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Flow and transport of Phenol in groundwater using PGWT equation

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ABSTRACT

With the increasing population, one has to depend on the groundwater for domestic, agricultural and industrial requirements. Hence conservation of groundwater in its pure form requires attention. Mismanagement of groundwater along with its deteriorating quality are major concerns in developing countries. The objective of this investigation is to understand the occurrence and degree of dissolved contaminants, as well as the rate and direction of contaminant's movement within the groundwater flow system. In this study, a Phenol Groundwater Transport (PGWT) equation is developed with Lagrangian interpolation function using a nine noded rectangular element. PGWT equation is used to determine the unknown concentration of a Phenol in the porous media for the range of concentrations and permeabilities. The equation is validated with the results of developed Physical Aquifer Model (PAM). It is observed that the transport equation of degree ten delivers the accurate concurrence with the physical model when contrasted with lower degrees of polynomial function.

1. Introduction

Landfills, surface waste ponds, underground storage tanks, land applications of pesticides, radioactive material disposal sites, salt water intrusion and mine evacuation have become the crucial sources of groundwater pollutions (Freeze and Cherry, 1979). With the diverse dangerous waste sites, occurrences of groundwater contamination has become major concern in last few decades.

Like many other contaminants Phenol primarily enters the groundwater from industrial effluent discharges. Phenol is degraded speedily in air by gas-phase chemical group reaction with estimated half-life of 14 h, but may persists in the groundwater for a longer period (Kadir and Suheyla, 2008). Groundwater contaminated with Phenol is considered to be hazardous.

Any groundwater pollution study involves identification of the source of pollution and the movement of the pollutants in the groundwater environment. Once the pollutants are introduced, appropriate management of resource utilization and preventive measures to ensure suitable development and remediation of polluted sites is needed (Eldho, 2001). The primary transport processes of concern in groundwater include advection, dispersion, diffusion, adsorption, biodegradation and chemical reaction (Bedient et al., 1999).

When groundwater transport investigation is carried out in 1D then the extent of concentration with distance is observed by plotting C/C_0 graphs where C is the concentration of contaminant and C_0 is the initial concentration of the contaminant. Controlled experimental conditions of temperature, pressure, hydraulic gradient, contaminant injection rate, and microbial populations are needed to simulate a wide variety of situations that may exist in the field (Boyraz and Alhan, 2017). Physical Aquifer Models (PAM) are developed for the simulation of the location of contaminant plume and its movement. They are fabricated to study and understand groundwater flow and transport. Multiple parameters can be introduced into physical model and better inference and conclusions can be achieved.

To understand the reactions involved and observation of the transport of contaminant may require several weeks (Karickhoff et al., 1979). Layered aquifer systems, sloping material interfaces, and heterogeneous hydraulic properties are a few examples of systems that have been studied in PAMs (Stauffer and Dracos, 1986; Nieber and Walter, 1981, Starr et al. (1985), Stoeckl et al. (2019)). Effluent concentrations measured in the physical model and simulated model are found in close agreement (Starr et al., 1985; Qayuum (2019)). The findings from the PAM can be used to validate the generated mathematical models.

In this study, Phenol is considered as a contaminant and its transport is observed in 1D with different initial concentrations and porous media.

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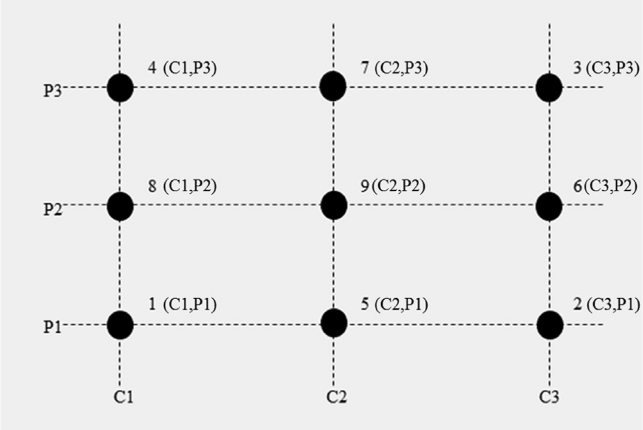

Figure 1. Nine noded element for Concentration and Permeability.

