# Water Quality Modeling Study for Umhlangane River, South Africa

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#### Abstract

Over the past few decades, river water quality has been a critical issue in many parts of the world due to various domestic, industrial and agricultural pollutants. The challenge lies in developing mechanisms and tools, that will assist us to mitigate, prevent or possibly reverse deteriorating river water quality. Water quality models are the most useful tools in describing river ecological conditions, assessing effects of water pollution and assisting decision makers for water quality management. They can be used to predict the changes of the water quality parameters and also contribute in reducing the cost of labor and time needed to conduct field studies or experiments to some degree. As the Hybrid Cells in Series model a conceptual mixing cells based water quality model that has an advantage over the Fickian based advection dispersion equation model, this paper aimed to assess pollutant transport characteristics of Umhlangane River north of Durban using the proposed model. A main advantage with this model is that it deals with first order ordinary differential equation and which can accommodate any reaction kinetics without any complexity in model equation unlike the Fickian model. Thus this paper derives a new model component and investigates its ability to simulate decaying pollutant decay and dissolved oxygen concentration under predefined condition. The proposed model in this study yielded positive outcome at the lower reach of Umhlangane River with an average agreement between simulation results and the observed data. The work is concluded by rendering a future potential scope of the proposed model to incorporate nutrient dynamics and non-point source pollution.

**Keywords:** Biochemical Oxygen Demand, Chemical Oxygen Demand, Dissolved Oxygen, Peclet Number, Umhlangane River, WQ Model

# 1. Introduction

Water plays an important role in the sustainability of all living beings and in meeting various domestic, agricultural and industrial demands. The increasing scale of water scarcity associated with water pollution problems, has turned water quality management into a pressing issue. Degrading water quality over the past decades has been a serious concern due to the rapidly growing population, resources abuse and industrial revolution<sup>1</sup>, and also for scientific, human and technological developments<sup>2</sup>. It needs to be realised that when water quality conditions worsen, the quantity of water available for usage decreases; however the human dependence on this natural resource remains the same<sup>3</sup>. The consequence of long term water

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pollution is a lack of availability and inadequacy of clean and safe water in many countries around the world<sup>4</sup>. The negative repercussions of water pollution continue to be experienced by the environment and human; it was reported that millions of people die every year as a consequence of water related diseases<sup>5.6</sup>. The main sources of water that are constantly being impaired by pollutants are largely rivers, streams, lakes and underground water. Despite rivers being a major source of water supply, they are commonly used as the primary disposal route for waste water<sup>2</sup>. The contamination of the rivers may lead to serious and costly consequences that might be impossible or difficult to reverse. To improve, protect and to avoid the ecosystem of our water sources being destroyed further, various preventative measures need to be devised. When employing suitable water quality management strategies having limited amount of field data is not feasible, modelling studies are often used to address water pollution problems and to design effective mitigation measures<sup>8</sup>. In order to understand and develop water quality models, it is vital to acquire knowledge about pollutants and pollutant transport processes. Since 1925, many water quality models have been formulated and applied to predict water quality of rivers, lakes and estuaries successfully. The Advection Dispersion Equation (ADE) model is one of the most widely used model for dealing with solute transport challenges. The argument is also owed to the limiting assumptions of the ADE model and estimation difficulties of its parameters<sup>9-12</sup>. The other models like Cells In Series (CIS) and Aggregated Dead Zone (ADZ) came into play because of the practical limitations and applications of the ADE model for the natural rivers<sup>10-18</sup>. Although there were some improvements brought by these alternative models, concerns were also raised about the inadequate advection in the concentration-time (C-t) profile produced by CIS and difficulties with the estimation of ADZ model coefficients. In addition, there are numerous water quality models available: Soil Water and Analysis Tools Model, Water Quality Analysis Simulation Program, MIKE 11, QUALs, the Hydrologic Engineering Centre River Analysis System and many others. The knowledge acquired from these models can be used to equip water managers with proper tools that will assist them to make reasonable water quality predictions and prevent further contamination in our rivers<sup>19</sup>. The use of a suitable model is a common practice for showing the cause and effect of the relationship between pollutants emissions and water quality<sup>20</sup>. This is also best addressed by improving the shortcomings of the existing models. The shortcomings of the CIS and ADZ models were addressed by using the Hybrid Cells In Series (HCIS) model<sup>21,22</sup>. This model has been conceptualised with a plug flow zone and two thoroughly mixed zones of unequal residence time connected in series in order to simulate advection dispersion pollutant transport. As HCIS model has a potential to adequately reproduce the impulse response<sup>21-23</sup>; it was further improved by considering pollutant decay<sup>24-25</sup>. Further to these, an attempt will be made in this paper to enhance the water quality modelling capabilities of the HCIS model by incorporating biochemical oxygen demand (BOD) and chemical oxygen demand (COD) to simulate dissolved oxygen (DO) and to carry out a case study with the pollutant transport along the Umhlangane River using the HCIS model as this is characterized by poor water quality.

