Comparative Study of an Experimental and Enalytical Eimulation to Predict the Contaminants Concentration along Transient Groundwater Flow in Homogeneous, Semi-Infinite Aquifers

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Abstract

An experimental and analytical investigation using Fourier Transform Technique (FTT) and Laplace Transform Technique (LTT) were applied to predict contaminants concentration along transient groundwater flow in homogeneous, semi-infinite aquifer. The solutions were obtained for sinusoidal and exponential form of velocity which represent the seasonal pattern in a year. MatLab software was used to determine values of solute concentration for different time intervals and different distances with the same initial and boundary conditions. The analytical concentration values were compared with the experimental obtained concentration. It was observed that the experimental pollutant concentration trends are consistent with the analytical simulations of the Laplace transform technique (LTT) and the Fourier transform technique (FTT). A new empirical equation was proposed to calculate a new concentration for all samples and all experimental parameters. The obtained new concentration results were in good agreement with both the Fourier Transform Technique (FTT) and the Laplace Transform Technique (LTT).

Keywords: Experimental, Analytical, Contaminants, Groundwater, Empirical equation.

الملخص

تم تطبيق دراسة تجريبية وتحليلية باستخدام تقنية تحويل فوريه وتقنية تحويل لابلاس للتنبؤ بتركيز الملوثات على طول تدفق المياه الجوفية العابر في طبقة المياه الجوفية المتجانسة وشبه اللانهائية. تم الحصول على الحلول للشكل الجيبي والأسي للسرعة التي تمثل النمط الموسمي في السنة. تم استخدام برنامج ماتلاب لتحديد قيم تركيز المادة المذابة لفترات زمنية مختلفة ومسافات مختلفة بنفس الظروف الأولية والحدودية. تمت مقارنة قيم التركيز التحليلي مع التركيز الناتج التجريبي. لوحظ أن اتجاهات تركيز الملوثات التجريبية تتوافق مع المحاكاة التحليلية لتقنية تحويل لابلاس وتقنية تحويل فوريه. تم اقتراح معادلة تجريبية جديدة لحساب تركيز جديد لجميع العينات وجميع المتغيرات التجريبية. حيث كانت نتائج التركيز الجديدة التي تم الحصول عليها في توافق جيد مع كل من تقنية تحويل فوريه وتقنية تحويل لابلاس.

1. Introduction

The contaminants in aquifer systems and advection. Generally, the solute transport from a source along the flow field through a medium of air or water is described by a partial differential equation of parabolic type, on the principle of conservation of mass, and it is usually known as advection-diffusion equation (ADE) [1]. Many experimental and theoretical studies were undertaken to improve the understanding, management, and prediction of the movement of contaminant behavior in groundwater system [2]. Analytical solutions are of fundamental importance in understanding and describing physical phenomena because they explicitly take into account all parameters of the problem [3-4]. In the deterministic approach, explicit closed-form solutions for transport problem can often be derived if the model parameters are constant with respect to time and position [5].
The objective of this research is to apply an analytical solution using Fourier Transform Technique (FTT) and Laplace Transform Technique (LTT), and to compare the result with the obtained experimental concentration data of the major cations and anions.

Research Methodology

Analytical solution used Fourier Transform Technique (FTT) and Laplace Transform Technique (LTT) were applied to estimate the distribution of the concentration of contaminants in one-dimension homogeneous semi-infinite aquifer.

- **Fourier Transform Technique (FTT) [4]:**

$$C(X,T) = 2 - QT + QX - \frac{1}{2}\left(2 - \frac{c_i}{c_o}\right)F_1(X,T) + \frac{Q}{2}\left[TF_1(X,T) - F_2(X,T) - e^X F_3(X,T)\right]; \qquad (1)$$

Where

$$F_1(X,T) = erfc\left(\frac{\sqrt{T}}{2} - \frac{X}{2\sqrt{T}}\right) - e^X erfc\left(\frac{\sqrt{T}}{2} + \frac{X}{2\sqrt{T}}\right); \qquad (2a)$$

$$F_2(X,T) = Xerfc\left(\frac{\sqrt{T}}{2} - \frac{X}{2\sqrt{T}}\right) + 2\sqrt{\frac{T}{\pi}}\, e^{-\left(\frac{\sqrt{T}}{2} - \frac{X}{2\sqrt{T}}\right)^2}; \qquad (2b)$$

$$F_3(X,T) = Xerfc\left(\frac{\sqrt{T}}{2} + \frac{X}{2\sqrt{T}}\right) - 2\sqrt{\frac{T}{\pi}}\, e^{-\left(\frac{\sqrt{T}}{2} + \frac{X}{2\sqrt{T}}\right)^2}; \qquad (2c)$$

