Three-Dimension Flow and Solute Transport Modeling of the Eolian Aquifer in a Uniform Flow Field of a Chemical Plant

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ABSTRACT

A numerical model consisting of 24 columns, 20 rows and 2 layers was developed for the chemical plant to solve the three-dimension flow and solute transport and to delineate the chromium plume dispersion along the longitudinal, transverse and vertical z directions. The PROCESSING MODFLOW (PM) was used in conjunction with the U.S. Geological Survey's "Modular Three-Dimension Finite-Difference Groundwater Flow Model", MODFLOW, and the transport model MT3D. From 1972 to 1992, plant liquid effluents with a chromate concentration of 2 to 3 ppm were discharged into the unlined evaporation ponds. In 1992, evaporation ponds were lined to control the process of infiltration of chromate liquid waste into subsoil and to avoid mixing in groundwater through vertical and lateral movement. The model predicted the flow pattern and movement of resultant plume developed in the Eolian aquifer. Heads distribution deduced by the models for the steady state case is in close harmony with the observed heads. In transient case model realizations were obtained with 4 stress periods identifying the chromate liquid waste plume (1972 - 1992) during stress period 1, which disappeared from the major flow system in 120 years during the remaining stress periods. Finally, plume appears to be oriented along the Dohar Wah Canal and discharges into it.

At specified nodes (1,11,6), (2,11,6), (1,7,6), (1,5,11) and (1,5,14) level of concentration monitored by the model for the simulation period of 80 to 140 years has assessed that chromium plume would arrive at village Kotla Mirza in year 2022.

Based on the most recent position of the contaminant plume, six monitoring well sites have been delineated at nodes (1,8,6), (1,8,8), (1,8,13), (1,11,6) (1,7,12) and (1,11,13) for future periodic water samplings.

INTRODUCTION

The PROCESSING MODFLOW (PM) has been used in conjunction with the U.S. Geological Survey's "Modular Three-Dimension Finite-Difference Groundwater Flow Model", MODFLOW, (McDonald and Harbaugh, 1988) and the transport model MT3D (Zheng, 1990) to delineate the configuration of chromate plume in the Eolian aquifer underlying a Chemical Plant. Strazimiri and Motz (1997) developed a groundwater flow model of the Lushnja aquifer in Albania and produced appreciable calibration results. Many more are discussed in the proceedings of the fifth international conference (1992) on the use of models entitled 'Solving Groundwater Problems with Models'.

Others include Pinder and Gray, 1977; Konikow and Bredehoeft, 1978 and Wang and Anderson, 1982. It is reported that plant liquid waste with a chromate concentration of 2 to 3 ppm had been drained into unlined evaporation pond for 20 years starting from 1972 to 1992. In 1992 evaporation pond was lined and since then liquid waste is being drained into lined evaporation pond. As a result of this long term process of liquid disposal waste, a plume of chromate concentration has been developed and it has started to travel along flow path towards the downstream hydraulic gradient. Prior to running MT3D, The PROCESSING MODFLOW (PM) and the 3-D groundwater flow model (MODFLOW) were run for 20 years period under steady-state condition. Under transient condition, the concentration distribution of chromate 140 years after beginning of chromate migration in the aquifer has been evaluated.

Evaporation pond lies at the central part of the model area while village Kotla Mirza is about 750 meters in west from the extreme boundary of the evaporation pond (Figure 1). There are six tubewells, belonging to Chemical Plant, exist outside the model boundary whose water quality is highly dependent upon the recharge of New Mahi Wah Canal. They are used for domestic and industrial purposes. A water treatment plant located adjacent to New Mahi Wah Canal is used to purify and remove suspended particles from the pumped water of these tubewells before delivering it by gravity to residence colony and plant.

