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VALIDATING RAINWATER QUALITY THROUGH MODELLING

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ABSTRACT

Research and design on runoff water through modelling have the potential to create accurate calibration and verification techniques to validate water quality. The potential contamination of rainwater harvesting systems and the need to have sustainable potable water management systems is gaining attention from water researchers, but still there is a paucity of research studies. Not enough attention has been paid to the integrity of rainwater quality and leaching of metals. This study shows how MATLAB software can be used to predict rainwater quality in an interactive and user-friendly way. The dynamic model employed in this study can be used to run and generate results by inputting data collected from harvested water to predict the level of contamination. Software that can be modified for future use when there are no experimental data to predict runoff water quality is a welcome development. The idea behind any water quality modelling is to explain and predict the effect of pollution in water from harvesting systems. In this study a modified model was used to analyse the quality of rainwater harvested from a rooftop

Key words: runoff**,** water quality, developed model, MATLAB, rainwater harvesting systems, rooftop

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1. INTRODUCTION

Water scarcity is a significant concern to human life and domestic animals who need it for drinking and feeding. Underground water is diminishing by the day, and the water reservoir is affected by seasonal changes. Hence the demand for rainwater has increased which has led to the design of various rainwater harvesting systems (RWHS). The critical role water plays in daily human life has led to its high-interest level among researchers worldwide [1]. This has resulted in the design and use of water quality modelling to have better and extensive data for reference purposes. Over the years, mathematical models have played a prime role in assessing the quality of water [2-4]. The model developed by the US Environmental Protection Agency

(EPA) known as QUAL2E is still relevant today [5]. However, QUAL2E as a modelling software is more applicable for water wells, stream water, and dam water than for rainwater. In 1998, Rauchi et al [3] provided an overview of water modelling software that has been used up until then to address water-related issues. Modelling software referred to most frequently in publications include WASP, SALMANQ and SIMCAT. Non-potable water modelling is usually classified from numerous perspectives starting from model complexity to the method of simulation, water quality and volume [4].

The majority of researchers use the QUAL2E application compared to other models [1,6]. Due to the dynamic nature of water bodies such as rivers and lakes, modification of water quality software is needed. Karadurmus and Berber (2004) [7] designed a unique dynamic modelling plan that is built on QUAL2E and integrated with an estimated technique. Karadurmus and Berber used this model (QUAL2E) to predict possible outcomes and compared their findings to a set of data compositions and the outcomes agreed well with the expected outcomes with some limitations. To test the authenticity of the modelling strategy, Karadurmus and Berber (2004) went further to test it against MATLAB, through a user-interactive software code called River Stream Dynamics and Simulation (RSDS) [7]. After running the suggested technique, the QUAL2E predictions were compared to experimental data, and compared very well [8].

Various models have been developed with improved features for better prediction of water qualities. A good example is the acquiring of a trade-off between computer load and prediction accuracy in Berber et al. (2009) [7]. However, the advancement made so far does not directly reflect several modelling studies involving software development for prediction of water (river water) quality [2]. The incorporation of geographical information system information to water quality models is gaining more attention [9]. Marsili-Libelli et al. in 2002 [10] showed how a MATLAB based quality water model interface can be integrated into a geographical information system (ArcViewTM).

The limitation of simulation software is the reason Marsili-Libelli et al. (2001) model has not experienced much development [9]. Most software in use today is as old as 30 years, so their uses are limited to specific sections and locations. The use of MATLAB in simulations and the development of modelling can now be used to predict a future outcome with high accuracy

Over the past 13 years accessible user interfaces have been developed to account for vital data that are not economically possible to derive. As such, graphical user interface (GUI) applications have gained more attention in quality information systems [11]. Such applications are believed to be of immense benefit in water quality analysis, and can be easily incorporated into critical decision-making. The appropriate use of GUI has been very useful in addressing the information management system of rivers and lakes, helping to predict the future quality of drinking and non-drinking water [6-7]. A good analysis of harvested rainwater is necessary to ascertain whether the harvested water is potable, because an increase in water pollution is a threat to available water resources. Any threat to water availability needs to be addressed before it becomes a global issue. The unavailability of data in most cases and the economic implications of extensive data collection have created room for modelling designs like those possible with MATLAB. This helps to broadcast and predict water quality which can also serve as a guide for future data collection. Some reference works show that mathematical models using MATLAB for water quality assessment in terms of the water quality index are suitable for natural and human-made water bodies (reservoirs) [2,11].