- **Laplace Transform Technique (LTT)** [6]

$$C(X,T) = \frac{1}{2}\left(2 - \frac{c_i}{c_o}\right)\cdot\left[erfc\left(\frac{X}{2\sqrt{T}} - \frac{\sqrt{T}}{2}\right) + e^X \cdot erfc\left(\frac{X}{2\sqrt{T}} + \frac{\sqrt{T}}{2}\right)\right] + \frac{c_i}{c_o} - \frac{Q}{2}\cdot\left[(T - X)\cdot erfc\left(\frac{X}{2\sqrt{T}} - \frac{\sqrt{T}}{2}\right) + (T + X)\cdot erfc\left(\frac{X}{2\sqrt{T}} + \frac{\sqrt{T}}{2}\right)\right] \qquad (3)$$

The analytical solutions were illustrated with the help of set of input data to understand the concentration distribution behavior in the sinusoidal and exponential forms of velocity expressions, which are valid for transient groundwater flow too. The sinusoidal and exponential forms of velocity can be written as follows [7]:

$$u(t) = u_o(1 - \sin mt); \qquad (4a)$$

$$u(t) = u_o e^{(-mt)}, \quad mt < 1 \qquad (4b)$$

The dimensionless time variable T can be written as follows:

$$T = \frac{u_o^2}{mD_o}[mt - (1 - \cos mt)];$$

$$T = \frac{u_o^2}{mD_o}\left[1 - e^{(-mt)}\right];$$

where $\mathrm{mt} = 3 \cdot \mathrm{k} + 2 \ldots\ldots\ldots\ldots.\mathrm{k} = 0 \text{ to } \mathrm{n}$

The values of *mt* represents the groundwater level and velocity minimum during June and maximum during December just after six months (Approximately 182 days) in one year and $6 \le K \le 13$. If the flow resistance coefficient m = 0.0165 day^{-1}, equation (21a) yields approximately t (days) = 182·k+121. So, we get the time t (days) in 4th, 5th, 6th and 7th, as t (days), (For the same set of inputs except m = 0.0002 day^{-1} as $mt < 1$):

Table 1. Time t (days) in 4th, 5th, 6th and 7th

K		**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**
T		**1213**	**1395**	**1577**	**1759**	**1941**	**2123**	**2305**	**2487**
mt	***m*=0.0165**	**20**	**23**	**26**	**29**	**32**	**35**	**38**	**41**
	***m*=0.0002**	**0.243**	**0.279**	**0.315**	**0.352**	**0.388**	**0.425**	**0.461**	**0.497**

2. Experimental data collection

The study area was on the north western side of Libya, from Sabratha to Al-Harsha, and is located between the following latitudes and Longitude:
latitudes 32°48'7.31"N to 32°46'48.52"N, Longitude 12°23'51.76"E to 12°41'14.48"E & latitudes 32°36'5.89"N to 32°36'11.51"N Longitude 12°24'13.31"E to 12°40'06.23"E.
One hundred and six samples (106) of groundwater were experimental determined by [8-11]. These samples were random collected from different sites of the selected study area. The concentrations of the major cations and anions, for some samples, are summarized in Table 2. Sample no. (37) was selected as the source, and thus the new ratio of the concentration for all samples and all parameters were calculated. The sample concentration was divided by the source concentration. For example, the calcium concentration in sample no. (1) was 310, and in the source, sample no. (37) the calcium concentration was 785.95, so the ratio was 0.3944.

In this way, all values were calculated for all samples as well as for each parameter. Then the average value was calculated for each parameter.

Table 2. Experimental concentrations of the major cations and anions.

