Mathematical model was developed and evaluated to monitor and predict the groundwater characteristics of Trans-amadi region in Port Harcourt City. In this research three major components were considered such as chloride, total iron and nitrate concentration as well as the polynomial expression on the behaviour on the concentration of each component was determined in terms of the equation of the best fit as well as the square root of the curve. The relationship between nitrate and distance traveled by Nitrate concentration by the model is given as \( P_c = 0.003x^2 - 0.451x + 14.91 \) with coefficient of determination, \( R^2 = 0.947 \), Chloride given as \( P_c = 0.000x^2 - 0.071x + 2.343 \), \( R^2 = 0.951 \) while that of Total Iron is given as \( P_c = 2E^{-05}x^2 - 0.003x + 0.110 \), \( R^2 = 0.930 \). All these show a strong relationship as established by Polynomial Regression Model. The finite element techniques are found useful in monitoring, predicting and simulating groundwater characteristics of Trans-amadi as well as the prediction on the variation on the parameters of groundwater with variation in time.

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Capsule Summary: The mathematical model developed was found useful in monitoring and predicting the rate of underground water characteristics upon the influence of diffusion and spreading on the concentration of chloride, total iron and nitrate. The concept of finite element method was applied on this study and result obtained revealed the significance of the developed model in simulating the variation on the concentration of components considered upon the influence of distance and the controlling factors.


INTRODUCTION

Water quality is what mankind needs, since the useful of water is paramount for once health as well as for agricultural purposes. In the Niger Delta area of Nigeria source of good water in some regions is becoming imposable due to high level of contamination of the surface and subsurface water. The degree of migration of these contaminants from one zone to the other leads to further contamination of regions that were not initially contaminated to experience high level of contamination as well. In this investigation some elements were monitored to evaluate the impact on the under groundwater characteristics as water travels from point to the other on the subsurface water environment and the
variation on the physicochemical parameters of these components are of paramount interest to the engineers.

British Standards Institution defines portable water as that suitable for drinking and culinary purposes as well as the water quality definition is a function of the intended use (Ukpaka et al., 2004, 2005, 2006). The main concern of the municipal water analyst is to ensure that corporate water supplies are wholesome and fit for human consumption (Ukpaka, 2006, 2005). A great number of natural waters are portable without the necessity of purification by man (Ukpaka et al., 2004a, 2005a, 2006a, 2007, Ogoni and Ukpaka, 2004, Tebbutt, 1979, Udom, 2002 and Ukpaka and Oboho, 2006; Iqbal, 2016).

Research conducted revealed that water can be classified as good water only if it must be free of pathogenic organisms, toxic substances and overdose of minerals and organic materials; to make it pleasant. It should be free of colour, turbidity, taste and odour, moreover it should contain high enough oxygen content and it should have a suitable temperature. Based on the definition of portable, natural well waters containing large amount of dissolved solids and gases may be considered wholesome and healthy. Such impurities are acceptable under the definition of portable water (Ukpaka and Ikonyiri, 2004., Ukpaka et al., 2004b, 2005b, 2006b, 2007 and ). It must be pointed out that portable water is not suitable for the recruitments of science, medicine and industry where it serves as the feed water or raw water for further purification (Ukpaka, 2004a, 2005a, 2006a, Udom et al. 1999, Short and Stauble, 1967, Nwaogazie, 1992., Derrick et al., 2005 and Jaco, et al., 2006)

For example, in pharmaceutical industries, purified water must be sterile, free from living micro-organisms and apyrogenic free from the fever producing products or microorganism as well as being of high chemical purity (Ukpaka, 2006b, 2005b). Portable water is, however, far from being chemically pure and may contain bacteria which are harmless when ingested orally but unacceptable for pharmaceutical uses. Also, in electronic industry, ultra-pure water is used in the manufacture of printed circuits, semiconductors, transistors and integrated circuits (DPR, 1990., Hallberg, 1989., Nwaogazie, 1991 and Offodile, 1992). It serves as single purpose-cleaning. Cleansing or decontamination of the active crystal surface is very important for the proper functioning and long term stability of electronic devise. Ultra – pure water proved to be the most efficient medium for the cleaning with purity of more than 99% (Etu-Efetor, 1981, Lawrence, 1990 and OCED, 1986).