Hydrogeological Setting for Model Operation

The hydrogeological setting used in the model operation of the Chemical Plant is illustrated in figure 2. The aquifer is unconfined and consists mostly of medium to fine sand exhibiting two hydraulic conductivities, about 6.94x10⁻⁴ m/sec in layer 1 and 2.3x10⁻⁵ m/sec in layer 2. In vertical view a thin confining layer of clay acts as a transition layer (it is called "quasi-3D confining layer" by MODPATH, a particle tracking program, Pollock, 1889). Its vertical leakance is calculated using the following formula:

where

$$\frac{1}{L} = \frac{\frac{d_1}{2} + \frac{d_2}{2} + d_c}{K_{N_1} + K_{N_2} + K_{N_c}}$$

L=vertical Leakance

 d_1 and d_2 = thicknesses of the upper and lower aquifers d_c = thickness of the semiconfining layer

 $K_{fv,1}$ = vertical hydraulic conductivity of the upper layer $K_{fv,2}$ = vertical hydraulic conductivity of the lower aquifer

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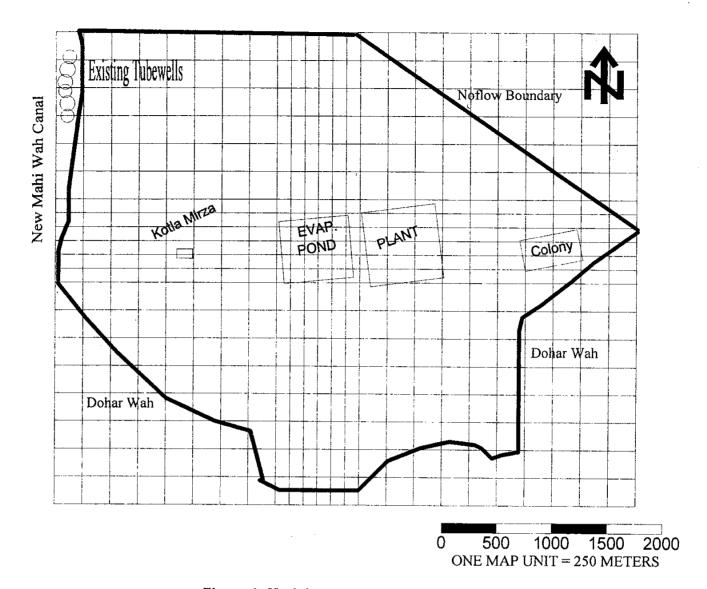


Figure 1- Model area - overlay of grid.

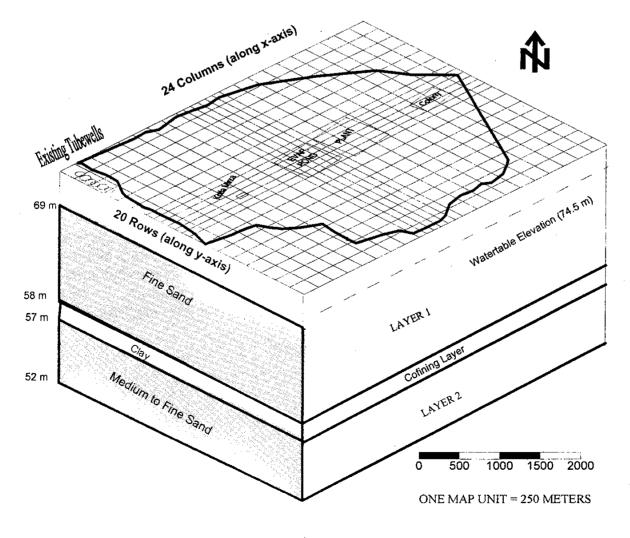


Figure 2- Subsurface lithological layers used in MT3D Transport Model.

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 $K_{\text{fv,c}}$ = vertical hydraulic conductivity of the semiconfined layer

The leakance calculated for the confining layer appears to be 2.6x10⁻⁸ m/sec.

Boundary Conditions

New Mahi Wah and Dohar Wah canals (Figure 1) are treated as constant head boundary and a no-flow boundary is assumed northeast of the plant site. Data for precipitation at the plant site are taken from the nearest meteorological observatory: the site receives 500 mm/year, out of which 15% is assumed to recharge the aquifer at a rate of 2.378x10⁻⁹ m/sec.

Description of Model

The model is consisted of two layers in the vertical direction as shown in figure 2. In plan view, 20 rows and 24 columns were used with a spacing of 250 meters in the x and y directions. However, cells falling in the evaporation pond and plant area are concentrated in the central part of the finite-difference mesh and also in area of the contaminant plume (125 meters in the x and y directions).

