A Numerical Model to Predict Vertical Diffusion of Contaminants in Open Channel Systems

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The representation of vertical transport of contaminants is a key issue in understanding proper remediation processes involving water systems. In this context, we present a numerical model to predict the rate of contaminants diffusion in open channel systems. The model was developed by discretizing the finite difference equations, implementing the numerical application of the lagged scheme and evaluating the diffusion term in the governing equation. Given the vertical diffusivity and the initial contaminant profile of the system, the developed model can be used to predict the vertical flow of contaminants and build a vertical diffusion model.

1. Introduction

Vertical diffusion of contaminants in open channels is of great importance in many fields of geosciences and engineering, and its accurate prediction is quite essential because of its implications on water quality and cleaning efforts. Natural channels like river, creek, run, branch, anabranch, and tributary are open conduits either naturally or artificially created, which periodically or continuously contains moving water or form a connecting link between two bodies of water while canal and floodway are some of the terms used to describe artificial channels. Water, which at any instant, is flowing into the channel system from surface flow, subsurface flow, base flow, and rainfall that directly falls onto the channel, is called a channel inflow.

According to US Environmental Protection Agency, 40% of the nation's open channels are too contaminated for use [1]. Most contaminants originate from industrial, municipal waste discharges, runoff from urban and agricultural areas and even individual households [2]. The understanding of contaminant flow is useful in estimating organic degradation in a pollution plume resulting from the disposal of industrial wastes and also to explain the role of colloids in transporting radio nuclides in an inter-granular aquifer [3, 4, 5]. Flow of contaminants in moving water has been variously explained by many authors including [6], [7] and [8], but very little has been done on the vertical diffusion of contaminants. The aim of this numerical experiment is, therefore, to develop a model to estimate the rate at which a contaminant diffuses vertically from the surface, and to ultimately build a flow profile at any instant of time.

2. Simulation procedure

In this section, the governing equations are presented, together with the controlling boundary conditions. The transformation of finite difference equations, leading to the method of computation is also described.

2.1 Governing equations

The contaminant concentration (ϕ) is a function of both the time duration (t) from when the contaminant is introduced and the depth (z) of the channel, i.e. $\phi = \phi(z,t)$. The numerical method used is based on the equation of diffusion given as [9, 10, 11]:

$$\frac{\partial \phi}{\partial t} = K_z \frac{\partial^2 \phi}{\partial z^2} \qquad (1)$$

where, K_z is the vertical diffusivity. The concentration at the surface is brought to C_s and maintained at that value with no flux at the base i.e.

$$\phi = C_s \text{ at } z = 0, \ \frac{\partial \phi}{\partial z} = 0 \text{ at } z = D \qquad (2)$$

where, D is the depth of the open channel.

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The initial concentration of the contaminant equals C_0 at other depths, i.e.

$$\phi(z,0) = C_0 \tag{3}$$

2.2 Discretization

The problem is solved by implementing the numerical application of the lagged scheme i.e., centered difference for the time derivative and evaluating the diffusion term at time (t) [12]. The finite difference scheme is constructed by replacing the derivatives with finite differences. From the Taylor's expansion of a function $f(x)$:

$$f'(x) \approx \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} \tag{4}$$

$$f''(x) = \frac{f(x+\Delta x) + f(x-\Delta x) - 2f(x)}{(\Delta x)^2} \tag{5}$$

where, Eqns. (4) and (5) are the first and second derivatives of $f(x)$.

Assuming $f(x,t) \equiv \phi(z,t)$, Eqn. (1) can therefore be written as

$$\frac{\phi_z^{t+1} - \phi_z^{t-1}}{2\Delta t} = \frac{K_z \left\{\phi_{z+1}^t + \phi_{z-1}^t - 2\phi_z^t\right\}}{(\Delta z)^2} \tag{6}$$

$$\phi_z^{t+1} - \phi_z^{t-1} = \frac{2K_z \Delta t}{(\Delta z)^2}\left\{\phi_{z+1}^t + \phi_{z-1}^t - 2\phi_z^t\right\} \tag{7}$$

