periodical simulations can be done. As mentioned by the Momblanch et al. (2015), analysis done by using SIMGES model shows the results of monthly time series which contains ratio of supply to demand, volume of the water in the reservoir, water flow etc. In addition to this, it also provides water supply feasibility and vulnerability and water demand over the entire time period of simulation. Simultaneously, GESCAL model provide the time series of the pollutant concentration along the reservoir.

2.2 Optimization model for groundwater management:

Range of groundwater optimization models have been used to identify and evaluate groundwater resources contamination and quality. The optimal use of the groundwater is useful to satisfy the need of the burgeoning population with limited groundwater resources. Optimization models are used to identify the specific conditions for specific use, such as, irrigation, industry or domestic. This can be determined by using optimization models (Gaur, Chahar & Graillot 2011).

As stated by Mohan and Jothiprakash (2003), linear programming based modelling techniques are widely used because of its easy formulation process and application. Optimization models was introduced and applied to identify the optimal use of the groundwater for the irrigation purpose in Pakistan back in 1992 (Afzal, Noble & Weatherhead 1992). The model was used under the poor groundwater quality. Furthermore, dual linear programming model was developed by Male and Mueller (1992) to fix the groundwater contamination and withdrawal. Dual linear programming model was used for the stream aquifer interaction which uses stream depletion factor to suggest the water body characteristics. According to Sedki and Ouazar (2011), Linear programming models are easy to use but cannot be used for the non-linear problems and also fail to attain the global optimization solution. This impotence caused the use of Non-linear programming models to be used in groundwater modelling. According to Mantoglou, Papantoniou and Giannoulopoulos (2004), the groundwater problem has been formulated by using the non-linear programming, in which flow system was treated as three dimensional and analyzed the optimal water quality for the aquifer problems. These non-linear programming modelling used widely across the world to identify the groundwater resources problems (Huang et al. 2012).

Moreover, genetic algorithm is also used as a vital tool for solving the groundwater issues. Genetic algorithm is based on the biological considerations and computational use to determine the optimal quality of the groundwater (Nicklow et al. 2009). Considering the uncertainties and multi criteria decision making process to identify water quality, cloud based model was proposed by Wang et al. (2016), in which randomness and fuzziness in the water quality has been evaluated by using eutrophication of different lakes. According to Loucks and Van Beek (2017), Eutrophication can be define as a gradual process of nutrient enrichment of the water system, which further leads to
increased productivity of the water system. In addition to this, physical interpretation of the parameters related to water quality can be evaluated using cloud model.

2.3 Spatiotemporal model to analyze groundwater contamination:

According to McLean et al. (2019), groundwater quality was analyzed by using spatial and spatiotemporal statistical modelling to assess the suitability of the methods and data collection of the groundwater quality. The analysis presents that a spatiotemporal model gives accurate predictions through the time period compared to spatial model used for individual time period. To achieve the same accuracy of spatiotemporal model by spatial model, the data should be collected much more extensively. Though, the results acquired by the spatiotemporal model are more efficient, there are certain limitations can be identified. Furthermore, spatiotemporal models are very much relying on how data are removed (McLean et al. 2019). Because of some unusually high or low data, it is difficult for the model to predict the steep gradient without data. For this reason, the data correction method should be used to remove the unusual data and to obtain shallow gradient (Evers et al. 2015).

2.3.1 Surrogate models for groundwater modelling:

The spatial and temporal parameters and inputs with complex groundwater modelling takes time and result into less comprehensive calibration and analysis. According to Asher et al. (2015), surrogate model provides faster, simple and comprehensive model which can give specified results of a more complex inputs and parameters. Similarly, Doherty and Christensen (2011) mentioned that the simple surrogate models reduce the mathematical instability which helps to calibration and uncertainty analysis of the water quality modelling. While using surrogate models, data-driven approaches are competent for the short runtime. In addition to this, projection-based modelling is also giving feasible results for the runtime reduction.