The importance of this work is to overcome the difficulty associated with most available software used for the prediction of water quality. MATLAB brings a whole lot to the prediction of the outcome because it is easy and has a very convenient GUI.

Most developing nations get their water from rivers. In most instances, little or no treatment is undertaken. Some rivers have been reported as non-suitable for drinking due to their high contamination by toxic, organic, and inorganic waste 12]. By extension, a highly polluted environment can affect the integrity of harvested rainwater from rooftops. Most water-polluting agents include physical, chemical and biological pollutants, and their presence lowers the quality of water [10, 12]. When such polluted water vaporises or mixes with air, it dissolves in falling rainwater and is deposited on the roofs then washed from the catchment area of the roof. After the wash down of deposited dirt, the pollutant will settle at the bottle of a water tank or be suspended. Either way, the harvested rainwater quality is affected. To account for these challenges, the graphical model based on MATLAB presented here is designed to assist in getting a solution through either graphics or estimated data. Only generated results are presented without the details of the actual model as this is not the aim of the study.

2. THEORETICAL BACKGROUND

Since the evolution of predictive software and MATLAB in water quality management, attention has turned to the modelling of river quality with biochemical oxygen demand (BOD) and dissolved oxygen (DO) in mind, according to Riyaj et al (2016) [12]. Here we apply the predictive software technique to the harvesting of rainwater, which contains few solid contaminants. The existing theoretical algorithm, based on a GUI, is used with all the necessary modifications to accommodate the difference between rainwater and river water without a complex user interface and computer language. This was made possible by the implementation of existing theory to predict the quality of harvested water. This made the method very economical, considering the time, resources, and cost usually involved in laboratory or field-based research work. With this technique, various vital parameters in water quality analysis were investigated.

3. ROOFTOP RAINWATER HARVESTING SYSTEM (RWHS)

Rainwater harvesting is a method of collecting rainwater during the raining season for consumption, therefore limiting runoff and waterlogging when there is heavy rain [13, 24-26]. This system is as old as a homo sapiens though it has not been practised extensively in most countries until recent times, brought on by the water scarcity crisis. The harvested water is usually stored in a tank reservoir, which could be for domestic or agricultural use. Figure 1 illustrates the collection channel through a piped network and storage in a typical

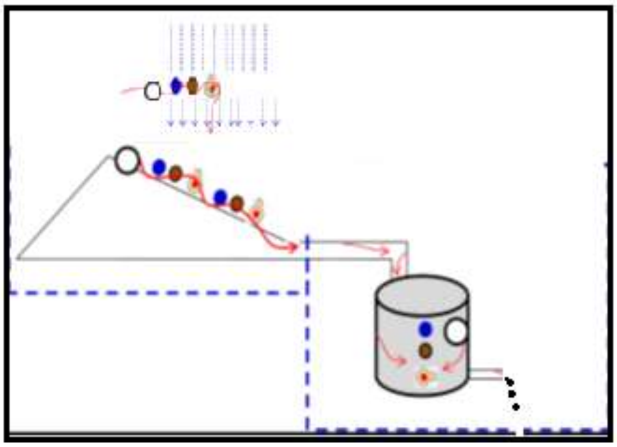

Figure 1 Conceptual depiction of a rainwater harvesting system indicating the key components (catchment, conveyance and storage and subsequent usage), nature and flow pathways of contaminants from source to the point of consumption

RWHS. Harvested water is a natural form of water resulting from the precipitation of condensed vapour; in its initial form, it is the purest form of water which can be classified as freshwater. However, no harvested water system (RWHS) is perfect, hence organic pollutants such as deposited bird faeces can contaminate its content. This study assumed that the storage tank area is divided into four regions of equal portions to examine water quality variables in the tank. In this way one can study the concentration of any selected water variable in any different region of the tank.