Let

$$K = {2K_z \Delta t}/{(\Delta z)^2} \tag{8}$$

Eqn. (7) can then be rewritten in the form

$$\phi_z^{t+1} + \phi_z^{t+1}K = K\left\{\phi_{z+1}^t + \phi_{z-1}^t - \phi_z^{t-1}\right\} + \phi_z^{t-1} \tag{9}$$

where,

$$\phi_z^t = \frac{\phi_z^{t+1} + \phi_z^{t-1}}{2} \tag{10}$$

Rearranging Eqn. (9) to a more convenient form gives

$$\phi_z^{t+1} = \phi_z^{t-1}\left\{\frac{1-K}{1+K}\right\} + (\phi_{z+1}^t + \phi_{z-1}^t)\left\{\frac{K}{1+K}\right\} \tag{11}$$

Let

$$K_1 = 1 - K \tag{12}$$

and

$$K_2 = 1 + K \tag{13}$$

$$\phi_z^{t+1} = \phi_z^{t-1}\left\{\frac{K_1}{K_2}\right\} + (\phi_{z+1}^t + \phi_{z-1}^t)\left\{\frac{K}{K_2}\right\} \tag{14}$$

A 20-m depth channel, having a 15 mg/cm^2 contaminant concentration introduced at the surface was simulated. A time step of 5 minutes, a depth step of 1 m, and a period of 500 hrs were considered as necessary simulation parameters of the numerical experiment. The required simulation inputs for the model were water depths (D (m)), depth step (dz (m)), time step (dt (hrs.)), diffusivity (K_z (m^2/s)) and the initial contaminant concentration profile across the depths, which assume a uniform initial value of 15 mg/cm^2 at 0.5m and 10 mg/cm^2 across other depths from 1.5m to 19.5m. The model generates future values for the concentration of the contaminants across the depths and their corresponding times, which were then compared analytically.

3. Results and discussion

The contaminant concentration maintained a uniform value of 10 mg/cm^2 from depths 1. 0m to 19.5m, while 15 mg/cm^2 of contaminant concentration was introduced at the surface. Figs. 1- 6 show the profile of contamination at different times, while Table 1 defines the initial and final values of time from the figures. Fig. 1 illustrates the flow dynamics at the beginning of the experiment between the hours of 0.08194 and 0.99861. As time was increased from the hours of 0.08194 to 0.99861 with a time step of 0.08334 hours as shown in Fig. 1, the concentration of the contaminant was still largely 15 mg/cm^2 and 10 mg/cm^2 at 0.5m and 19.5m depths, respectively. However, at 2.5m depth, the original concentration of 10 mg/cm^2 increased by 0.23374, 0.49149, 0.73884, 0.96296, 1.16255, 1.33926, 1.49589, 1.63525, 1.7599, 1.87201, and 1.97339, respectively, after every 5mins.

From Fig. 2, the flow movement between the hours of 4.08194 and 4.99861 was illustrated as the concentration at depth 1.5m increased from 10 to 14 mg/cm^2 and from 10 to 13 mg/cm^2 at 2.5m. The concentration at 4.5 m depth was 12.01760 at 3.75 hrs, and 12.80659 at 7.74 hrs (not shown). At 19.5m depth, the concentration increased by

0.00128 and 0.07840 at the hours of 3.08 and 7.74, respectively, indicating the rate of increase.