Well	Ca^{2+}	Na^{+}	Mg^{2+}	K^{+}	HCO_3^-	SO_4^{2-}	NO_3^-	Cl^-
no.	Ratio	Ratio	ratio	ratio	ratio	ratio	ratio	ratio
1	0.3944	0.1497	0.3978	0.0789	0.4547	0.2921	0.6081	0.1806
2	0.4453	0.1164	0.4310	0.0632	0.4667	0.2708	0.5405	0.1711
9	0.1781	0.0665	0.2210	0.0316	0.1867	0.1062	0.4730	0.0722
10	0.1718	0.0366	0.1923	0.0368	0.3080	0.0956	0.4054	0.0741
21	0.4836	0.1563	0.2966	0.0711	0.5477	0.1832	0.5946	0.1807
35	0.1126	0.0544	0.0431	0.0463	0.2035	0.2225	0.6014	0.0619
36	0.3728	0.1414	0.2527	0.0595	0.3527	0.2262	0.6486	0.1748
37	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
38	0.4500	0.1852	0.5263	0.1463	0.3527	0.3840	0.5135	0.2492
39	0.6500	0.1330	0.2105	0.0711	0.1899	0.2554	0.8243	0.2430
63	0.5093	0.1124	0.3474	0.0337	0.2973	0.3797	0.0039	0.0728
64	0.2243	0.0948	0.2316	0.0337	0.2980	0.1375	0.0001	0.0890
76	0.3257	0.1111	0.3359	0.0500	0.3307	0.2469	0.0001	0.0985
77	0.8156	0.2581	0.7161	0.1368	0.4133	0.5560	0.0230	0.3158
92	0.1832	0.1586	0.2106	0.0632	0.2813	0.1322	0.0000	0.1551
93	0.3868	0.5604	0.4089	0.1316	0.4293	0.2411	0.0000	0.4725
105	0.7799	0.3851	0.9188	0.1895	0.1411	0.6771	0.1459	0.5867
106	0.1966	0.0969	0.2312	0.0384	0.1688	0.1377	0.0365	0.1477
Avr.	0.3598	0.1534	0.3131	0.0809	0.3025	0.2521	0.2598	0.1587

3. Result and discussion

The numerical values, used for plotting the Matlab graph for both analytical and experimental solutions, were as follows: initial concentration (theoretical) $c_{i,th} = 0.1$, initial concentration (experimental) $c_{i,ex} = \{Na^+ = 0.1534, K^+ = 0.0809 \text{ and } Cl^- = 0.1587\}$, solute concentration $c_o = 1.0$, initial groundwater velocity $u_o = 0.01$ km/day, initial dispersion coefficient $D_o = 0.1$ km^2/day, decay rate coefficients $q = 0.0001$ day^{-1} and distance $x = 100$ km.
The following Figures show the contaminant concentration distribution obtained from the analytical and experimental solution with the same boundary condition along uniform groundwater flow with the sinusoidal and the exponential form of the temporally dependent dispersion equations (21a-b). Figure (1) and (2) plot the curves showing contaminant

concentration distribution in the aquifer at the 4th and 7th year, using Laplace Transform Technique (LTT) and Fourier Transform Technique (FTT), compared with experimental contaminant concentration for $\{Na^+ = 0.1534,\ K^+ = 0.0809 \text{ and } Cl^- = 0.1587\}$.

