Modelling and Simulation of Inorganic Ions Migration in Soil Water

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Abstract

This paper proposes some developed mathematical model equations for predicting the migration of ions in soil water in Minna, Nigeria using the principle of conservation of mass. The model was simulated for four ions (Na^+, K^+, Ca^{2+} and NO_3^-) at seven different sites (Jebba, Bida, Shiroro, Izom, Kutigi, Agaie, and Borgu) for five consecutive years using Mathcad 14 software. The simulated results were compared numerically with the experimental results. The result of the comparison shows that the simulated results compares favourably with the experimental results with slight variation which could be attributed to certain assumptions taken during the development of the model. The developed model is a good representation of the migration of four ions in soil water. This model predictions are a welcome development for the river basin authorities, which give greater control of the migration of these ions within the affected regions and indication of concentration depletion of the ions for effective management.

Key words: Migration, soil water, sodium, potassium, calcium, nitrate.

1. Introduction

Soil water contains dissolved ions that are in constant migration from one area or site to another within the soil profile. The concentration of a particular ion in soil water depends on the solubility of the ion in soil and the rate of migration of this ion in the soil water (Anderson, 1984). Some of these ions are essential plant mineral nutrient elements existing in soil solution while others are toxins resulting from various pollution activities on the soil. Traditionally, soil and agricultural scientist have been interested in an effective usage of the available resources to

maximize product yield (Feike and Martinus, 2001). The recent concern by the Federal Government of Nigeria on the quality of farming is a major impetus for the study of ion migration in soil water (Daniel and Ihechituru, 2011).

The migration of ions through soil is determined by the transference of water and different forms of chemical and physical interactions between the ions and the soil (Adeniyi et al., 2005; Odigure and Adeniyi 2003a, Davidson, 1989; Kinzelbach, 1987). Some basic mode of ion transportation process in soil water are mass flow and diffusion (Charles and David, 1991). The mass flow called advection transport is responsible for the vertical displacement of soluble ions through the soil and it involves the movement of the bulk fluid. Diffusion on the other hand is the movement of the ions as a result of concentration gradient occurring between two points in the soil. Most ions in the soil water move by this mechanism, movement taking place from areas of higher concentration to areas of lesser concentration. The movement of ions in soil water is affected by the principle of adsorption which causes the immobilization of solute in soil water (Adeniyi *et al*., 2005; Odigure and Adeniy 2003a,b; Adeniyi, 2005; Joan and Bert, 1992). This paper focuses on the development and simulation of the migration of ions present in soil water in Minna, Nigeria using MATHCAD 14.

2. Conceptualisation of the Model

Some assumptions were made in the development of the models these include: Ion transport in the soil is governed by the principle of diffusion and advection. Ion transport is impeded by retardation due to linear equilibrium adsorption and ion exchange. Reaction is negligible. Diffusion transport is defined by Fick's law. Ion responds only to concentration gradient, electric field gradient is negligible. Transport takes place in the z-direction only and there is no fertilizer application and human activities on the soil during the years under consideration.

2.1 Development of the Model Equation

The material balance on the soil water system is given below:

(Rate of accumulation of ions) = (rate of ion inflow by advection + rate of inflow by diffusion) − (Rate of outflow by advection + Rate of outflow by diffusion) ± (rate of generation)   (1)

Equation (1) can also be represented by Equations (2 - 7)

Accumulation = Input − output ± generation   (2)

$$\text{Rate of accumulation} = \frac{\partial C}{\partial t}(A\,dz) \tag{3}$$

$$\text{Rate of inflow by advection} = FC|_z \tag{4}$$

$$\text{Rate of inflow by diffusion} = -(DA)\frac{\partial C}{\partial z}\Big|_z \tag{5}$$

$$\text{Rate of outflow by convection} = FC|_{z+dz} \tag{6}$$

$$\text{Rate of outflow by diffusion} = -(DA)\frac{\partial C}{\partial z}\Big|_{z+dz} \tag{7}$$

Where C is ion concentration, A is soil surface area, F is volumetric flow rate, D is diffusion coefficient and z is distance in z-direction. Assuming that generation is equal to zero. Substituting equations (3) to (7) into Equation (1), we obtain Equations (8-10).

$$\frac{\partial C}{\partial t}(A\,dz) = FC|_z - (DA)\frac{\partial C}{\partial z}\Big|_z - FC|_{z+dz} + (DA)\frac{dC}{dz}\Big|_{z+dz} \tag{8}$$