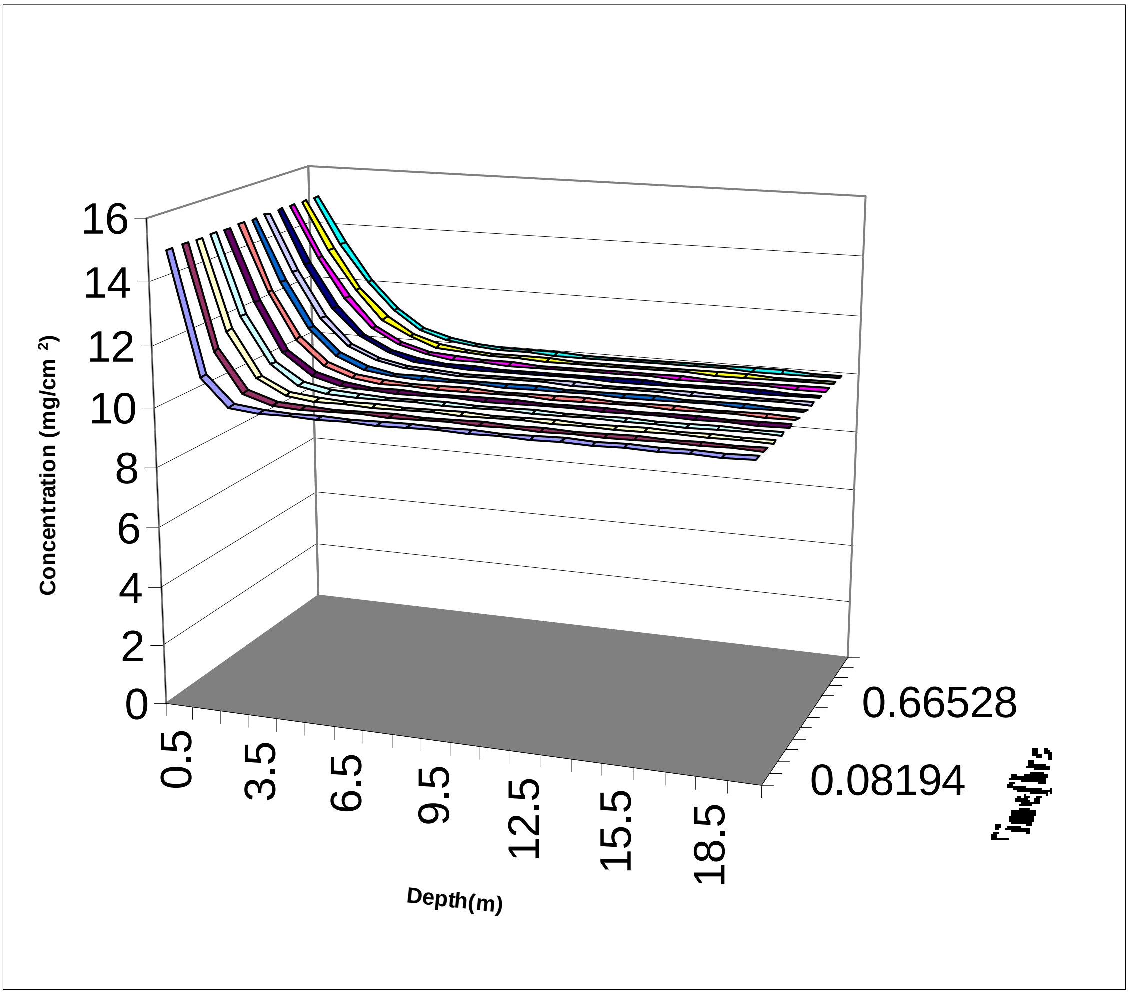

Fig.1: Concentrations at depths from T_1 to T_2.

At 12.00 hrs (not shown), the concentration at depths 1.5m and 19.5m increased by 4.08228 and 0.31342, respectively, while at 30.00 hrs. (Fig. 3), the increase was 4.42990 and 1.65619, respectively. The concentration at depth 19.5m increased by 1.64532 and 3.02285 at the hours of 29 and 53, respectively (Fig. 3 and Fig. 6). 3.77593 mg/cm^2 and 3.89864 mg/cm^2 of contaminant concentration had reached the depth of 6.5 m at hours 42.30 and 48.00, respectively (Fig. 4 and Fig. 5). With increase in time from the hours of 50.10 to 54.00 as shown in Figure 6, the contaminant concentration was approximately 14.83533, 14.51087, and 13.06152 mg/cm^2 at 0.5, 2.5 and 19.5m depths, respectively, suggesting that the tracer had diffused largely over a 2-day period. At about 500 hrs (not shown), the concentration of contaminants increased by 4.999 across the depths, which indicates a considerable spread of vertical diffusion between the surface and the base i.e., the base concentration is about 99 % of the surface concentration.