Phenol Groundwater Transport Equation (PGWT) is developed using Lagrangian interpolation function with nine noded rectangular element. Three distinctive initial concentrations of 50 ppm, 75ppm and 100 ppm and three diverse permeability of 0.32, 0.38 and 0.42 of porous media are used to develop the equation. This equation predicts the spread of Phenol in the porous media with respect to distance from the point of injection.

A Physical Aquifer Model (PAM) is likewise developed to verify the results of PGWT equation. It is found that there is a good agreement between the results of PGWT and PAM.

2. PGWT equation

Three initial concentrations of Phenol as 50 ppm, 75ppm and 100ppm are considered to develop PGWT equation. Three values of permeability of porous media as 0.32, 0.38 and 0.42 are taken into consideration thereby generating nine combinations. Figure 1 shows the nine noded element for the nine combinations.

Using Lagrangian interpolation function for a nine noded rectangular element the equation is developed. The interpolation functions for ith node of nine noded element is given by

$$N_{i\ (C,P)} = N_{i,1}C^2P^2 + N_{i,2}C^2P + N_{i,3}C^2 + N_{i,4}CP^2 + N_{i,5}CP + N_{i,6}C + N_{i,7}P^2 + N_{i,8}P + N_{i,9} \tag{1}$$

When the concentration C1 = 50 ppm; C2 = 75 ppm and C3 = 100

Table 1. Coefficient for interpolation functions of ith node of nine noded element.

i	$N_{i,1}$	$N_{i,2}$	$N_{i,3}$	$N_{i,4}$	$N_{i,5}$	$N_{i,6}$	$N_{i,7}$	$N_{i,8}$	$N_{i,9}$
1	0.1212	-0.0982	0.0198	-21.2121	17.1818	-3.4660	909.0909	-736.364	148.5455
2	0.1212	-0.0982	0.0198	-15.1515	12.2727	-2.4757	454.5455	-368.182	74.2727
3	0.1455	-0.1018	0.0176	-18.1818	12.7272	-2.2109	545.4545	-381.818	66.3272
4	0.1455	-0.1018	0.0176	-25.4545	17.8181	-3.0952	1090.909	-763.636	132.6545
5	-0.2424	0.1963	-0.0396	36.3636	-29.4545	5.9418	-1212.12	981.8182	-198.061
6	-0.2667	0.2000	-0.0366	33.3333	-25	4.5866	-1000	750	-137.6
7	-0.2909	0.2036	-0.0353	43.6363	-30.5455	5.3061	-1454.55	1018.182	-176.873
8	-0.2667	0.2000	-0.0366	46.6666	-35	6.4213	-2000	1500	-275.2
9	0.5333	-0.4000	0.0733	-80	60	-11.008	2666.667	-2000	366.9333

Table 2. Coefficient *Bi* for transport equation using 10th degree polynomial for different combinations of C and P.

Combination	B_0	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9	B_{10}
C = 50ppm, P = 0.32	0.94	40.9055	-797.899	6113.818	-25174.2	62062.87	-95887.3	93569.84	-55975.1	18728.96	-2682.81
C = 100ppm, P = 0.32	0.92	12.7567	-251.259	1919.004	-7904.32	19473.49	-30045	29279.38	-17499.2	5852.633	-838.377
C = 100ppm, P = 0.43	0.93	5.36993	-119.25	965.7012	-4194.9	10785.53	-17217.3	17246.58	-10541.1	3590.539	-522.08
C = 50ppm, P = 0.43	0.92	29.1239	-576.302	4498.361	-18814.6	46915.24	-73081.3	71750.38	-43123.3	14482.2	-2080.7
C = 75ppm, P = 0.32	0.96	-12.5941	245.6567	-1902.76	7827.899	-19166.4	29285.93	-28189.5	16612.94	-5474.51	772.6405
C = 100ppm, P = 0.38	0.9	4.5118	-87.569	629.9993	-2470.36	5787.478	-8495.22	7900.827	-4526.32	1457.823	-201.973
C = 75ppm, P = 0.43	0.95	-11.8723	222.1547	-1682.03	6800.338	-16408.7	24745.93	-23528.7	13703.32	-4464.17	623.0664
C = 50ppm, P = 0.38	0.94	21.1484	-414.481	3190.304	-13220.6	32766.99	-50858.5	49843.24	-29940.9	10058.05	-1446.2
C = 75ppm, P = 0.38	0.96	-1.2357	17.7860	-109.83	300.4696	-257.919	-506.227	1482.258	-1507.28	712.2393	-130.838

Table 3. Coefficient *Bi* for transport equation using 5th degree polynomial for different combinations of C and P.