Rearranging to obtain Equation (9) and (10),

$$\frac{\partial C}{\partial t}(A\,dz) = FC|_z - FC|_{z+dz} - (DA)\frac{\partial C}{\partial z}\Big|_z + (DA)\frac{dC}{dz}\Big|_{z+dz} \tag{9}$$

$$\frac{\partial C}{\partial t}(A\,dz) = -[FC|_{z+dz} - FC|_z] + DA\left[\frac{\partial C}{\partial z}\Big|_{z+dz} - \frac{\partial C}{\partial z}\Big|_z\right] \tag{10}$$

Dividing through by Adz, we have Equation (11);

$$\frac{\partial C}{\partial t} = -\frac{F}{A}\left[\frac{C|_{z+dz} - C_z}{dz}\right] + D\left[\frac{\frac{\partial C}{\partial z}\Big|_{z+dz} - \frac{\partial C}{\partial z}\Big|_z}{dz}\right] \tag{11}$$

Taking limit as dz tends to zero gives Equations (12 and 13),

$$\frac{\partial C}{\partial t} = \lim_{dz \to 0}\left[-\frac{F}{A}\left[\frac{C|_{z+dz} - C_z}{dz}\right] + D\left[\frac{\frac{\partial C}{\partial z}\Big|_{z+dz} - \frac{\partial C}{\partial z}\Big|_z}{dz}\right]\right] \tag{12}$$

$$\frac{\partial C}{\partial t} = -\left(\frac{F}{A}\right)\frac{dC}{dz} + D\frac{d^2C}{dz^2} \tag{13}$$

The ratio of volumetric flow rate to area, $\left(\frac{F}{A}\right)$ gives velocity, *u*, so that we have Equation (14)

$$\frac{dC}{dt} = -u\frac{dC}{dz} + D\frac{d^2C}{dz^2} \tag{14}$$

Modifying Equation (14) to include the adsorption term of Equation (15), (Eliezer, 1992)

$$\frac{dC}{dt} = -\frac{\rho K_d}{\theta}\frac{dC}{dt} \tag{15}$$

Where $\rho =$ density, $K_d =$ distribution coefficient, $\theta =$ effective porosity. Incorporating the adsorption term into Equation (14), we have (16);

$$\frac{dC}{dt} = -u\frac{dC}{dz} + D\frac{d^2C}{dz^2} - \frac{\rho K_d}{\theta}\frac{dC}{dt} \tag{16}$$

Collecting like terms gives Equation (17),

$$\left(1 + \frac{\rho K_d}{\theta}\right)\frac{dC}{dt} = -u\frac{dC}{dz} + D\frac{d^2C}{dz^2} \tag{17}$$

If we denote the term in the bracket by R, then we have Equation (18)

$$R = \left(1 + \frac{\rho K_d}{\theta}\right) \tag{18}$$

This is called the retardation factor. Equation (17) becomes (19),

$$R\frac{dC}{dt} = D\frac{d^2C}{dz^2} - u\frac{dC}{dz} \tag{19}$$

The independent variables can be transformed from (z, t) by using characteristic transformation to a spatial coordinate that transform with the velocity, (y, t)

$$y = z + ut \tag{23}$$

$$\frac{dy}{dz} = 1 \tag{24}$$

$$\frac{dy}{dt} = u \tag{25}$$

The total differential expressed either in the form (z, t) or (y, t) are equal. This implies that;

$$dc = \left(\frac{\partial C}{\partial t}\right)_z dt + \left(\frac{\partial C}{\partial z}\right)_t dz \tag{26}$$

$$dc = \left(\frac{\partial C}{\partial t}\right)_y dt + \left(\frac{\partial C}{\partial y}\right)_t dy \tag{27}$$

From Equation (27), we can infer that the partial derivative

$$\left(\frac{dC}{dt}\right)_z = \left(\frac{\partial C}{\partial t}\right)_y + \left(\frac{\partial C}{\partial y}\right)_t\left(\frac{\partial y}{\partial t}\right)_t \tag{28}$$

Recall from Equation (25), $\frac{dy}{dt} = u$

This implies that Equation (28) becomes Equations (29-30);

$$\left(\frac{dC}{dt}\right)_z = \left(\frac{\partial C}{\partial t}\right)_y + u\left(\frac{\partial C}{\partial y}\right)_t \tag{29}$$

$$\left(\frac{dC}{dz}\right)_t = \left(\frac{dC}{dy}\right)_t \left(\frac{dy}{dz}\right)_t \tag{30}$$