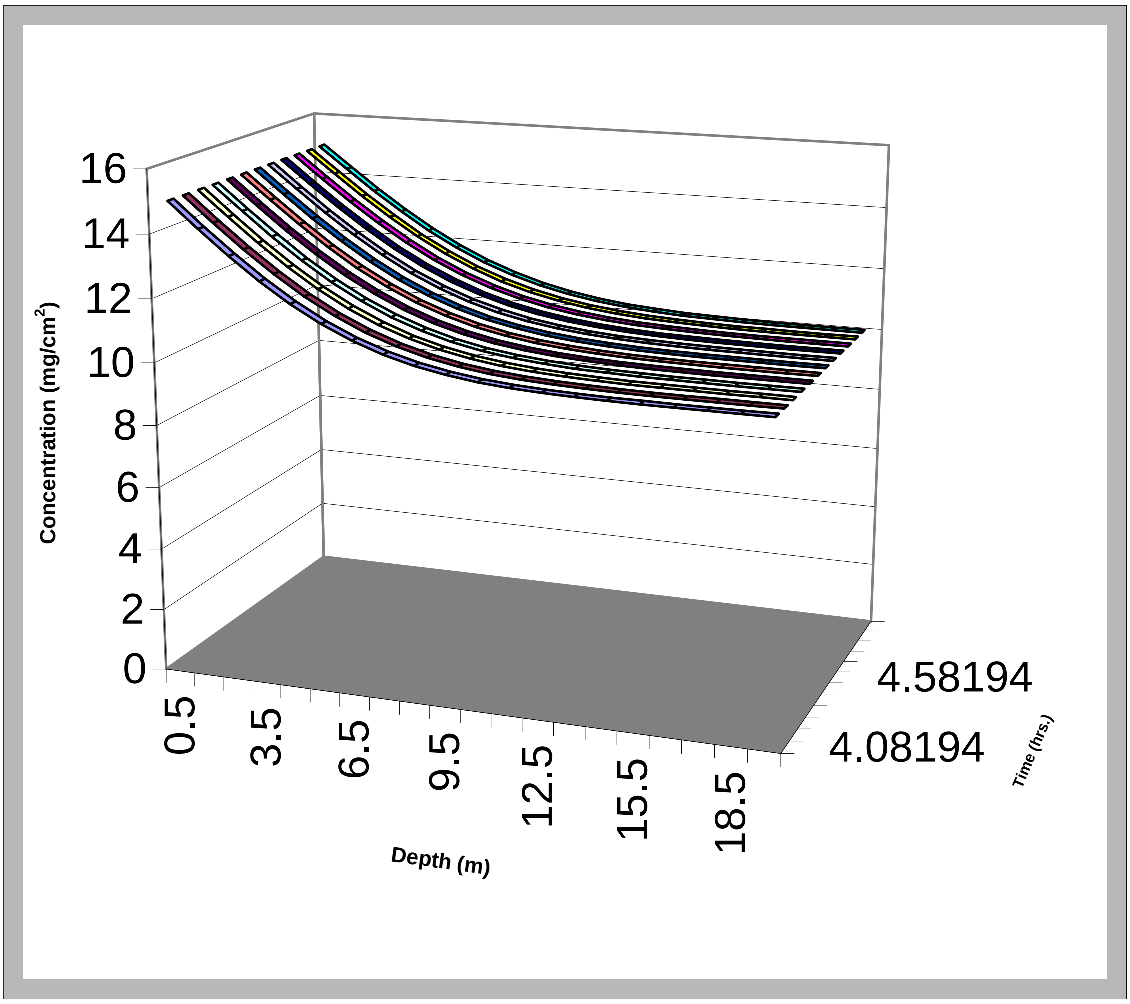

Fig.2: Concentrations at depths from T_3 to T_4.

The key requirement in contaminant remediation processes is to be able to predict with an appreciable accuracy, the time when a little fraction (say 0.0001 – 0.0003 %) diffuses to a particular depth. Fig. 7 presents a graphical relationship between t (time taken to reach a particular depth (z), i.e., the time at which the contaminant concentration increases by the smallest concentration at depth (z) and z^2/K_Z. Linearly regressing, the relationship yields the equation

$$y = 0.00234x - 0.1767 \qquad (15)$$

which, predicts the time the contaminant enters any depth, where $y = t$ and $x = z^2/K_z$.