4. MATERIAL AND METHODS

4.1 Application

The water quality curve of a rooftop as a function of time is the velocity across the top through the catchment and the amount of BOD. There is one-dimensional water quality downflow of a roof harvesting water to the catchment base downstream. A mathematical model can be used to define the tracer concentration transformation movement so as to assess contaminants. Specific parameters have to be defined such as average depth of flow, H, average surface width, B, the average frictional velocity of flow, u. The processing time, which produces the tracer concentration, is defined in Equation 1. Contaminants originate from bird faeces deposition on the roof surface, dust particle accumulation, decay of fallen leaves from trees and particles from rusting roofing material. Assuming two points along the roof with a depth H (0.5 m), average surface width B (5 m) the pollutant concentration can be calculated. From one-dimensional downflow water quality primary equation, the concentration of the migrated tracer at point x is given as:

$$C(x,t) = \frac{M}{\sqrt{4\pi \mathrm{Edt}}} \exp\left[-\frac{(x-ut)}{4Edt}\right] \quad (1)$$

where C is the concentration of pollutant, u is the water flow velocity, E is the longitudinal dispersion coefficient, d is distance, and t is time [14, 23].

In a one-dimensional differential for longitudinal water, flow direction assumes the following:

Dispersion is transverse and vertically very small; a pollutant is miscible entirely in water; no chemical reaction between pollutants and its surroundings; and pollutant mass remains constant as it moves in the water. Table 1 is a description of a building rooftop.

Table 1 Description of a building rooftop

Si/i	Description	units
1	East-west roof length (width)	m
2	North-south roof length (length)	m
3	Building roof area	m2
4	Average minimum depth	m
5	Average maximum depth	m
6	Roof slope	
7	Average minimum temperature	°C
8	Average maximum temperature	°C

4.2 Data and Simulink Process

First, the simulation was verified by testing against standard data without laboratory testing in compliance with the standard method (American Public Health Association) [15] to analyse the quality parameters. For this study, the following water quality parameters were simulated: pH, DO, electrical conductivity (EC) and total dissolved solids. However, only pH, DO, dissolved solids and EC are presented in the results section because of insufficient verification of the other parameters. The simplified form of the MATLAB Simulink associated model used is presented in Figure 2.

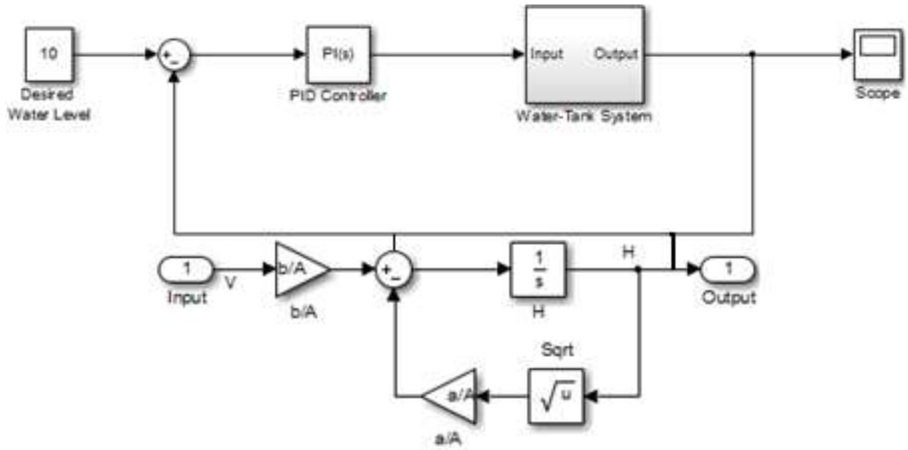

Figure 2 Model block diagram

The two classes of data defined in the model are the variables and parameters. Variables: *H* is the height of water in the tank. *Vol* is the volume of water in the tank, *V* is the voltage applied to the pump. Parameters: *A* is the cross-sectional area of the tank, *b* is a constant that relates the flow rate into the tank, while *a* is the constant relating to flow rate out of the tank. The increase in water scarcity in most regions has provided the need for a fast and reliable model to test the potability of water and manage the sustainability of water resources. Being able to assess water quality will boost water availability to consumers and should be regarded as a priority. The use of water quality modelling is an impetus as a supporting tool for evaluation purpose.