# 2. Development of the New Model Component of the HCIS Model

### 2.1 Scope of the Modeling Study

Monitoring and modelling water quality are essential in understanding the behaviour of water pollutants and for devising effective mitigation strategies<sup>26</sup>. The traditional importance of measuring pollutants concentration in a river is to determine their influence on DO. In general, pollutants are measured according to their oxygen demand, which is BOD or COD. These parameters are relatively convenient to measure<sup>8</sup>. In order to achieve and maintain good water quality for a river system, it is important to understand ways of self-purification and governing pollution processes<sup>27,28</sup>. The self-purification process depends on a wide range of parameters. For example, if water is not overloaded with pollutants, an aerobic process will take place and no unpleasant odour will be produced. However, if heavily loaded with pollutants, the biological process becomes anaerobic (i.e. bacteria not utilising free oxygen) producing noxious gases that could be harmful to life<sup>29</sup>. The relation between biological, chemical and physical processes is critical in predicting the impact of an effluent on a river. When organic pollutants are discharged into a water body depletion of dissolved oxygen occurs<sup>30,31</sup> in addition, the decay of pollutants is widely acknowledged and follows the first order reaction kinetics<sup>32</sup>. This is because of the high demand for oxygen by the bacteria responsible for decomposing the pollutants<sup>33</sup>. DO is generated by diffusion of oxygen from the atmospheric air into water and production of oxygen from photosynthesis by aquatic plants. Diffusion from the atmosphere is a relatively slow process, but it is responsible for most of the dissolved oxygen in our rivers. Atmospheric pressure and water temperature affect the ability of water to retain dissolved oxygen. Warm water at low atmospheric pressure holds less dissolved oxygen than cold

water at high atmospheric pressure. Oxygen levels are also affected by the degree of water turbulence or wave action and level of light penetration as well as turbidity, colour and water depth. The dissolved sag curve demonstrates how the DO concentration in a volume of water changes with time and distance after organic material is introduced into water. DO Sag was developed by Burke in the late 1980s<sup>34</sup>. The model is based on a modified version of the Streeter and Phelps equation. The majority of DO models including DO sag is based on the concept of the dissolved oxygen sag curve and the Streeter-Phelps Equation. The following section explains the development of model component of the HCIS model considering decay of pollutants, oxygen depletion and re-aeration processes.

#### 2.2 Conceptualization of the HCIS Model

The HCIS is chosen to be modified for this study, based on the advantages it demonstrated over some of the mixing cells based models. A single unit of this model is capable of reproducing an asymmetric pattern of concentrationtime profile showing a rising limb and a falling limb<sup>22</sup>. This model's behavior is identical to that of the analytical solution of the advection-dispersion equation when the size of the basic hybrid unit is more than  $4D_1/u$ , where  $D_{I}$  = longitudinal dispersion coefficient and u = mean flow velocity. The model comprises of a plug flow zone and two thoroughly mixed zones of unequal residence times as shown in Figure 1. The initial concentration of non-conservative pollutants in each zone is assumed to be zero and the boundary concentration changes from 0 to  $C_{p}$  at t = 0. The fluid is substituted in a time  $\alpha$  in the plug flow zone, and is equal to the ratio of the volume of plug flow zone to the flow rate. The residence time of the



Figure 1. Conceptual Hybrid-Cells-in-Series model<sup>25</sup>.

fluid in the first and second thoroughly mixed zones are denoted as  $T_1$  and  $T_2$  respectively. The flow rate is Q m<sup>3</sup>/ unit time and flow is assumed to be under a steady-state condition.