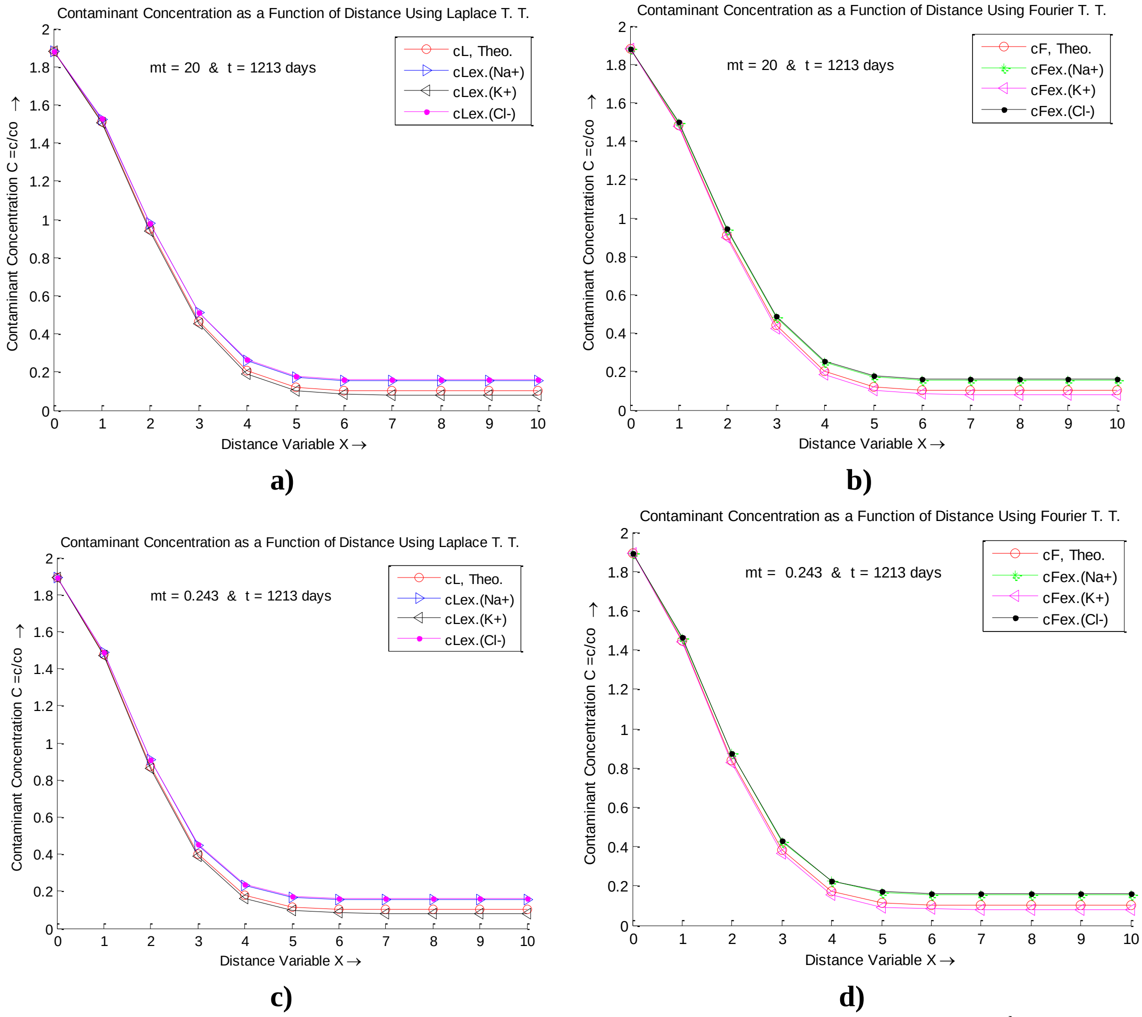
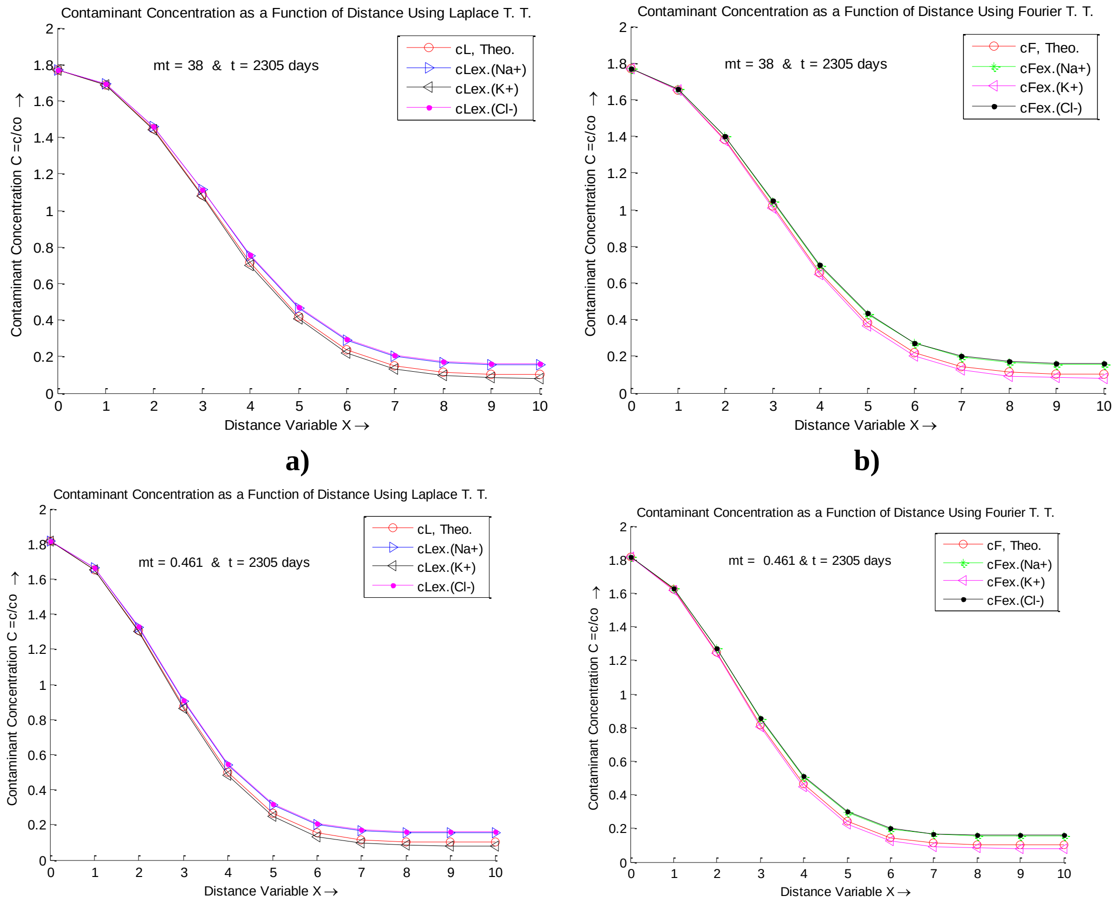