Combination	B_0	B_1	B_2	B_3	B_4	B_5
C = 50ppm, P = 0.32	0.9460	-0.6124	-2.5800	3.6145	-1.4183	0.1192
C = 100ppm, P = 0.32	0.9164	0.1543	-4.6724	6.4912	-3.3828	0.5959
C = 100ppm, P = 0.43	0.9259	0.0110	-3.8697	4.4981	-1.4864	0.0000
C = 50ppm, P = 0.43	0.9380	0.2214	-4.8615	5.4240	-1.7342	0.0000
C = 75ppm, P = 0.32	0.9568	0.2387	-1.2499	0.7069	-0.8021	0.4281
C = 100ppm, P = 0.38	0.8960	0.3637	-5.2064	6.6017	-2.9297	0.3576
C = 75ppm, P = 0.43	0.9546	0.0768	-1.1608	1.2690	-1.5132	0.6555
C = 50ppm, P = 0.38	0.9390	0.1233	-4.3590	4.2947	-0.7168	-0.2210
C = 75ppm, P = 0.38	0.9643	0.2370	-2.0458	3.0451	-2.8594	0.9932

Table 4. Coefficient *Bi* for transport equation using 3rd degree polynomial for different combinations of C and P.

Combination	B_0	B_1	B_2	B_3
C = 50ppm, P = 0.32	0.9748	-1.3424	0.0699	0.3002
C = 100ppm, P = 0.32	0.9712	-0.9507	-0.2275	0.3094
C = 100ppm, P = 0.43	0.9789	-1.0032	-0.2277	0.3355
C = 50ppm, P = 0.43	0.9446	-0.9525	-0.6681	0.6244
C = 75ppm, P = 0.32	0.9403	0.5596	-2.0388	0.8179
C = 100ppm, P = 0.38	0.9657	-0.9161	-0.3392	0.3801
C = 75ppm, P = 0.43	0.9272	0.3757	-1.6808	0.6591
C = 50ppm, P = 0.38	0.9857	-0.9761	-0.6715	0.539
C = 75ppm, P = 0.38	0.9416	0.3013	-1.445	0.522

Table 5. Coefficients for transport equation using 10th degree polynomial.

i	$A_{1,i}$	$A_{2,i}$	$A_{3,i}$	$A_{4,i}$	$A_{5,i}$	$A_{6,i}$	$A_{7,i}$	$A_{8,i}$	$A_{9,i}$
0	0.0067	-0.0050	0.0008	-0.7757	0.5763	-0.0982	18.1818	-13.7273	3.2509
1	10.5269	-8.04509	1.5595	-1639.81	1253.139	-243.113	60116.58	-45984	8943.405
2	-209.156	159.7805	-30.9446	32512.48	-24837.7	4814.567	-1190250	910083.8	-176852
3	1641.717	-1253.18	242.3766	-254746	194464.1	-37647	9313816	-7115531	1380897
4	-6887.82	5254.038	-1014.97	1067000	-813958	157399.4	-3.9E+07	29741833	-5765394
5	17277.12	-13171.3	2541.535	-2672144	2037302	-393545	97425581	-7.4E+07	14394285
6	-27139.6	20679.9	-3986.08	4191185	-3193981	616354	-1.5E+08	1.16E+08	-2.3E+07
7	26906.47	-20493.8	3946.19	-4149370	3160906	-609388	1.51E+08	-1.1E+08	22220655
8	-16338.1	12439.98	-2393.13	2516361	-1916301	369114.6	-9.1E+07	69587969	-1.3E+07
9	5543.131	-4219.38	811.0098	-852760	649235.8	-124954	30898339	-2.4E+07	4542720
10	-804.226	612.0243	-117.548	123595.9	-94077.1	18093.33	-4471959	3406316	-656886

ppm while Permeability P1 = 0.32; P2 = 0.38 and P3 = 0.43 then the coefficients N_i are given in Table 1.