Similarly, for most applications in food and drink industries, portable water supply has to be further upgraded or purified to a quality level acceptable to the production of canned or frozen food and drinks (Davis and Weist, 1966., Joseph, 1989., Reymert, 1965., Kuichling, 1989., Domenico, 1972 and Ukpaka, 2004b, 2005c, 2006c). The Port Harcourt bore holes are intended for drinking and culinary purposes. The supplies are abstracted from deep wells and are low in suspended solid. Water loach explains that deep water are safe to drink without sterilization— in contrast to water from shallow wells, because during percolation, the water loses its organic matter live or dead, and so comes out of the ground with low level of organic and bacteria impurity. Water, (1987) further explains that the percolation let the water leach soluble materials out of the minerals using acidity due to dissolved CO2 (carbondioxide). These waters tend to have high total dissolved solid (TDS) values and most of the TDS will be calcium bicarbonate. The percolation and its associated leaching process eliminate acidity and hence the pH will be on alkaline side (Ababio, 2004, Reghunath, 1985., John, 1992, Edet, 1993., Ukpaka, 2004,2005, 2006d, 2007a, 2009 and Nwaogazie, 1990). In contrast, borehole water from Port Harcourt sites in however not alkaline, it is acidic with very low TDS values it appears that the Port Harcourt acidic rain retains its acidic pH during percolation through the earth into the borehole. The low quantity of carbonate content of Port Harcourt borehole sites evaluated might be an indication that there is low or no presence of limestone or dolomite in the geological formation of the area (Ukpaka, et al., 2005c,d., 2006 c,d). From the synopsis above, the quality of water therefore for various purposes depends on the concentration of these substances. However, excess concentrations of these substances have posed a great environment danger to life.

MATERIAL AND METHODS

Groundwater parameters distribution prediction through Finite Element Method

The assessment and prediction of groundwater parameters is simulated using the governing equation of groundwater mass transport defined as;

$$\frac{\partial c}{\partial t} = D_x \frac{\partial^2 c}{\partial x^2} + u \frac{\partial c}{\partial x}$$  \(1\)

Equation (1) is the governing differential equation for one dimension flow state mass transport model. Let $C = P_c = \text{Groundwater Parameters } \text{concentration}$  

Equation (1) becomes, 

$$\frac{\partial P_c}{\partial t} = D_x \frac{\partial^2 P_c}{\partial x^2} + u \frac{\partial P_c}{\partial x}$$  \(2\)

$D_x$ = hydrodynamic dispersion, $U_x$ average fluid velocity in x – direction

Galerkin’s Finite Element Formulation Method

Applying the finite element method to obtain a solution to equation (1), the mass transport functions and the domains are dieselized into elements and groundwater concentration are determined at each node. For this investigation linear shape function is chosen and is given as:

Step A: Linear element approach

$$p_c(x) = N_{ie} P_{ci} + N_{ie+1} P_{ci+1} = [N] [P_c]$$  \(3\)

Note, 

$$N_{ie} = 1 + \frac{x}{l}$$  \(4\)
Considering that the linear shape or approximation functions of element at nodes $i$ and $i+1$.

**Step B: Formation of element Equation**

Galerkin’s Weighted Residual Method is the basis of the element formation equations of the governing equation (equation (2)), by Galerkin’s Principles is as follows;

$$\int_{0}^{1} N^T \left( D_x \frac{\partial^2 p_c}{\partial x^2} - \frac{u_x \partial p_c}{\partial x} - \frac{\partial p_c}{\partial t} \right) dx = 0$$

(6)

**Step C: Assembling element equation in global equation**

Assuming one-dimensional stretch, the divided element generated were assemble to produce the element assemblage for the governing equation (1) which gives the prediction of groundwater parameters interaction at each node.

**Evaluation of groundwater velocity**

Velocity in equation (1) was determined using Darcy’s Law. The hydraulic gradient of the study areas in Port Harcourt was investigated and evaluated. Discharge velocity equation by Darcy’s is given as:

$$V = K I$$

(7)

Where, $I$ = state hydraulic gradients (m/m), $V$ = groundwater velocity and $K$ = state permeability ($m$/day).