A mass balance equation is formulated for a control volume within the pollutant front considering decay of both BOD and COD to simulate DO concentration as given below Eq. (1).

$$Q\Delta t C_{DO}(x,t) - k_1 A \Delta x C_B(x,t) \Delta t$$
  
- $k'_1 A \Delta x C_C(x,t) \Delta t + k_2 A \Delta x \left[ S_{DO} - C_{DO}(x,t) \right] \Delta t$   
=  $Q\Delta t C_{DO}(x + \Delta x, t + \Delta t)$  (1)

where,  $S_{DO}$  = saturated DO concentration, A = cross sectional area of the flow,  $C_B(x, t)$  = BOD concentration,  $C_C(x, t)$  = COD concentration,  $\Delta x$  = length of the hybrid cell,  $C_{DO}(x, t)$  = DO concentration,  $k_1$  = Decay rate coefficient of BOD,  $k_1'$  = Decay rate coefficient of COD,  $k_2$ = Re-aeration rate coefficient. Eq. (1) is subjected to the initial and boundary conditions as, C(x, 0)=0 for x > 0;  $C(0,t)=C_R$  for t ≥ 0;  $C(\alpha u, t)$ =0 for 0< t<  $\alpha$ ;  $C_{DO}(x, 0)=S_{DO}$ for x > 0 and  $C_{DO}(0,t)=S_{DO}-D_O$  for t ≥ 0, where  $D_O$  is the boundary deficit of DO.

It needs to be noted that the effluent (Solution of Eq. (1)) from the plug flow becomes the influent for the first thoroughly mixed cell. A similar mass balance equation is formulated for first thoroughly mixed cell after solving Eq. (1).

$$V_{1} \Delta C_{DO} = \begin{cases} C_{B} \left( \frac{k_{1}}{k_{2} - k_{1}} \right) \left[ e^{-k_{1}\alpha} - e^{-k_{2}\alpha} \right] U(t - \alpha) \\ + C_{C} \left( \frac{k_{1}'}{k_{2} - k_{1}'} \right) \left[ e^{-k_{1}'\alpha} - e^{-k_{2}\alpha} \right] \\ U(t - \alpha) + D_{0}e^{-k_{2}\alpha}U(t - \alpha) \end{cases} \end{cases} \begin{cases} Q\Delta t \\ - C_{DO}Q\Delta t - k_{1}V_{1}C_{B}\Delta t - k_{1}'V_{1}C_{C}\Delta t + k_{2}V_{1}(S_{DO} - C_{DO})\Delta t \end{cases}$$

$$(2)$$

Effluent concentration from first thoroughly mixed cell is derived by solving Eq. (2) which forms influent to the second. Successively, a mass balance equation is formulated for the second thoroughly mixed cell as follows:

$$\begin{cases} S_{DO} - \left\{ C_{B}U(t-\alpha) \left( \frac{k_{1}}{k_{2}-k_{1}} \right) \left( \frac{1}{1+k_{2}T_{1}} \right) \left( e^{-k_{1}\alpha} - e^{-k_{2}\alpha} \right) \left[ 1 - e^{-\left( \frac{1+k_{2}T_{1}}{T_{1}} \right) \left[ t-\alpha \right]} \right] \right] \\ + C_{B}U(t-\alpha) e^{-k_{1}\alpha} \left( \frac{T_{1}k_{1}}{1+k_{1}T_{1}} \right) \left( \frac{1}{1+k_{2}T_{1}} \right) \left[ 1 - e^{-\left( \frac{1+k_{2}T_{1}}{T_{1}} \right) \left[ t-\alpha \right]} \right] \\ - C_{B}U(t-\alpha) e^{-k_{1}\alpha} \left( \frac{k_{1}}{k_{2}-k_{1}} \right) \left( \frac{1}{1+k_{1}T_{1}} \right) \left[ e^{-\left( \frac{1+k_{1}T_{1}}{T_{1}} \right) \left[ t-\alpha \right]} - e^{-\left( \frac{1+k_{2}T_{1}}{T_{1}} \right) \left[ t-\alpha \right]} \right] \\ + C_{C}U(t-\alpha) \left( \frac{k_{1}'}{k_{2}-k_{1}'} \right) \left( \frac{1}{1+k_{2}T_{1}} \right) \left( e^{-k_{1}\alpha} - e^{-k_{2}\alpha} \right) \left[ 1 - e^{-\left( \frac{1+k_{2}T_{1}}{T_{1}} \right) \left[ t-\alpha \right]} \right] \\ + C_{C}U(t-\alpha) e^{-k_{1}\alpha} \left( \frac{T_{1}K_{1}'}{1+k_{1}'T_{1}} \right) \left( \frac{1}{1+k_{2}T_{1}} \right) \left[ 1 - e^{-\left( \frac{1+k_{2}T_{1}}{T_{1}} \right) \left[ t-\alpha \right]} \right] \\ - C_{C}U(t-\alpha) e^{-k_{1}\alpha} \left( \frac{K_{1}'}{k_{2}-k_{1}'} \right) \left( \frac{1}{1+k_{1}'T_{1}} \right) \left[ e^{-\left( \frac{1+k_{1}T_{1}}{T_{1}} \right) \left[ t-\alpha \right]} - e^{-\left( \frac{1+k_{2}T_{1}}{T_{1}} \right) \left[ t-\alpha \right]} \right] \\ + D_{0}U(t-\alpha) e^{-k_{1}\alpha} \left( \frac{k_{1}'}{k_{2}-k_{1}'} \right) \left( \frac{1}{1+k_{1}'T_{1}} \right) \left[ e^{-\left( \frac{1+k_{1}T_{1}}{T_{1}} \right) \left[ t-\alpha \right]} - e^{-\left( \frac{1+k_{2}T_{1}}{T_{1}} \right) \left[ t-\alpha \right]} \right] \\ - \frac{C_{DO}'X - \frac{1}{12} B\Delta - k_{1}' 2 C\Delta + \frac{2}{2} \left( DO - DO \right) \Delta$$