A transport equation for a combination of C and P in the form of polynomial function is defined as shown below. It is in the form of C/C_0.

$$\left(\frac{C}{C_0}\right)_{(X)} = \sum_{i=0}^{i\leq 10} (B_i)X^i \tag{2}$$

where X is the distance from point of injection and B_i is the coefficient of polynomial for different combinations of C and P and are tabulated in Table 2 for 10th degree polynomial, Table 3 for 5th degree of polynomial and Table 4 for 3rd degree of polynomial.

The PGWT equation for the concentration, permeability and distance from point of injection was derived using the relation as follows,

$$\left(\frac{C}{C_0}\right)_{(C,P,X)} = N_{i\,(C,P)} \cdot \left(\frac{C}{C_0}\right)_{(X)} \tag{3}$$

$$\left(\frac{C}{C_0}\right)_{(C,P,X)} = \sum_{i=0}^{i\leq 10} \left(A_{1,i}C^2P^2 + A_{2,i}C^2P + A_{3,i}C^2 + A_{4,i}CP^2 + A_{5,i}CP + A_{6,i}C + A_{7,i}P^2 + A_{8,i}P + A_{9,i}\right)X^i \tag{4}$$

where, A_i is the coefficients for different degrees of transport equation and tabulated in Table 5 for transport equation of 10th degree polynomial, Table 6 for transport equation of 5th degree of polynomial, and Table 7 for transport equation of 3rd degree of polynomial.

Table 6. Coefficients for transport equation using 5th degree polynomial.

i	$A_{1,i}$	$A_{2,i}$	$A_{3,i}$	$A_{4,i}$	$A_{5,i}$	$A_{6,i}$	$A_{7,i}$	$A_{8,i}$	$A_{9,i}$
0	0.0121	-0.0090	0.0016	-1.6717	1.2505	-0.2234	54.0545	-40.5582	8.2142
1	-0.1054	0.0864	-0.0176	15.7653	-13.1082	2.7078	-618.406	517.1509	-107.285
2	-0.0487	0.0244	-0.0066	10.22	-5.2966	1.1768	-211.073	49.2709	-13.6508
3	0.8459	-0.6439	0.1264	-136.924	103.4282	-20.0615	4833.555	-3621.7	699.4944
4	-0.9683	0.7481	-0.1427	154.9553	-119.09	22.5856	-5618.12	4299.799	-812.881
5	0.2854	-0.2226	0.0418	-45.2357	35.1163	-6.5786	1639.797	-1269.14	237.2876
6	0.0121	-0.0090	0.0016	-1.6717	1.2505	-0.2234	54.05455	-40.5582	8.2142

Table 7. Coefficients for transport equation using 3rd degree polynomial.

i	$A_{1,i}$	$A_{2,i}$	$A_{3,i}$	$A_{4,i}$	$A_{5,i}$	$A_{6,i}$	$A_{7,i}$	$A_{8,i}$	$A_{9,i}$
0	-0.0002	0.00018	1.5E-05	0.2784	-0.20596	0.0294	-22.5242	16.4086	-1.70428
1	-0.1420	0.1116	-0.0239	21.91642	-17.2871	3.7049	-791.8	627.06	-134.962
2	0.3326	-0.260	0.0522	-51.4151	40.28186	-8.10164	1852.039	-1455.33	292.1028
3	-0.1432	0.1122	-0.0220	21.5163	-16.92	3.3344	-738.476	583.8014	-115.01

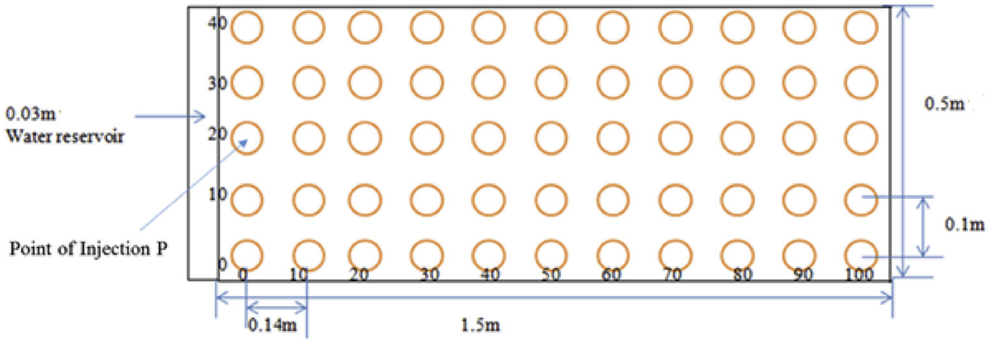

Figure 2. Plan view of the Physical Model.