Recall , $\frac{dy}{dz} = 1$, Equation (30) becomes,

$$\left(\frac{dC}{dz}\right)_t = \left(\frac{dC}{dy}\right)_t \tag{31}$$

Also, since Equations (26) and (27) are equal, then;

$$\left(\frac{dC}{dt}\right)_z = \left(\frac{dC}{dt}\right)_y \tag{32}$$

Therefore, Equation (29) becomes

$$0 = u\left(\frac{\partial C}{\partial y}\right)_t \tag{33}$$

Equation (32) can also be written as (33)

$$u\left(\frac{\partial C}{\partial z}\right)_t = 0 \tag{34}$$

From Equation (31), we can also write

$$\left(\frac{d^2 C}{dz^2}\right)_t = \left(\frac{d^2 C}{dy^2}\right)_t \tag{35}$$

Substituting Equations (32, 34 and 35) into Equation (22), we have

$$R\frac{dC}{dt} = D\left(\frac{d^2 C}{dy^2}\right) - 0 \tag{36}$$

$$R\frac{dC}{dt} = D\frac{d^2 C}{dy^2} \tag{37}$$

Equation (37) can be solved using Laplace transform with appropriate boundary conditions to obtain Equation (38) (Shapiro, 2011; Eliezer, 1992).

$$C(z,t) = C_0 erfc\left[\frac{\left[\frac{1}{D}\left(1+\frac{\rho}{\theta}K_d\right)\right]^{\frac{1}{2}}}{2\sqrt{t}}(z+ut)\right] \tag{38}$$

The migration of the ions can be studied by varying the concentration with distance or time or both. If time alone is considered, Equation (38) thus becomes Equation (39):

$$C(t) = C_0 erfc\left[\frac{\left[\frac{1}{D}\left(1+\frac{\rho}{\theta}K_d\right)\right]^{\frac{1}{2}}}{2\sqrt{t}}(ut)\right] \tag{39}$$

3. Results and Discussion

The experimental and the simulation results are presented in Figures 1-4. Figure 1 show the results of the comparison between the simulated and the experimental concentrations of Na^+ for all the sites.
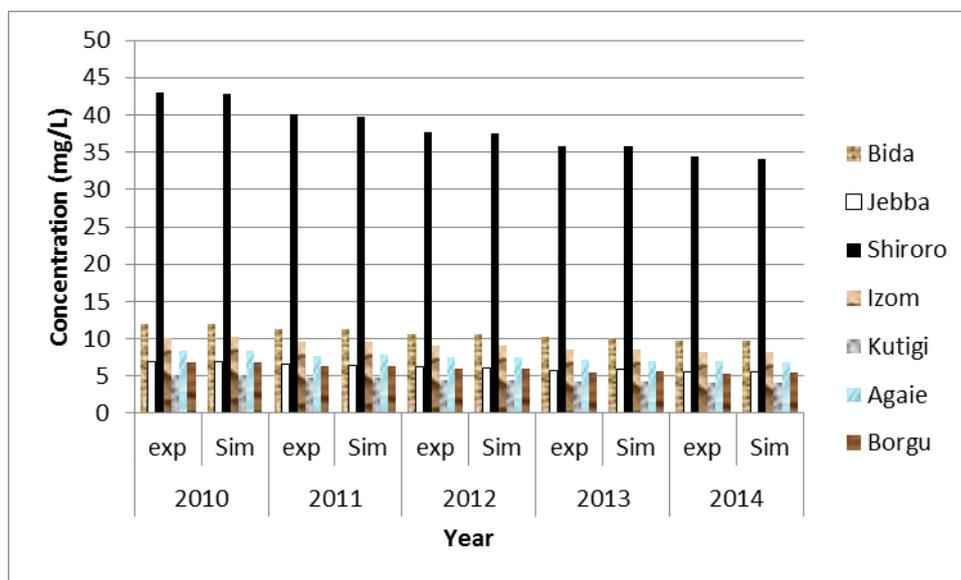

Fig. 1: Experimental and simulation Concentrations of Na^+ in the sites.