Therefore, the actual velocity of flow of the studied area,

$$V_a = \frac{V}{\eta}$$

(8)

Where, $\eta$ = Porosity (%) and $V_a = U_x$

The individual terms of equation (6) is evaluated by linear shape functions of finite element method as follows:

1st term evaluation

$$\int_{0}^{1} N^T \left( D_x \frac{\partial^2 p_c}{\partial x^2} \right) dx = \int_{0}^{1} N^T \frac{\partial}{\partial x} \left( [N] [p_c] \right) dx$$

(9)

2nd term evaluation

$$\int_{0}^{1} N^T \left( U_x \frac{\partial p_c}{\partial x} \right) dx = \int_{0}^{1} N^T \left( U_x \frac{\partial}{\partial x} [N] [p_c] \right) dx$$

(11)

3rd term evaluation

$$\int_{0}^{1} N^T \frac{\partial p_c}{\partial t} dx = \frac{L}{6} \left[ \begin{array}{c} 2 \\ 1 \\ 2 \end{array} \right]$$

(13)
Putting equation (10), equation (12) and equation (13) into equation (6), we have

\[
\begin{vmatrix}
\frac{dx}{t} & 1 & -1 & 0 & 0 & 0 \\
1 & -1 & \frac{u_c}{2} & 1 & \frac{L}{2} & 1 \\
\end{vmatrix}
\begin{vmatrix}
|p_c_1| \\
\end{vmatrix}
= \begin{vmatrix}
|p_c_2| \\
\end{vmatrix}
\]

(14)

Considering \(k_1 = \frac{D_x}{L}\) and \(\frac{u_c}{2}\)

\[
\begin{vmatrix}
-k_1 + k_2 & 0 & 0 & 0 & 0 \\
-k_1 + k_2 & 2k_1 & -k_1 - k_2 & 0 & 0 \\
0 & -k_1 + k_2 & 2k_1 & -k_1 + k_2 & 0 \\
0 & 0 & -k_1 + k_2 & 2k_1 & -k_1 - k_2 \\
0 & 0 & 0 & -k_1 + k_2 & k_1 - k_2 \\
\end{vmatrix}
\begin{vmatrix}
|p_c_1| \\
|p_c_2| \\
|p_c_3| \\
|p_c_4| \\
|p_c_5| \\
\end{vmatrix}
= 0
\]

(15)

\[
\begin{vmatrix}
36.16 & 15.26 & 0 & 0 & 0 \\
14.32 & 72.32 & 15.26 & 0 & 0 \\
0 & 14.32 & 72.32 & 15.26 & 0 \\
0 & 0 & 14.32 & 72.32 & 15.26 \\
0 & 0 & 0 & 14.32 & 36.16 \\
\end{vmatrix}
\begin{vmatrix}
|p_c_1| \\
|p_c_2| \\
|p_c_3| \\
|p_c_4| \\
|p_c_5| \\
\end{vmatrix}
= 0
\]

(16)

**RESULTS AND DISCUSSION**

Prediction of Groundwater parameters for trans-amadi groundwater velocity of trans-amadi area

\[
V = \frac{kdh}{dx}
\]

\[
V = K \times 100 = 0.009 \frac{m}{day} \times 65.5
\]

\[
V = 0.563 \frac{m}{day}
\]

Actual velocity, \(U_x = 2.81 \frac{m}{day}\) and \(D_x = 0.025 \frac{m^2}{day}\)

\[
k_1 = 0.001 \frac{m}{day}\] and \(k_2 = 1.41 \frac{m}{day}\)

Substituting the values of \(L\), \(k_1\) and \(k_2\) into equation (16), we have

\[
\begin{vmatrix}
1 & 0 & 0 & 0 & 0 \\
14.32 & 72.32 & 15.26 & 0 & 0 \\
0 & 14.32 & 72.32 & 15.26 & 0 \\
0 & 0 & 14.32 & 72.32 & 15.26 \\
0 & 0 & 0 & 14.32 & 36.16 \\
\end{vmatrix}
\begin{vmatrix}
|p_c_1| \\
|p_c_2| \\
|p_c_3| \\
|p_c_4| \\
|p_c_5| \\
\end{vmatrix}
= 0
\]

(17)

Predicting Nitrate interaction of Trans-amadi from the borehole to a considered distance of 100 m

Substituting initial concentration \(p_{c_1} = 2.5\) mg/l and applying upstream boundary condition to equation (18), we have

\[
\begin{vmatrix}
1 & 0 & 0 & 0 & 0 \\
14.32 & 72.32 & 15.26 & 0 & 0 \\
0 & 14.32 & 72.32 & 15.26 & 0 \\
0 & 0 & 14.32 & 72.32 & 15.26 \\
0 & 0 & 0 & 14.32 & 36.16 \\
\end{vmatrix}
\begin{vmatrix}
|p_c_1| \\
|p_c_2| \\
|p_c_3| \\
|p_c_4| \\
|p_c_5| \\
\end{vmatrix}
= 0
\]

(18)

Solving equation (19), we have

\[
\begin{vmatrix}
p_{c_1} \\
p_{c_2} \\
p_{c_3} \\
p_{c_4} \\
p_{c_5} \\
\end{vmatrix}
= \begin{vmatrix}
2.5 \\
-0.52 \\
0.11 \\
-0.02 \\
0.009 \\
\end{vmatrix}
\]

Predicting Chloride \((\text{cl}^-)\) concentration from the borehole to a considered distance of 100 m.