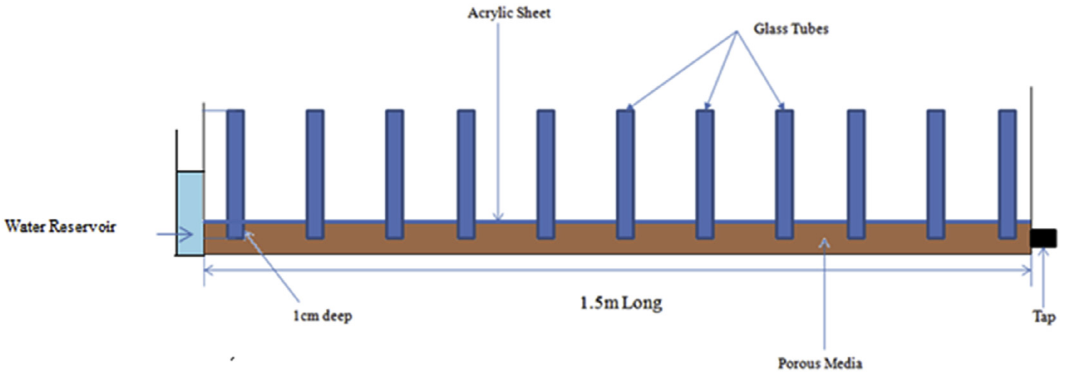

Figure 3. Cross section of the physical aquifer model.

It is observed that the transport Eq. (4) using 10th degree polynomial provided the accurate results with the number of coefficients as 99. However, the number of coefficients using 5th degree polynomial and 3rd degree polynomial are 63 and 36 respectively.

3. Physical Aquifer Model (PAM)

A Physical Aquifer Model (PAM) is developed to conduct the experiments to understand Phenol transport in groundwater. A tank of 1.5 m × 0.5 m is developed with sand as a porous media. Locations of monitoring wells in the PAM are shown in Figure 2 and the cross section of PAM is shown in Figure 3.

Table 8. Material used for PAM.

Material	Size/No.
Glass Tray	1.5 m × 0.5 m x 0.07 m
Acrylic Sheet with laser cut grid	1.5 m × 0.5 m x 0.01 m
Glass Tubes	4 mm dia. 7 cm long 55Nos
Rubber Stoppers	55 Nos

Table 9. Compositions of porous media for PAM.

Sieve Size	% Retained		
	P1	P2	P3
4.75 mm	5	10	—
2.36mm	10	5	15
1.18mm	40	40	40
600 micron	40	40	40
150 micron	5	5	5

3.1. Physical model specifications

PAM has a glass base and sides. The grid patterned acrylic sheet with 4mm diameter holes at fixed points is placed inside the glass base. Table 8 gives the material used for PAM.

3.2. Preparation of porous media

Sand is selected as the porous media in PAM for conducting experiments. Sand is washed and sundried. It is sieved through 4.75 mm, 2.36 mm, and 1.18 mm, 600 micron, and 150 micron sieves and stored in different bags for further use. The mixing of different proportions of sand for arriving at the defined porosities of P1 (0.32), P2 (0.38) and P3 (01.43) for PAM are given in are given in Table 9.

3.3. Methodology

Initially, the porous media for the experimental work is prepared. In the first stage experiments are conducted for simulating steady state flow conditions. In the second stage, experiments are conducted to understand the transport of contaminant Phenol.

Table 10. Absorbance values for standard Phenol solution.