In order to simulate water quality in a typical storage tank, a linear dynamic model illustrating the process is needed [16-17]. In this study, as previously stated, MATLAB Simulink was used to predict the quality of harvested water. All the outcome of this research was simulated in a MATLAB environment, and Figure 2 gives the brief block diagram of the model used. This model is patterned after Steeter-Phelps model [18-24], after inputting the necessary data (predictors). The model is run in order to generate results, and this model works by combining re-oxidation and de-oxidation rate constants to produce an oxygen sag curve, also known as classical resolution.

5. RESULTS

The conditions depicted above assisted in the acquiring of water quality parameters, such as pollutant and pH level of the harvested rainwater. The process incorporates some subsystems. First is reference temperature (Tref), roof size, nature of rooftop material (chemical constituents of the roof), catchment area, duration of storage and tank condition, hence no fixed value is assigned to these variables. Each block in Figure 3 represents a particular variable, which are the predictors with an assumption and verified by the QUAL2E model.

The results presented in Figure 3 show that these parameters are determinant factors when considering the quality of potable water. The model used did not provide which data gives the highest variability; however, it shows which data affects water quality the most. The turbidity parameter proves to be easily influenced by change in other factors, and it is the parameter with the highest variability. This shows that the model-simulated results can compare accurately with other techniques. As seen in Figure 3, each parameter is place side by side with the WHO values at standard condition of 1 atmospheric pressure and at room temperature.19

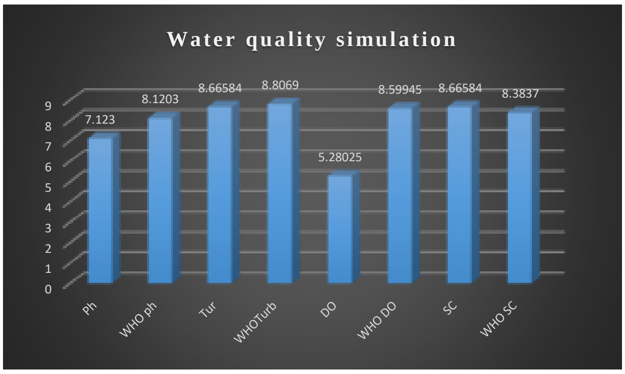

Figure 3 Water quality parameter calculated by verifying the other variables

As stated by USF (University of South Florida) water atlas publisher, dissolved oxygen (DO) is the most important indicator of water quality. A high level of DO indicates a better quality of potable water. Also, high DO concentrations give drinking water a better taste. A high DO concentration is healthy for human and aquatic life, especially fishes that need DO for survival. At the same time, a low level of DO can be detrimental to the health of the consumer. The only drawback is that high DO leads to rapid corrosion of domestic water supply pipes. This is one source of contamination. In Figure 4, it is evident that a DO range of 7.5 mg/L to 9.1 mg/L is best for drinking water. The results show that at elevated temperatures DO decreases and at lower temperatures it increases. The simulation was run by setting a temperature rise in intervals of 2.5 °C from 0 °C to 45 °C. The outcome fitted correctly with the existing standard relationship of DO and temperature. Another DO result was run for 12 months at 30 days interval to see how its concentration performed with time. It was found that DO decreases as time increases, which is possibly due to an increase in the number of organisms such as algae. These organisms consume DO through photosynthesis, considering that most water storage systems are positioned outside rather than in buildings.