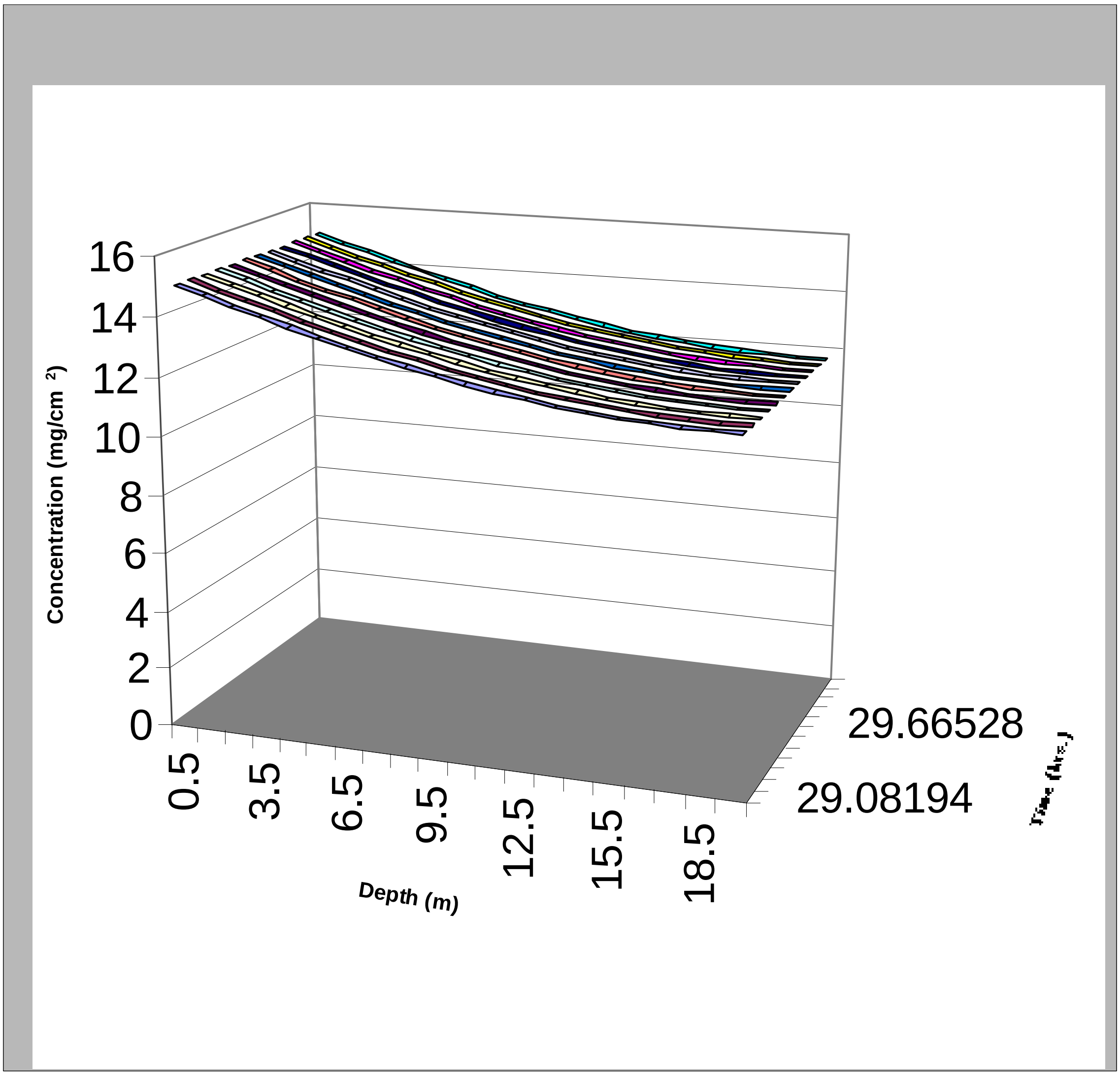

Fig.3: Concentrations at depths from T_5 to T_6.

4. Conclusion

In this paper, a numerical model to predict the vertical diffusion of contaminants in an open channel system was presented, thereby assisting the contamination cleaning efforts and improving water quality. The model predicts the rate at which a tracer diffuses vertically down from the surface and the time the contaminant reaches any depth within the profile. Given the vertical diffusivity of a tracer, the developed vertical diffusion model can be used to build the diffusion profile across the depths. For further work, we intend comparing experimental results with numerical prediction.