Concentration-mg/l	Set I	Set II	Average
6	0.02	0.03	0.015
12	0.07	0.06	0.065
18	0.10	0.09	0.095
24	0.17	0.18	0.175
30	0.21	0.20	0.205

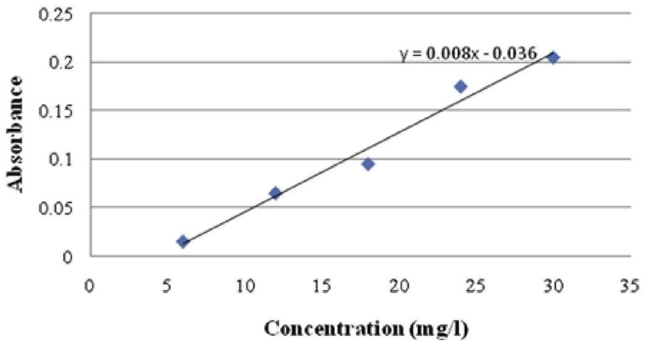

Figure 4. Graph of absorbance and concentration of phenol.

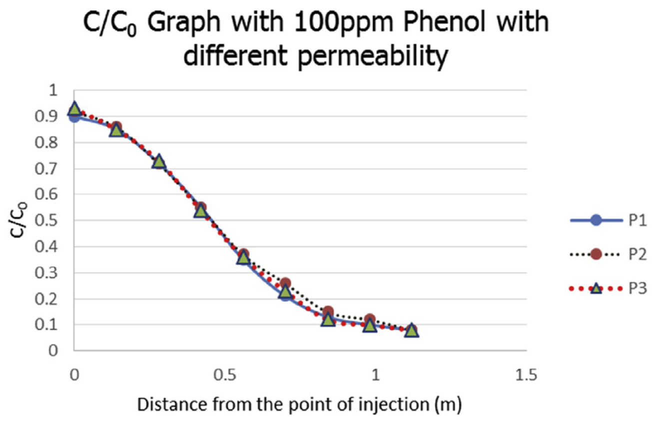

Figure 5. C/C_0 graph with 100ppm Phenol with permeability P1, P2 and P3.

3.4. Flow conditions

In the glass tank, the selected porous media is spread up to 2cm thickness at the bottom. An Acrylic sheet with the glass tubes grid is placed in the tank. The glass tubes are arranged such that each tube is inserted 1cm into the porous media. The porous media is saturated with water by maintaining the water level slightly above 2 cm. After 24 h, the level of water is reduced to 2 cm. Readings are taken for the changes in water level in the tank. Contaminant solution is prepared with 100 ppm Phenol concentration. 100 ml of the contaminant solution is introduced into the tank from fixed point P as shown in Figure 2a. Readings are recorded for the changes in water level in the tank. After 24 h, readings are recorded for the changes in water level in the tank. 100 ml of the contaminant solution is again injected into the tank from point P (Figure 2a). Readings are recorded for the changes in water level in the tank. After 24 h. Readings are recorded for the changes in water level in the tank.

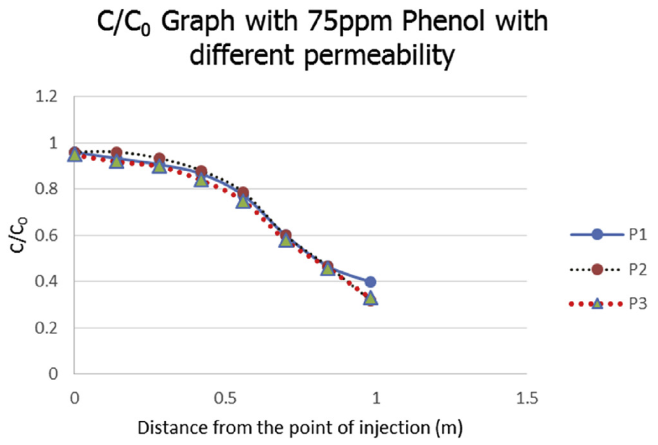

Figure 6. C/C_0 graph with 75ppm Phenol with permeability P1, P2 and P3.