Figure 1. Contaminants concentration along unsteady ground water flow 4th year
a) Sinusoidal, LTT and experimental b) Sinusoidal, FTT and experimental
c) Exponential, LTT and experimental d) Exponential, FTT and experimental

The contaminants concentration distribution behaviour along unsteady flow of sinusoidal form of velocity are depicted in the Figures (1a-b) and Figures (2a-b) and of exponential form in the Figures (1c-d) and Figures (2c-d). It is observed that the contaminant concentration (theoretical for LTT and FTT and experimental) decreases with distance traveled in presence of source contaminants and follows almost the same trend in obtained theoretical and experimental contaminant concentration. This decreasing tendency of contaminant concentration with distance traveled may help to rehabilitate the contaminated aquifer.



a) b) c) d)

Figure 2. Contaminants concentration along unsteady ground water flow 7th year
a) Sinusoidal, LTT and experimental b) Sinusoidal, FTT and experimental
c) Exponential, LTT and experimental d) Exponential, FTT and experimental

Figure (3) plots the curves showing contaminant concentration distribution in the aquifer at the 4th and 7th year together, using Laplace Transform Technique (LTT) and Fourier Transform Technique (FTT), compared with experimental contaminant concentration for {$Na^+ = 0.1534$, $K^+ = 0.0809$ and $Cl^- = 0.1587$}. The contaminants concentration distribution behaviour along unsteady flow of sinusoidal form of velocity are depicted in the Figures (3a, b) and of exponential form in the Figures (3c, d). It is observed that the concentration at the origin of the aquifer is decreasing for the both unsteady velocities with time. Nearby the origin, it starts slightly decreasing and emerging at the common point.

It goes on decreasing and the rate of decreasing tendency for sinusoidal form of velocity is slightly slower than the exponential form of velocity. In both cases, the decreasing tendency of the concentration levels of contaminants with time and distance travelled, may help to rehabilitate the contaminated aquifer. It was observed that the experimental pollutant concentration trends are consistent with the analytical simulations of the Laplace transform technique (LTT) and the Fourier transform technique (FTT).