Dissolved oxygen concentration at the end of all the cells of the model are derived by solving Eq. (3).

The convolution technique is applied for the dissolved oxygen of second and subsequent hybrid units using discrete kernel approach as follows:

$$D(n,t) = \int_{0}^{t} C[(n-1),\tau] k_{D}(t-\tau) d\tau$$
(4)

where C(n-1) is the concentration of pollutant at the end of (n-1)th cell and  $K_D$  is the impulse deficit of DO. Dissolved oxygen concentration along the river is the simulated by substituting solution of Eq. (4) in  $C_{DO} = S_{DO} - D$ .

The HCIS model parameters have to be estimated as descripted in<sup>21-23</sup> to simulate pollutant transport with prior estimation of mean flow velocity and longitudinal dispersion coefficient. This paper estimates  $D_L$  using empirical relationship suggested by Etemad-Shahidi and Taghipour<sup>35</sup>.

### 3. Results and Discussions

The Umhlangane River in South Africa is considered in this paper for applying the proposed model to simulated DO concentrations. The river is encircled by areas with industrial activities especially from Phoenix, Avoca, Effingham and a portion of the Springfield flats. There are also commercial areas in KwaMashu Town Centre, Inanda MR93, Phoenix, Mt. Edgecombe and various institutional areas as shown in Figure 2.



**Figure 2.** Google image of Umhlangane River and various data collection points and location of study area.

Having the data collected from this study area, the reaeration rate<sup>32</sup> and longitudinal dispersion coefficient<sup>35</sup> are estimated as 0.22 per day and 212.58m<sup>2</sup>/min respectively. The estimation of  $k_2$  and  $D_L$  require flow and channel characteristic for all the reaches. Due to the lack of channel depths along the river, having one set of measured values

at the upper reach,  $D_L$  has been estimated and assumed the same for all the reaches. The reach lengths along the river are measured from Google image. The flow and water quality data were collected from Ethekwini water and sanitation division and are listed in Table 1. Table 1 also shows the reach-wise lengths and the HCIS model's time parameters for these reaches and number of hybrid units required for each reach of the river.

The model parameters were calculated based on the data ( $D_1$ , u and  $\Delta x$ ) using the empirical relationships suggested in<sup>22</sup>. Thus those values vary reach-wise. The model simulations have been carried out using the model developed with having above set data provided and COD and DO concentrations are plotted in Figures 3a and 3b. This is noted that the BOD concentrations are not available from the data source, thus BOD input was taken as zero in the model for the simulation. The simulation results for the model were produced reach by reach in terms of COD and DO ie., spatial variation. In Figure 3(a), it can be seen that the graph starts at a high COD concentration and then decreases until it reaches a distance of 15000m at which it then vertically increases due to WWTW discharge and then decreases again.

From Figure 3(a) the observed and simulated data are closely matching each other except at 3130m. The observed COD concentration is 49mg/l whereas the simulated COD concentration is 36mg/l. This could also be due to the variation in rate constants in the river reaches or pollutant discharge into the river from other point or non-point sources that were not investigated in this research. However in this research, the geometry was taken to be prismatic and the flow was taken to be fixed throughout the entire river that resulted in a decay rate used that could have been slightly different from the actual decay rate. The section of river passes through an area that is high in urban and industrial activities. There are also reports of informal settlements that lead directly into the river. The increase in COD concentration due to these activities were no considered as inputs into the model and could as be the reason as to why there is a difference in the simulated and observed results at 3130m. The reason that these inputs were not considered is due to