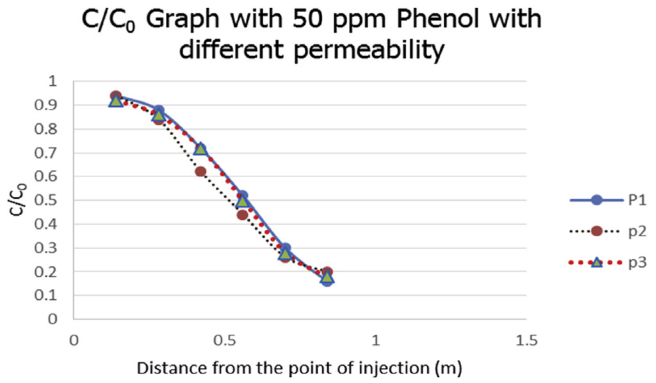

Figure 7. C/C_0 graph with 50ppm Phenol with permeability P1, P2 and P3.

3.5. Transport condition

50 ml of contaminant solution with 100 ppm Phenol concentration is added at fixed point in the tank. After 24 h. Phenol concentrations are recorded using colorimetry. Colorimetry uses absorbance between control sample and contaminated sample to check the level of contaminant concentration. It is a standard method of checking concentrations of contaminants with application in different fields of science (Jones and Johnson (1973); Varadraju et al. (2018)). .4-aminoantipyrine (4AAP) method is used for finding the absorbance of control flasks and test flasks. For taking the absorbance values, the wavelength of the colorimeter is adjusted to 530 nm by rotating the filter disc. Initially, cuvette is washed with distilled water, reagent blank in the cuvette is inserted in colorimeter and absorbance is adjusted to zero. Test solution in the cuvette is inserted in colorimeter and absorbance is checked. Sample is diluted if the absorbance goes beyond the maximum absorbance of standard graph. 4AAP in the presence of potassium ferricyanide at a pH of 10 to form a stable reddish-brown colored antipyrine dye. The amount of color produced is a function of the concentration of Phenolic material.

Table 10 represents the absorbance values for standard Phenol solution. The average of two sets of readings of the absorbance of Phenol with different concentrations is noted.

Graph between absorbance and concentration of Phenol contaminant is plotted as shown in Figure 4. The trend line of the standard graph is used for calculating unknown concentrations of Phenol contaminant from known absorbance values.

Reagents are prepared using 4 AAP and Sodium Hydroxide and Borax Buffer. The standard equation for the graph is:

$$y = 0.008\,x - 0.036 \tag{5}$$

where y is the absorbance and x is concentration of contaminant Phenol in ppm.

4. Results and discussion

The results of PGWT equation for Phenol transport in groundwater are validated with the observation in PAM developed. C/C_0 graphs are

Table 11. Accuracy of PGWT Equation for different degrees of polynomial.

Degree of Transport Equation	10	5	3
% of nodes having less than 2% Error	100%	43%	20%
% of nodes having less than 5% Error	100%	67%	52%
% of nodes having less than 10% Error	100%	84%	72%

plotted for the 100ppm, 75ppm and 50ppm Phenol concentrations for understanding the transport of Phenol in groundwater aquifer. All the graphs are following S-curve pattern as shown in Figures 5, 6, and 7.

It is observed that there is a good agreement of PGWT equation using 10th degree polynomial as compared to 5th or 3rd degree polynomial with the observations of PAM. The accuracy of PGWT equation is elaborated in Table 11.

However, the study is limited to the Phenol contaminant with sand as porous media. The intermediate values of concentrations between 50 ppm to 100 ppm and permeabilities between 0.32 to 0.42 can be calculated using PGWT equation. Different equations can be developed for different permebilities and concentrations of contaminants in groundwater.

5. Conclusions

The process of identifying the spread of contaminant like Phenol in the groundwater is tedious because of the hydrological parameters and complex geological strata. The concentration of contaminant at a distance can be predicted using the PGWT equation presented in the study. This equation is based on the Lagrangian interpolation function using nine noded element for initial contaminant concentrations values of 50 ppm, 75 ppm and 100 ppm with porous media of porosity 0.32, 0.38 and 0.43. The equation is developed with the polynomials of degree ten, five and three. The present study also demonstrates the usefulness of Physical Aquifer Model (PAM) for understanding the transport characteristics of Phenol as contaminant under simulated *in situ* conditions. Phenol concentration levels are found to get affected by the permeabilities of the aquifer.

The results of PGWT equation are validated with the observations of PAM. It is observed that the accuracy of the equation increases with the degree of polynomial.

Declarations

Author contribution statement

Kamat Sahajanand & Mategaonkar Meenal: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

Gharat Prasad: Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

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Competing interest statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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