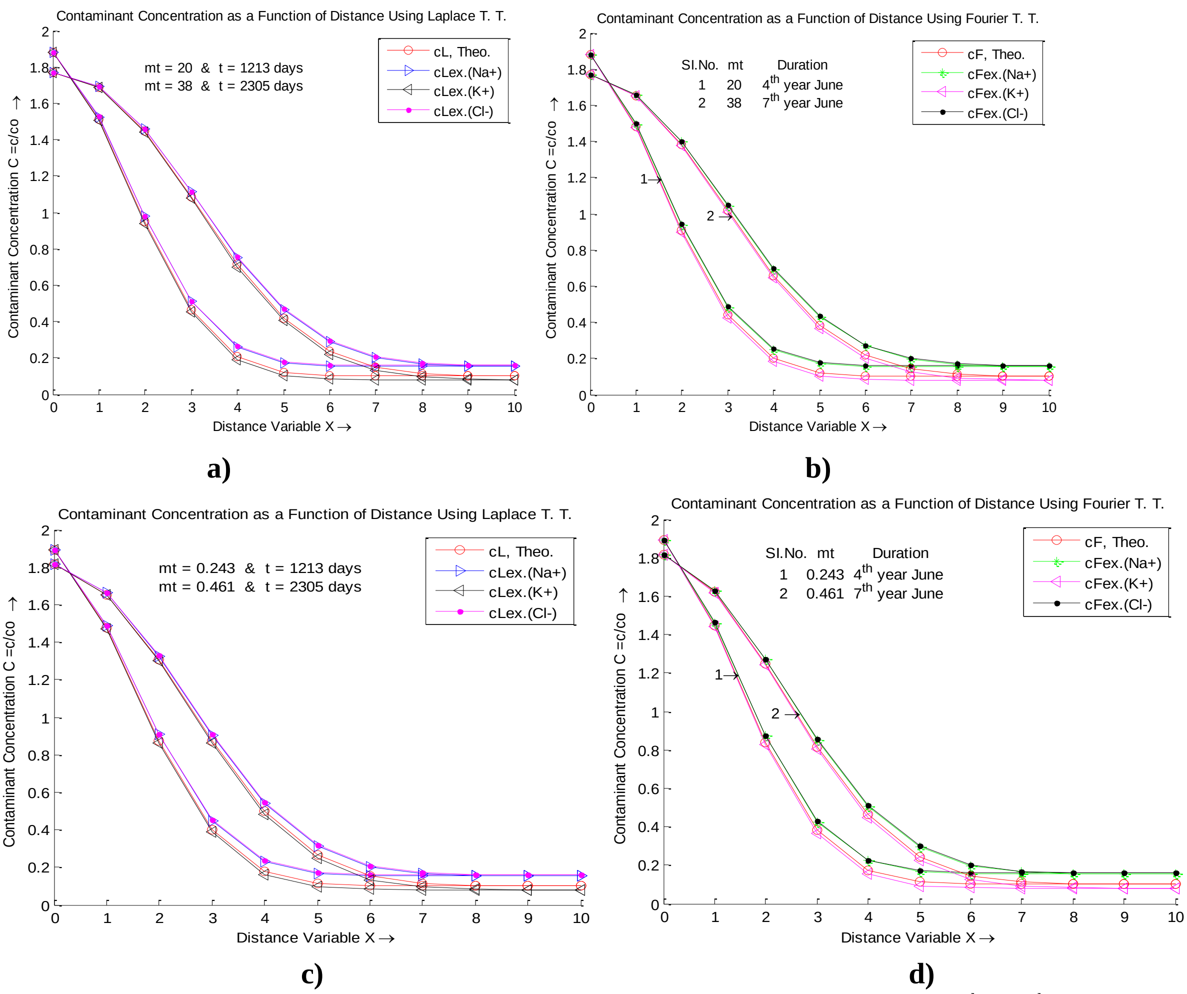


Figure 3. Contaminants concentration along unsteady ground water flow 4th & 7th year
a) Sinusoidal, LTT and experimental b) Sinusoidal, FTT and experimental
c) Exponential, LTT and experimental d) Exponential, FTT and experimental

There is still variation, especially at the end of the path, so a new empirical equation were proposed to calculate the new concentrations for all samples and for all experimental parameters as follows:

$$\boldsymbol{C_{i,exnew} = C_{i,th}.C_{i,ex} + C_{i,th}} \tag{5}$$

Figure (4) plots the curves showing contaminant concentration distribution in the aquifer at the 4th year, using LTT and FTT, compared with all obtained new experimental contaminant concentration equation (5). The contaminants concentration distribution behaviour along unsteady flow of sinusoidal form of velocity are depicted in the Figures (4a, b) and of exponential form in the Figures (4c, d). It is observed that the contaminant concentration (theoretical for LTT and FTT and the new experimental concentration data $C_{i,exnew,}$ obtained by equation (5) decreases with distance traveled in presence of source contaminants and follows almost the same trend in obtained theoretical and experimental contaminant concentration.