2.4 Inter comparison design for large scale water quality modelling:

According to van Vliet et al. (2019), large scale water quality models considered as models which are capable of simulating more than one water quality parameters. Many inter comparison modelling studies have been done by several modelling communities such as hydrological, climate, irrigation etc. Figure 1 is representing the several large-scale models capable of simulating more than one water quality parameters since 1990s.

Previous large-scale models were focused on the nutrient loads and can assess water quality trends for current and future scenarios. These models analyzed consistent load predictions with different level of model complexity and distinct input data source (Strokal 2016). Furthermore, Large scale quality models provide consistent output which helps to decision making and water policy as well. According to McCrackin, Harrison and Compton (2013), It also assist to improve the understanding of the pollution process and its source, especially in the regions where water quality data are sparse.

Large scale models have certain limitations. The major challenge is that there are limited numbers of models per parameters available to compare and provide efficient results. Furthermore, when comparing models for different resolution, methods should be aggregated according to temporal scale to compare quality predictions. Simultaneously, different models use distinct data set and assumptions, which complicates the direct comparison and simulation of the water quality results. Therefore, while using large scale models using similar input dataset is recommended (van Vliet et al. 2019; Weedon et al. 2011).
3 Discussion, Conclusion and future outlook:

Review is proposed to identify the key gaps and application of the different modelling approaches for the groundwater quality. The article is presenting summary of the current models in practice and drawbacks associated with those models. Firstly, simulation models are competent for periodical analysis and only efficient when using one-point data source, such as SIMGES and GESCAL. However, despite of being feasible at predicting the likely behavior of groundwater for policy decisions, simulation models are unable to identify the best possible option for the given set of data. This led to use of optimization models for the groundwater management. Secondly, optimization models are vital to identify optimal water usage and quality of the water based on its application. Thus, it is helpful for multiple decision-making processes in industrial, domestic and agriculture sectors. Thirdly, while using spatiotemporal models, it is important to have correct set of the data. It is also time consuming and less comprehensive when used without appropriate data correction method. Furthermore, as mentioned in the review several surrogate models are used for reduced the mathematical complexity and short water runtime as well.

Finally, inter-comparison models are most feasible amongst all, considering its ability to analyze more than one parameter at a time with constant output. Though, inter-comparison design modelling is more competent compared to others it is believed that more integrated effort is needed to achieve more efficient results. The review has tried to highlight all possible gaps and findings related to modelling techniques. It provides the base for the selection of the appropriate model for groundwater quality management. It can be said that the gaps can be filled by further contribution.
<table>
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<tr>
<th>Modelling approach</th>
<th>Key findings</th>
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<tbody>
<tr>
<td>Simulation modelling</td>
<td>• Dependent on data set quality</td>
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<td>• Inefficient with the one-point data collection</td>
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<td>• Periodical simulation can be done</td>
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<td></td>
<td>• Periodic analysis of the pollutant concentration is possible</td>
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<td>Optimization modelling</td>
<td>• It can be used to identify water quality according to water application, such as, domestic, irrigation etc.</td>
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<td>• Multi criteria decision can be made</td>
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<td></td>
<td>• Interpretation of the biological and physical water quality parameters can be evaluated.</td>
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<tr>
<td>Spatiotemporal modelling</td>
<td>• Largely relying on the how data is used, data ballooning can have significant impact on the results.</td>
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<td></td>
<td>• Less comprehensive calibration and analysis</td>
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<td></td>
<td>• Time consuming</td>
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<td>Surrogate modelling</td>
<td>• Reduced statistical complexity</td>
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<td>• Feasible while using short water runtime</td>
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<td>Inter-comparison design modelling</td>
<td>• Possible to simulate more than one water quality parameters at one time</td>
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<td></td>
<td>• Consistent output</td>
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<td>• Method use is dependent on temporal scale</td>
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*Table 1. Summary of the review*

Data Availability Statement:

Figure 1 for this research are included in (Van Vliet, MT, Flörke, M, Harrison, JA, Hofstra, N, Keller, V, Ludwig, F, Spanier, JE, Strokal, M, Wada, Y & Wen, Y 2019, 'Model inter-comparison design for large-scale water quality models', vol. 36, pp. 59-67.)
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