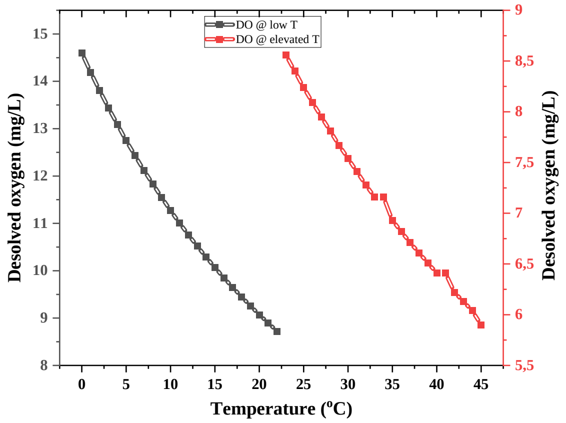

Figure 4 Effect of pressure, temperature on dissolved oxygen

Assuming a linear compensation temperature coefficient of 2.1 %/°C, harvested water quality can be calculated at any specific temperature. At 25 °C the specific conductivity (SC) is defined by Equation 2, the relationship between dissolved oxygen with temperature was analysed and the results showed that as the temperature rises, the DO decreases. Another variable that affects the quality of drinking water which needs to be defined is salinity which is the concentration of salt in any particular water. To assess that the SC was simulated and the results are presented in Figure 5. More results of DO are presented in Figure 6 by running the programme for a temperature range of 0 °C to 40 °C at 2.5 °C intervals. Another important information is the distribution of net contaminants in a storage tank after a long period. In Figure 7 shows the net contaminant concentration in a storage tank, using a tracer.