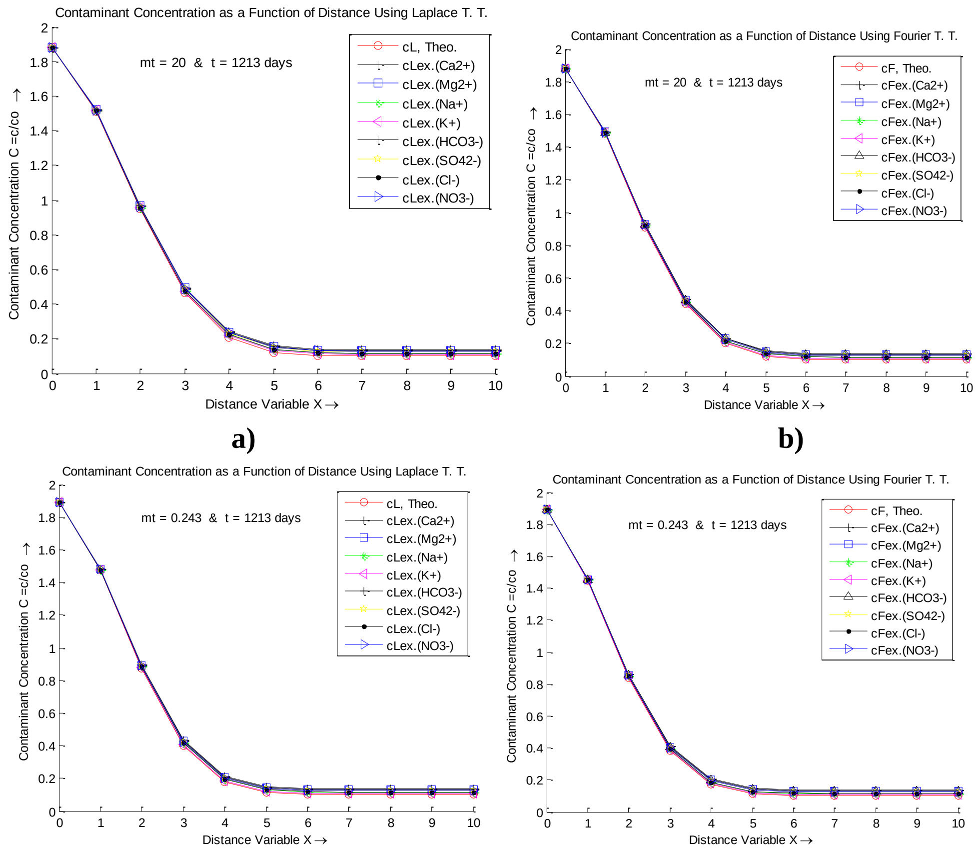


Figure 4. Contaminants concentration along unsteady ground water flow 4th year.
a) Sinusoidal, LTT and experimental b) Sinusoidal, FTT and experimental
c) Exponential, LTT and experimental d) Exponential, FTT and experimental

Table (3) shows the difference percentage(%) between theoretical and analytical simulations of both (LTT and FTT) for Sodium Na. The maximum deviation of both was around 13%.

Figure (5) plots the curves showing contaminant concentration distribution in the aquifer at the 4th, 5th, 6th & 7th year together, using Laplace Transform Technique (LTT) and Fourier Transform Technique (FTT), compared with all obtained new experimental contaminant concentration equation (22). The values of *mt* represents the groundwater level and velocity minimum during June and maximum during December are summarized in Table 1. It is also observed that the contaminant concentration (theoretical for LTT and FTT and the new experimental concentration of all data $C_{i,exnew,}$ obtained by equation (22) decreases with time and distance traveled in presence of source contaminants. It goes on decreasing and the rate of decreasing tendency for sinusoidal form of velocity is slightly slower than the exponential form of velocity. In both cases, the decreasing tendency of the concentration levels of contaminants with time and distance travelled, may help to rehabilitate the contaminated aquifer.

Table 3. Difference percentage(%) between theoretical and analytical simulations.

mt = 20	t = 1213 days										
X	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
C Fourier Theo.	1.8824	1.4839	0.9104	0.4405	0.1995	0.1198	0.1027	0.1002	0.1000	0.1000	0.1000
C Fourier Exp. Na^+	1.8824	1.4876	0.9190	0.4530	0.2140	0.1350	0.1180	0.1156	0.1154	0.1153	0.1153
% to Fouier	0.0	0.2	0.9	2.8	6.8	11.2	13.0	13.3	13.3	13.3	13.3
C Laplace Theo.	1.8824	1.5130	0.9493	0.4663	0.2097	0.1224	0.1031	0.1003	0.1000	0.1000	0.1000
C Laplace Exp. Na^+	1.8824	1.5167	0.9580	0.4788	0.2243	0.1376	0.1184	0.1156	0.1154	0.1153	0.1153
% to Laplace	0.00	0.25	0.90	2.62	6.48	11.03	12.94	13.27	13.30	13.30	13.30