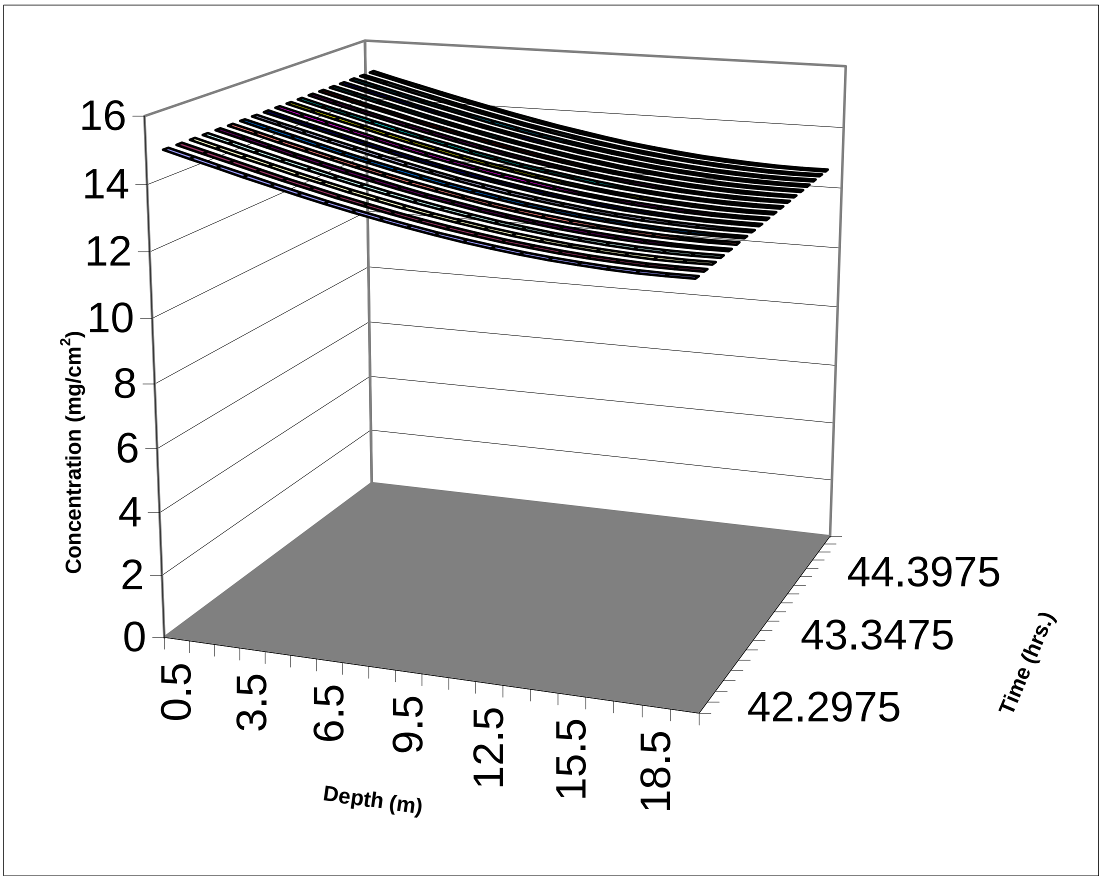

Fig.4: Concentrations at depths from T_7 to T_8.

Table 1: Initial and final values of time.

Figures	Initial Time (hrs)	Final Time (hrs)
Figure 1	T_1 = 0.08194	T_2 = 0.99861
Figure 2	T_3 = 4.08194	T_4 = 4.99861
Figure 3	T_5 = 29.08194	T_6 = 29.99861
Figure 4	T_7 = 42.2975	T_8 = 44.99750
Figure 5	T_9 = 47.0975	T_{10} = 49.94750
Figure 6	T_{11} = 50.0975	T_{12} = 53.9975