$$SC = \frac{Ye}{(1-(25-T)\,x\frac{a}{100})} \tag{2}$$

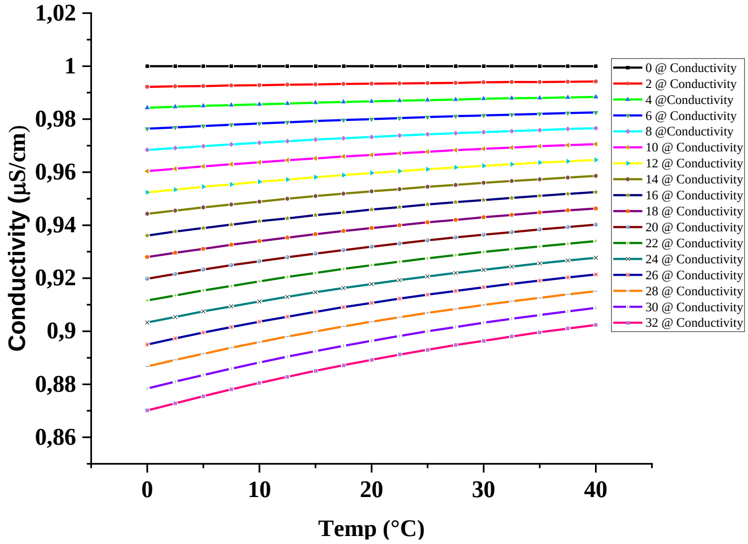

Figure 5 Specific conductivity against Temp

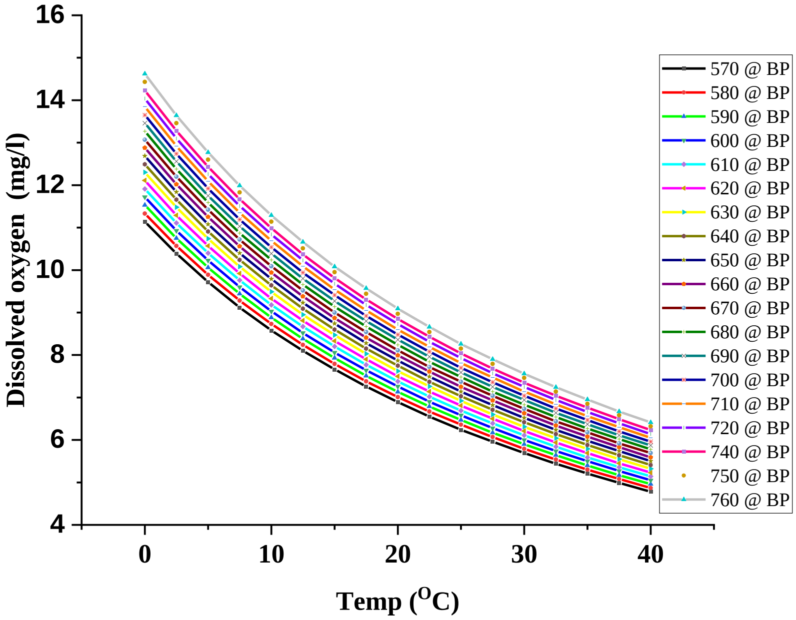

Figure 6 Relative dissolved oxygen in relation to Temp

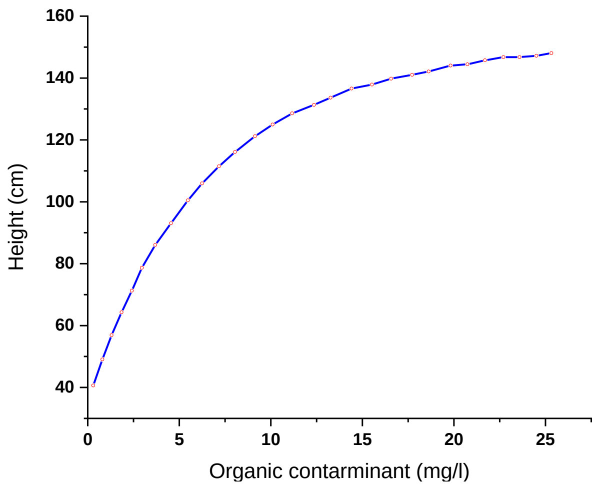

Figure 7 Concentration of net contaminant in a storage tank

5.1 Assuming Flushing Principle

The result in Figure 7 can be explained by the flushing principle. According to flushing principle, for any inflow and outflow of water system, the pollutant concentration is affected because of the mixing process that occurs. The principle is mostly applicable when rainwater is stored in a tank for a long time before usage begins. As water runoff from the tank occurs, the ability of the flushing to clean the tank water is proportional to its runoff velocity, which depends on the height of water and height above the ground with regards to its volume.20 This is a discontinuous and periodic flow, unlike the flow in streams and lakes. Considering any pollutant such as biochemical oxygen demand (BOD), the exponential flushing decay can be defined as in Equation 3:

$$\frac{dL}{dt} = \frac{QLin}{V} - \frac{QL}{V} - K^{\times}L \qquad (3)$$

where L, Lin, Q, V, t, K* are BOD leftover, BOD inflow, tank flow rate, time of flow/runoff and absolute reaeration constant respectively. K* is the process of oxygen transfer from the atmosphere via the air-water boundary into the water tank that does not have a natural flow rate.21 It is slightly different for a body that has a continuous inflow and outflow flush. This theory was initially used for natural water bodies like stream inflow and wastewater inflow. The volume per time gives the concentration change. However, the concentration transformation is derived from differentiating the volume change. Finally, the concentration per time is expressed in Equation 4 and Equation 5; in the model it is the same as the component of mass balance22 where Ci is the change in concentration for i component. The non-smooth nature of the curve in Figure 7 is due to the negligible mass of rainwater pollutants compared to river pollutants.

$$\frac{dV}{dt} = Qin - Q \qquad (4)$$

$$\frac{dCi}{dt} = \frac{Qin}{V}(Cin, i - Ci) + ri \qquad (5)$$

The value 0 mg/l corresponds to freshwater (0 salinity), oxygen solubility of 35 mg/l means seawater.22 Figure 7 shows the DO in harvested water from a pressure range of 567 mm Hg to 760 mm Hg. The theory behind the simulation assumes the tank inflow and outflow are similar to stream conditions. However, this is not a perfect stream system, due to its discontinuous and periodic inflow and outflow as stated previously.