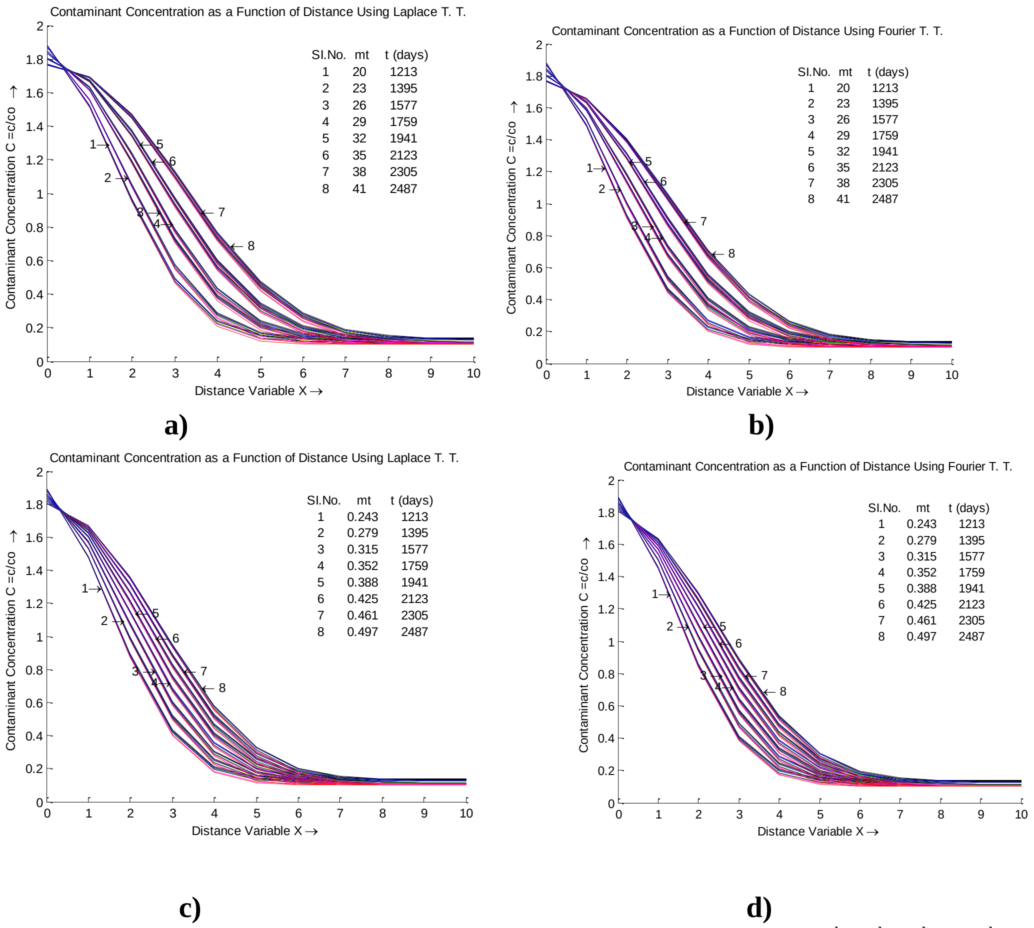


Figure 5. Contaminants concentration along unsteady ground water flow 4th, 5th, 6th & 7th year
a) Sinusoidal, LTT and experimental   b) Sinusoidal, FTT and experimental
c) Exponential, LTT and experimental   d) Exponential, FTT and experimental

4. Conclusions

A comparative Study of an experimental and analytical simulation using Fourier Transform Technique (FTT) and Laplace Transform Technique (LTT) was applied to predict the contaminants concentration along transient groundwater flow in homogeneous, semi-infinite aquifers. The analytical solutions were illustrated with the help of set of input data to understand the concentration distribution behavior in the sinusoidal and exponential forms of velocity expressions. The obtained concentration values are depicted graphically in the presence of time-dependent source of contaminant concentration at $mt = 3 \cdot k + 2$ and $6 \leq K \leq 13$ which represents minimum and maximum records of groundwater level and velocity during June and December in 4^{th}, 5^{th}, 6^{th} and 7^{th}. The analytical concentration values were compared with experimental obtained concentration. It was observed that the experimental pollutant concentration trends are consistent with the analytical simulations of the LTT and the FTT. A new empirical equation was proposed to calculate a new concentration for all samples and all experimental parameters. The obtained new concentration results were in good agreement with both the Fourier Transform Technique (FTT) and the Laplace Transform Technique (LTT).

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