Figure 1 shows considerable similarities between the simulated results and the experimental results with the exception of Shiroro recording a higher concentration of about 40 mg/L. Figure 1 also show similar trend in the migration of sodium ion in soil water in agreement with the fact that the migration of ion in the soil is a function of the properties of the ions. It can also be observed that the concentration of the ions in the soil water decreases with time. This trend of the variation of the ion concentration with time confirms the migration of the Na^+ ion in the soil water. The high concentrations of Shiroro could be attributed to the facts that River Kaduna which passes through Shiroro come along with a lot of saline product contributing to the higher level of sodium ions (Adeniyi, 2005; Odigure and Adeniyi, 2003a,b).

Figure 2 show the results of the comparison between the simulated and the experimental concentrations of K^+ for all the sites. A similar pattern of migration was observed for K^+ as with Na^+ .The result show considerable similarity between the simulated and the experimental results. However, slight variations were observed in some sites as shown in Figure 2.
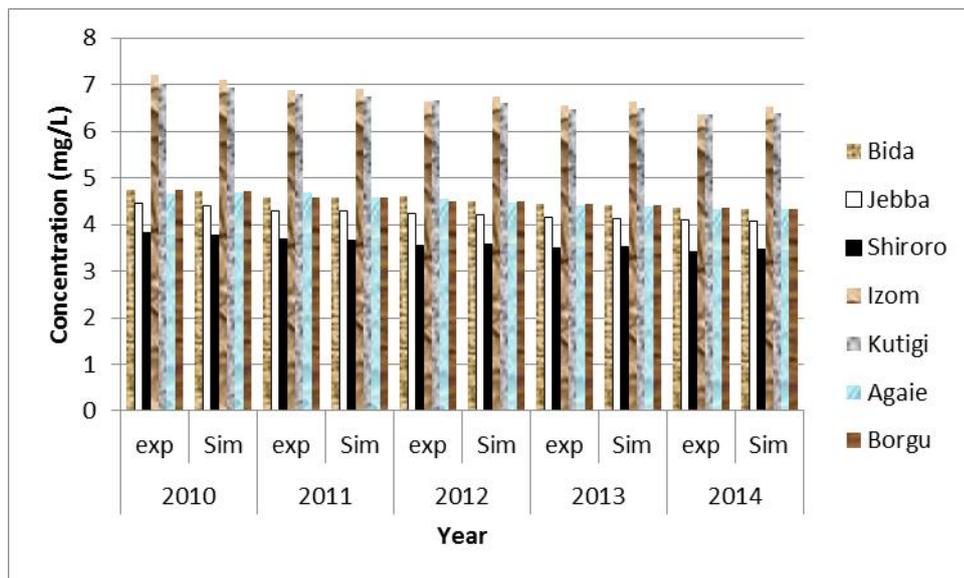
Fig. 2. Experimental and simulation Concentrations of K^+ in the sites.

It can also be seen that the values of the concentrations of K^+ at Bida and Izom sites for 2010 to 2014 is higher than those of other sites. This could be attributed to farming activities on the soil which include the application of fertilizers on the sites. These fertilizers, when applied, are leached into the soil water zone by rainfall and therefore augment the concentrations of the component ions in the soil water (Adeniyi, 2005; Odigure and Adeniyi, 2003a,b; Clain and Jeff, 2001).