Initial chloride concentration \(p_{c_1} = 15.9\) mg/l, Putting this values into equation (18) and solving it gives,
Predicting Total iron \( (F_c) \) concentration from the borehole to a considered distance of 100m.

Initial total iron concentration \( p_{c1} = 0.12 \text{mg/l} \), solving equation (18) for 0.12mg/l gives:

\[
\begin{array}{c|c}
p_{c1} & 0.12 \\
p_{c2} & -0.02 \\
p_{c3} & 0.006 \\
p_{c4} & 0.001 \\
p_{c5} & 0.0004 \\
\end{array}
\]

\[
\frac{mg \text{ Total Iron}}{m}
\]

Predicting Total iron \( (F_c) \) concentration from the borehole to a considered distance of 100m.

Initial total iron concentration \( p_{c1} = 0.12 \text{mg/l} \), solving equation (18) for 0.12mg/l gives:

\[
\begin{array}{c|c}
p_{c1} & 15.96 \\
p_{c2} & -3.30 \\
p_{c3} & 0.68 \\
p_{c4} & -0.15 \\
p_{c5} & 0.06 \\
\end{array}
\]

Prediction of groundwater parameters interaction by Galerkin’s finite element

Figure 1 shows the relationship between groundwater parameter concentration and distance traveled by parameters for Trans-Amadi area in Port Harcourt. The relationship between nitrate and distance traveled by nitrate concentration by the model is given as \( P_c = 0.003x^2 - 0.451x + 14.91 \) with coefficient of determination, \( R^2 = 0.947 \), chloride given as \( P_c = 0.000x^2 - 0.071x + 2.343 \), \( R^2 = 0.951 \), while that of Iron is given as \( P_c = 2E-05x^2 - 0.003x + 0.110 \), \( R^2 = 0.930 \). All these show a strong relationship as established by Polynomial Regression Model.

The Figure 1 illustrates the behavior of groundwater parameters concentration upon distance traveled and also, this indicate that water parameters can migrate from a point to another. Based on this fact, that is the reason why simulation, prediction and monitoring of groundwater parameters using Galerkin’s Finite Element Method were used to simulate the mass transport of groundwater parameters concentration within Trans-Amadi area in Port Harcourt upon a given distance. The pollution is increasing and resultantly groundwater is contaminating (Adrover et al., 2017; Bishop et al., 2017; Bradley et al., 2016; Bricker et al., 2017; Fackrell et al., 2016; Fisher et al., 2016; K’Oreje et al., 2016; LaGro et al., 2017; Lamastra et al., 2016; Ma et al., 2016a; Ma et al., 2016b; Richardson et al., 2017; Robertson et al., 2016; Sanciolo and Gray, 2017; Yan et al., 2017a; Yan et al., 2017b). The integration of finite element techniques is proved to efficient technique for evaluation of trans-Amadi groundwater parameters and could possibly be used for the monitoring of ground water to evaluate the effect of pollution on water quality (Alaboodi and Hussain, 2017; Awais et al., 2017; Boffi and Stenberg, 2017; Hedayat et al., 2017; Jacques et al., 2017; Jeong et al., 2017; Keith et al., 2017; Lee et al., 2017; Liu et al., 2017; Lostado Lorza et al., 2017; Mironova et al., 2017).

CONCLUSIONS

The finite element technique is found useful in monitoring and predicting groundwater characteristics upon the influence of migration of contaminants from point to the other. The velocity of groundwater charge is a contributing factor that influences the rate of contaminants filtration. The degree of the functional parameters decreases with increase in the distance. The investigation can be validated by applying numerical evaluation on the experimental obtained data, to predict the concentration of each component in between points with variation in distance as well as variation in time. The trans-amadi zone of Port Harcourt is an industrial area where the level of contaminants generated is high as well as the groundwater characteristics is induced by these activities. The individual terms was evaluated by linear shape functions of finite element method.

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