6. DISCUSSION

In order to know the salt content of any water the salinity is required, this is important in roof-harvested water to discern any possible metal leaching from the roof material. The most direct method of doing this is to test for the specific conductive (Cs), and this is defined by Equation 6.

$$\mathrm{Cs} = \frac{Ys}{[1-(25-T)\, x\frac{a}{100})]} \tag{6}$$

where Cs, Ys, a and T are specific conductance, electrical conductivity, temperature coefficient and water temperature respectively. Assuming standard room temperature of 25 °C, a linear temperature compensation coefficient of 2.1 %/°C was used. One of the limitations of this calculation is that the linear coefficient temperature compensation used is for river water. Oxygen solubility is also derived from temperature versus pressure curve, depending on pollutant concentration. Values-based on published equations by Benson and Krause23 are the basic equations used. Most of the constants used in the model utilised in the simulation presented are from freshwater except when stated otherwise. The reason is that freshwater is natural water which contains less salt or heavy metals except when there is leachate. The conclusion drawn from this work applies only to less than 3 % of global water because global water makes up 3% of the total water and not all freshwater is potable. There is a need to draw a balance on the potability of freshwater quality. Drinking water accounts for less than 1.21 % of net freshwater.

From this study, Simulink MATLAB has proven that it is possible to simulate preselected water parameters required to assess the potability of water. This helps to limit excessive time use in most water analytical processes, thereby making the process cost-effective. This has shown that any dimensional quality model can be modified to suit any desired model without involving high-level programming language as seen from the above results. A subsystem model (Figure 2) is needed to understand the quality of water and to study the different influencing scenarios that can affect water quality. Unlike streams and rivers, modelling of rainwater quality is yet to gain significant attention. In the harvested water storage system model in this study, the similarity of tank inflow to that of a stream was used. Here specific water quality parameters were generated and calculated from the Simulink model, and the input parameter was generated from software in order to be able to run the model. The outcome of the simulation presented above compares reasonably well with basic known standards.

7. CONCLUSION

As the guidelines for potable water become more stringent, and the demand for fast and reliable certification becomes urgent, modelling techniques that utilise tested methods and processes are needed for modification process analysis and control in the quality of drinking water. This will provide robust alternative methods compared to traditional laboratory testing before certification for consumption. More importantly, such modelling gives room for knowledge improvement without time-wasting. The applicability is promising, considering it can easily be accessed and directed to specific needs, thereby increasing the availability of useful data for future modelling of water treatment and analysis. Finally, the results presented here can help in water sustainability by eliminating waste.

CONFLICT OF INTEREST

The authors declare no conflict of interest

AUTHOR CONTRIBUTIONS

All authors had contributed to the study and approved the manuscript.

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REFERENCES

[1] B. A. Cox. A review of available in-stream water quality models and their applicability for simulating dissolved oxygen in lowland rivers. The Science of the Total Environment. 314-316. 2003.

[2] J. Vojtesek. L. and Spacek. Modeling, Simulation and PID Control of Water Tank Model Using Matlab and Simulink, Proceedings of the 33rd International ECMS Conference on Modelling and Simulation (ECMS 2019. 2019, 33(1), 177-183.

[3] W. Rauch, M. Henze, L. Koncsos, P. Reichert, P. Shanahan, L. Somlyody and P. Vanrolleghem. River water quality modelling: I. State of the art. IAWQ Biennial Int. Conf. Vancouver-Canada, 1998. 21-26.

[4] M. K. Yetik, M. Yüceer, R. Berber, E. Karadurmu. River water quality model verification through a Gis Based Software, IFAC Proceedings, 2009, 42(11), 798-803,

[5] P. Shanahan, M. Henze, L. Koncsos, W. Rauch, P. Reichert, L. Somlyody and P. Vanrolleghem. River water quality modelling: II. Problems of the art. IAWQ Biennial Int. Conf. Vancouver-Canada. 1998. 21-26.