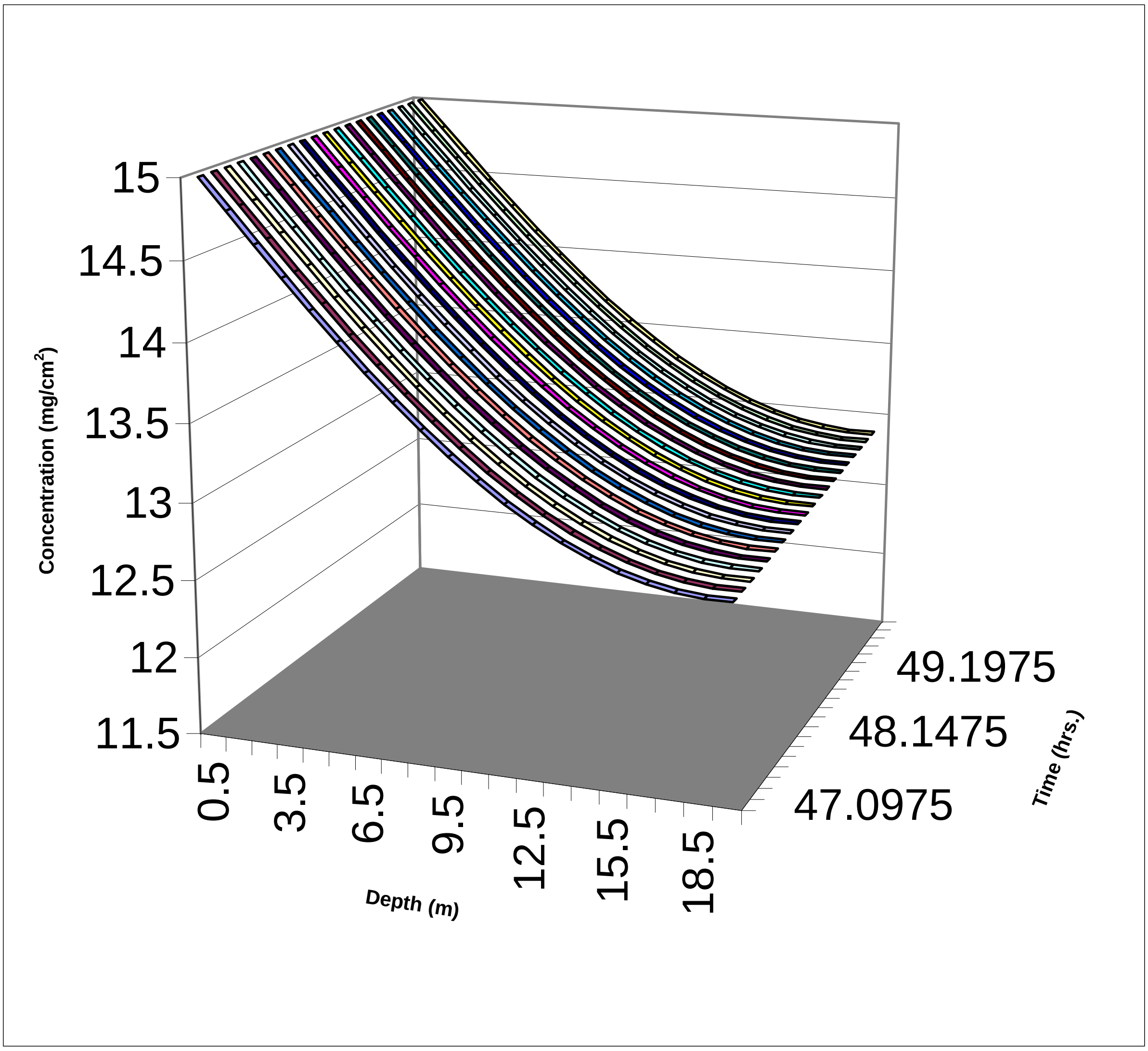

Fig.5: Concentrations at depths from T_9 to T_{10}.