Table 1. HCIS parameters for calibration and observed WQ data

Parameters \ Reaches	R15-R14	R14-R13	R13-R12.9	R12.9-R12.8	R12.8-R12.7
COD (mg/L)	64	49.5	68	67	50.5
DO (mg/L)	4.7	6	6.4	4.3	5.1
Flow velocity (m/min)	8.4	8.9	7.9	8	8.3
$D_{L}$ (m <sup>2</sup> /min)	212.58	212.58	212.58	212.58	212.58
P <sub>e</sub>	8.36	8.36	8.36	4.36	8.36
K <sub>1</sub> (BOD) (1/min)	0.001	0.001	0.0019	0.001	0.001
$K_1(COD)$ (1/min)	0.0015	0.0015	0.019	0.0015	0.0015
K <sub>2</sub> (re-aeration)(1/min)	0.22	0.22	0.22	0.22	0.22
Reach length (m)	2130	1420	11480	500	1900
Number of Hybrid units	10	7	54	4	9
Size of Hybrid unit	211.5	200.0	215.2	115.8	214.1



Figure 3. COD concentration, (b) DO concentration along Umhlangane River.

no data on these activities. For more accurate representation of the simulated results, the model will have to be improved to incorporate the geometry and flow conditions of the river as being non-uniform so that the decay rate can be determined as the geometry and flow velocity of the river changes. Figure 3(b) shows DO concentration along the river reaches. It is noted from the Figure 3(b) that the simulated data does not reach the saturated DO level of 9.1mg/l. This is due to continues discharge of pollutant into the river and the decay rates of the pollutants being much higher than the re-aeration rate. These impacts negatively on the ecosystem of the river. The low DO concentration of less than 3.9mg/l is of concern as continuous exposure to such conditions impacts negatively on the rivers ecosystem.



**Figure 4.** Temporal variation of DO concentration at the end of reach R12.9

Having the same set of model parameters as shown in Table 1 and with the continuous measurement of DO concentration over a period of 9 months were compared with simulated results by the HCIS model. This comparison was carried out to understand temporal variations of DO and HCIS model performance for a given point (R12.9) temporally and shown in Figure 4. It can be noted from the Figure 4 that the HCIS responses are in agreement with observed temporal data collected from R12.9 except few dates. That could be due to rain events or increased effluent discharge from WWTW or catchment flush due to rains for example on 02/03/2014, the DO concentration was very low due to high pollutant entry into the river. These results demonstrate that the proposed model component reasonably simulates which matches with observed data set under limited conditions.

### 4. Conclusion

The performance of the HCIS model was evaluated by comparing the model simulations with the observed data. The simulation results were then assessed in view of the possibility of improving water quality of Umhlangane River. In meeting the objectives of this paper, the HCIS model was upgraded by modified from<sup>25</sup>, to incorporate BOD and COD into the original mass-balance equation and investigated by performing a water quality analysis of Umhlangane River. The analysis of the simulated water quality results generated by this model yielded some promising outcomes when compared to the actual recorded data. The modified HCIS model with the inclusion of BOD and COD into the mass balance equation yielded positive outcome at the lower reach, where there was a reasonable agreement with the observed data. With this kind of performance, any user who chooses to employ this model should be able to run it with some degree of confidence in predicting future water quality of the river under investigation. The utilities such as WWTW that are built along the rivers to reduced level of water deterioration, however, sometimes create water quality problems. The use of chloramines for disinfection can result in excessive growth of nitrifying bacteria. The continuous oxidation of nitrites into nitrates and of ammonia into nitrites can result in serious negative effects in water bodies<sup>36,37</sup>. Another cause of water quality changes is orthophosphate. It is found in wastewater and naturally as Phosphates. If discharged in large quantities it may stimulate the growth of aquatic organisms in an undesirable manner<sup>38</sup>. Therefore testing and removal of phosphorus from effluent is critical to these rivers' water quality. The effect of acid deposition can also be harmful to most aquatic systems if it is lower than 5. The pH, oxygen and alkalinity reduction is a result of chloramine residuals that increase in heterotrophic bacteria by autotrophic creation of soluble microbial products<sup>39</sup>. The high level of nutrients produced above the levels of their consumption increases biological oxygen demand at bottom layer of the water column where density stratification interferes with reaeration<sup>40</sup>. Therefore, serious caution needs to be exercised when considering the variation of re-aeration, decay rates of BOD and COD coefficients. The advantage with this model is that any specific point of interest along the river could be chosen and analysed in terms of DO, BOD and COD. The disadvantage with this model is that the BOD and COD inputs of the pollutants are assumed to be of average constant values. This neither reflects nor takes into account the fluctuations of the pollutants loading which take place at different times. The model is flexible enough and has the capacity for the addition of any other parameters.

Due to the complexity of the processes involved in river systems, continuous research is essential for further develop the models focusing nutrient dynamics, nonpoint source pollutions and channel and flow variations.

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