[6] Li, Xiuli, Zhou Wen and Dedong Liu, Water Quality Simulation in River Based on Matlab, Nature Environment and Pollution Technology, 2015, 14(1), 2015.

[7] R. Berber, M. Yuceer, and E. Karadurmus, A parameter identifiability and estimation study in Yesilirmak River. Water Science and Technology, 2009, 59(3), 515–521.

[8] M. Yuceer, E. Karadurmus, and R. Berber. Simulation of river streams: Comparison of a new technique to QUAL2E. Mathematical and Computer Modelling. 2007, 46(1-2), 292–305.

[9] S. Marsili–Libelli, E. Caporali, S. Arrighi, and C. Becattelli, A georeferenced water quality model. Water Sci. Tech. 2001, 43(7), 223-230.

[10] S. Marsili–Libelli, G. Pacini, C. Barresi, E. Petti, and F. Sinacori. An interactive georeferenced water quality model. Hydroinformatics: Proc. of the 5th Int. Conf. on Hydroinformatics, Cardiff, UK. 2002.

[11] N. A, Rahim, Z. Ahmad, Graphical user interface application in matlabtm environment for water and air quality process monitoring, Chemical Engineering Transactions, 2017, 56, 97-102 DOI:10.3303/CET1756017

[12] K. Riyaj Mulla and M. Shrikant Bhosale. Water quality Analysis and simulation of Panchaganga River using Matlab. International Journal of Engineering Sciences & Research Technology, 2016, 5(8), 613–620. http://doi.org/10.5281/zenodo.60106

[13] S. Rahman and F. Hossain. Spatial assessment of water quality in Peripheral Rivers of Dhaka City for optimal relocation of water intake point, Water Resources Management, 2008, 22 (3). 377–391.

[14] L. C. Brown, T. O. Barnwell, The Enhanced Stream Water Quality Models Qual2e and Qual2e-Uncas: Documentation and User Manual; Environmental Research Laboratory, Office of Research and Development, US Environmental Protection Agency: Athens, GA, USA, 1987.

[15] J. Graf. PID Control Fundamentals. Create Space Independent Publishing Platform. 2016.

[16] C. Rosen, D. Vrecko, K. V. Gernaey, M. N. Pons, & U. Jeppsson, Implementing ADM 1 for plant-wide benchmark simulations in Matlab/Simulink.Water Science & Technology, 2006, 54(4), 11-19.

[17] D. Vrecko, K. V. Gernaey, C. Rosen, & U. Jeppsson, Benchmark simulation model No 2 in Matlab-Simulink: towards plant-wide WWTP control strategy evaluation, 2006, 54 (8), 65-72.

[18] W. H. Streeter and E. B. Phelps. A study of the pollution and natural purification of the Ohio River. Public Health Bulletin 146, US Public Health Service: Washington D.C. 1925.

[19] World Health Organization, Guidelines for drinking-water quality, vol. 1, Recommendations, 3rd edition, 2006.

[20] S. E, Jorgensen, B. Halling Sorensen and S. N. Nielsen. Handbook of environmental and ecological modeling Lewis publisher 1993.

[21] M. Chadwick and M. J. Bovd. A water quality modeling tutorial using Simulink, water research lab University of New South Wales and department of Civic Mining and Environmental Eng, University of Wollongong, 1995.

[22] Ramesh Saagi, Modelling River Water Quality For System-Wide Benchmark Simulation Model, Industrial Electrical Engineering And Automation Faculty Of Engineering, Lund University, Coden:Lutedx/(Teie-7249)/1-22/(2014)

[23] US EPA Dissolved Oxygen and Biochemical Oxygen Demand.http://water.epa.gov/type/rsl/monitoring/vms52.cfm

[24] ESRI ArcView GIS. The geographic information system for everyone. Environmental Systems Research Institute, USA. 1996a

[25] E. Karadurmus, and R. Berber. Dynamic simulation and parameter estimation in river streams. Environmental Technology. 2004, (25), 471-479.

[26] The Math Works Inc. Simulink User Guide, 2015.