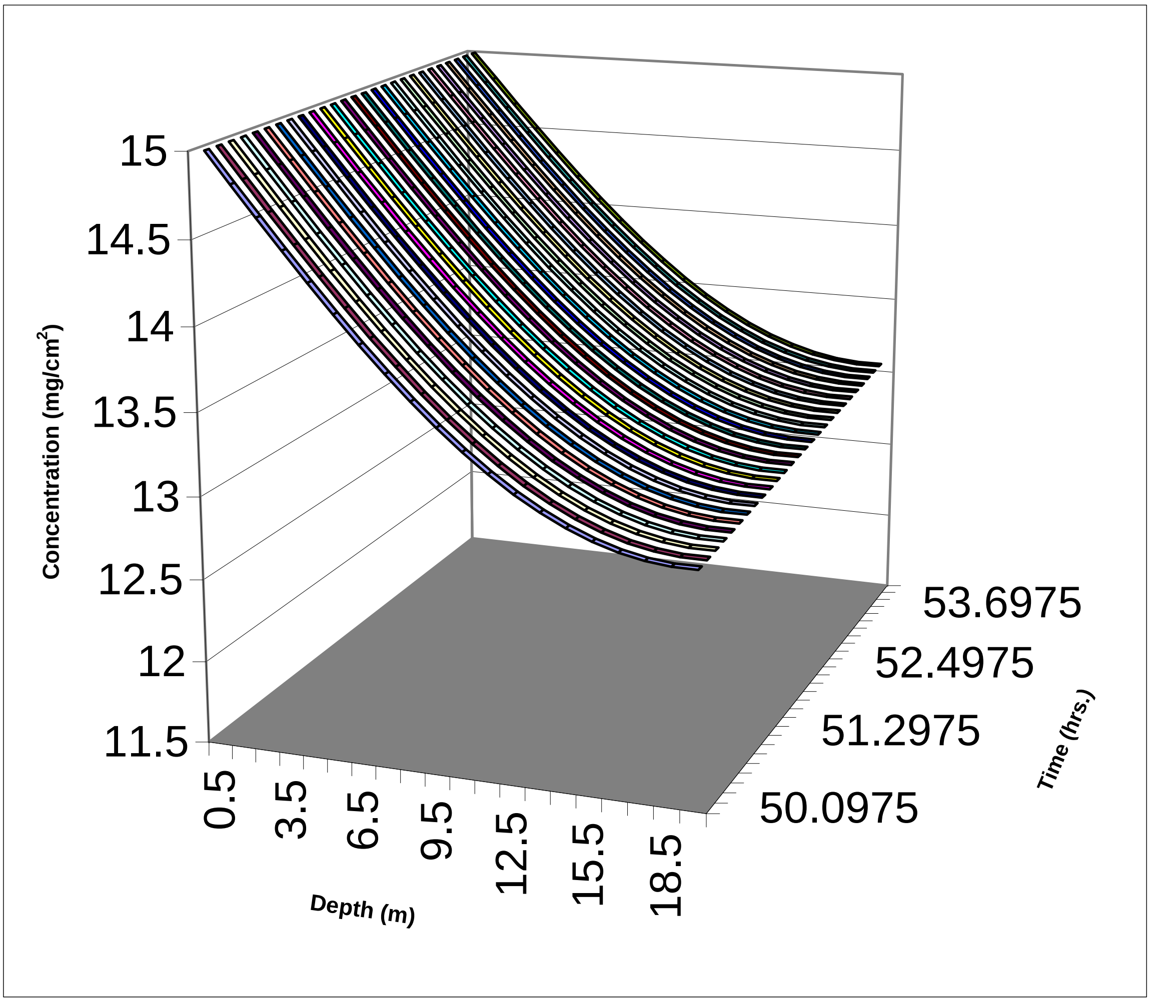

Fig.6: Concentrations at depths from T_{11} to T_{12}.

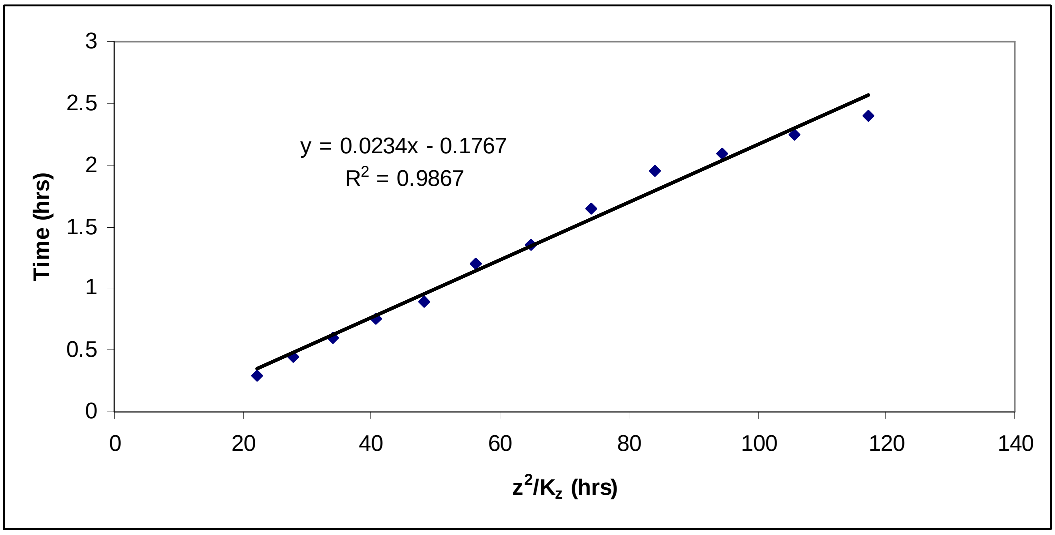

Fig.7: Relationship between time and z^2/K_Z.

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