Figure 3 show the results of the comparison between the simulated and the experimental concentrations of Ca^{2+} for all the seven sites. There are similar trends in the migration of Ca^{2+} ion. Notable are the sites of Shiroro and Bida, these sites are riverine areas with many fishing activities going on as well as farming activities. These activities could be more in these two sites than in other sites presented in the figure. The peak concentrations gradually reduces from 2010 to 2014, indicating some seasonal effects of various activities occurring at the sites (Odigure and Adeniyi, 2003a,b)
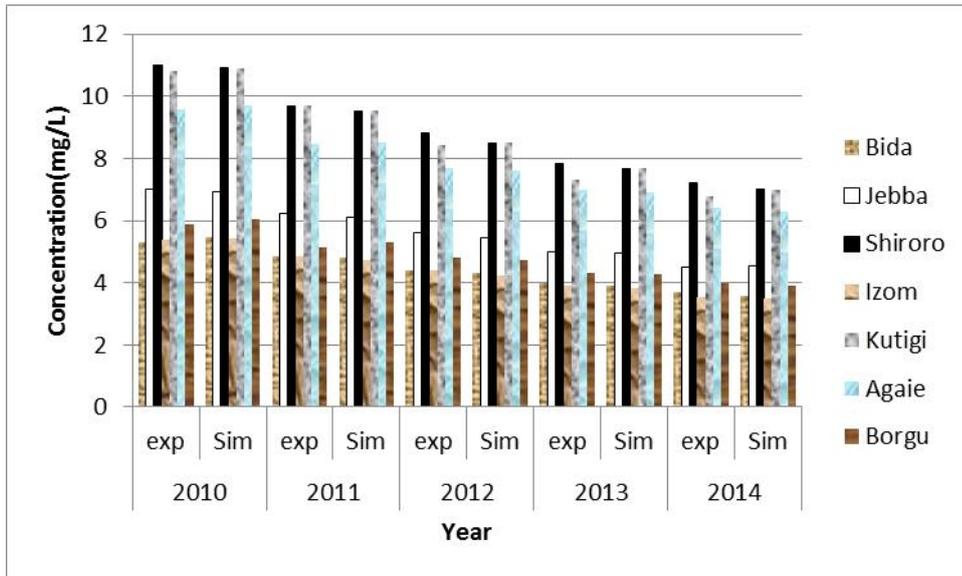
Fig. 3. Experimental and simulation Concentrations of Ca^{2+} in the sites.

Figure 4 show the results of the comparison between the simulated and the experimental concentrations of NO_3^- for all the sites. The concentration of Jebba was the highest followed by that of Agaie and Shiroro. This is an indication of the nature of farming activities and associated with the use of different kinds of fertilizers. The concentration in Jebba was much higher than other sites.
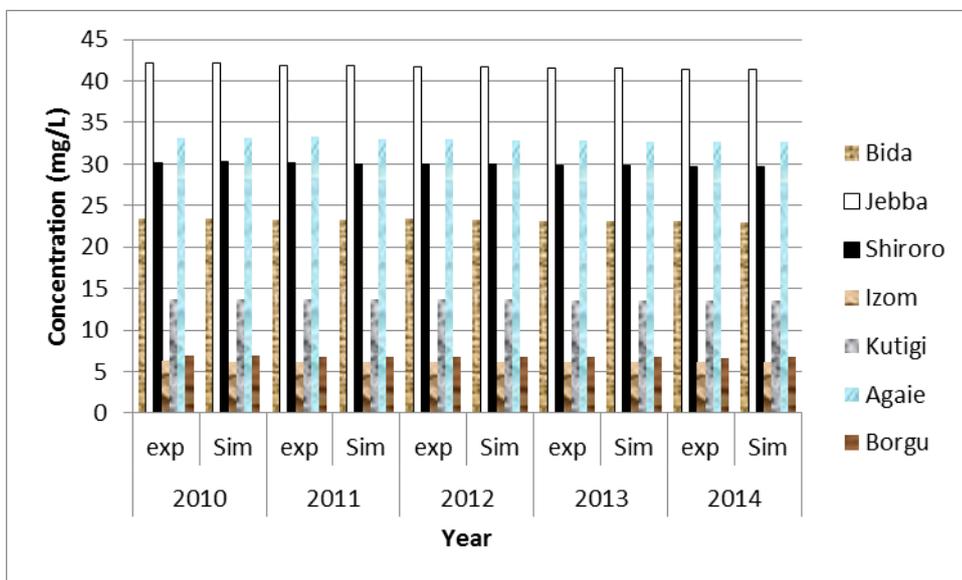

Fig. 4. Experimental and simulation Concentrations of NO_3^- in the sites.

It could be observed that Figures 4 shows a wide variation in the migration trend of NO_3^- in all the seven sites considered. Similar reason of fertilizer application and a lot of farming

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activities could also be stated as the reasons for these variations (Adeniyi, 2005; Odigure and Adeniyi, 2003a,b; Clain and Jeff, 2001).

4. Conclusion

The model of the Na^+, K^+, Ca^{2+} and NO_3^- ion migration in soil water was developed based on the principle of conservation of mass. The model shows that the migration of ions in the soil is dependent on some factors which include the diffusivity of the ions and the rate of flow of the soil water. The model was simulated using Mathcad 2014 software. The simulated result was then compared with the result of the experimental analysis. The result of the comparison shows that the simulated results give good predictions of the experimental results with slight variation which may be as a result of the assumptions taken during the development of the model. The model prediction and simulation tools developed form an effective tool for environmental management for the developing world.

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