In figure 2, central mesh area is the main source of contamination located adjacent to Chemical Plant in southwest. A concentration of 2x10⁻³ Kg/m³ (2 ppm) is assumed to enter the aquifer system via layer 1 as recharging source since 1972. Under steady-state flow conditions, the concentration distribution of chromate twenty-five years after beginning of chromate migration in the aquifer has been evaluated. Under transient flow conditions, the same procedure is repeated with four period of stress with variable time duration.

Input Parameters used in MT3D

The following aquifer parameters and solute properties are used in the model:

Effective Porosity = 0.2

Hydraulic conductivity = 6.94x10⁻⁴ m/sec and 2.3x10⁻⁵ m/sec

Recharge = $2.37x10^{-09}$ m/sec

Longitudinal dispersivity = 2 m

Distribution coefficient of chromium = .0002 and .00002 m³ /Kg

Bulk density of the porous medium = 1600 to 1900 Kg/m³ (medium to fine, and fine sand)

Leakance for the confining bed = $K_L = 2.6 \times 10^{-8}$ m/sec

MODELING RESULTS

The output of the flow modeling for the steady state and transient simulation is shown in figure 3 and figure 4. In figure 3 head distribution for the three selective nodes in layer 1 are shown. Three-dimension representation of the groundwater flow in layer 1 (Figure 4) indicates very little change in the hydraulic heads varying from 74.0 m to 72.20 m. The groundwater flows southwest from the evaporation ponds (concentration source). There is no significant change in the hydraulic heads in layer 2.

The effect of plume dispersion in layer 1 with 20 years simulation time is shown in figure 5. In this test,

concentration plume has spread about 700 meters beyond the pond limit but has not reached Village Kotla Mirza. The extending front has a concentration of $1x10^{-5}$ Kg/m 3 (.01 ppm) which is below WHO's drinking water permissible limit of 0.05 ppm.

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The transport model produced realistic results when simulated under transient condition (Figure 6). In practice, plant liquid effluents with 2 to 3 ppm chromate concentrations are not disposed off continuously throughout the day. Therefore, the time period and the process of simulation (in the transient condition) with selective stress period are important criteria in accurate prediction.

Under transient simulation, the extending front has a concentration of $7x10^{-6}$ Kg/m 3 (.007 ppm) and it stays at about 500 meters beyond the pond limit. Kotla Mirza is about 250 meters away from the edge of the dispersion plume. A three-dimension view of the transient simulation in layer 2 is shown in figure 7.

From the results of this study, it appears that liquid waste disposal has effected no significant degradation in the groundwater around the evaporation pond. The plume has not expanded to a significant distance either laterally or vertically. The values of chromium concentration within the plumes in layer 1 and layer 2 are given in table 1. In the contour column, the contour lines are numbered consecutively from 1 (the outermost contour) to 9 (the innermost).

Table 1. Values of Chromium Concentration (Kg/m3).

Contour	Layer 1	Layer 2
1	4.86E-6	1.22E-6
2	9.75E-6	2.45E-6
3	1. 4 6E-5	3.68E-6
4	2.44E-5	4.91E-6
5	2.93E-5	6.14E-6
6	3.41E-5	7.37E-6
7	3.91E-5	8.60E-6
8	4.39E-5	9.83E-6
9	4.88E-5	1.10E-5

FUTURE SCENARIOS OF PLUME DISPERSION

To navigate the dispersion of plume along the flow path in layer 1 and layer 2, different time increments comprising 60, 75, 105, and 120 years stress periods were used and the model was run under transient conditions. The output of these forecasting simulations is shown in figure 8, figure 9, figure 10, figure 11, and figure 12. The level of concentration tends to decline with each incremental change in time. Figure 8 and figure 9 give a 3-D view of plume dispersion in the flow field. In figure 10 and figure 11, the plume's configuration is shown on the finite-difference grid with respect to surface features where it appears to be discharging into the Dohar Wah Canal. Figure 12 shows the plume's configuration with respect to the equipotential surface after 120 years of simulation.

From the forecast scenarios, the rate of plume dispersion has been evaluated at about 17 m/year. Dispersion will take place in the southwest direction and the plume will arrive at Kotla Mirza in 2022. Kotla Mirza is located at node (1,5,11).

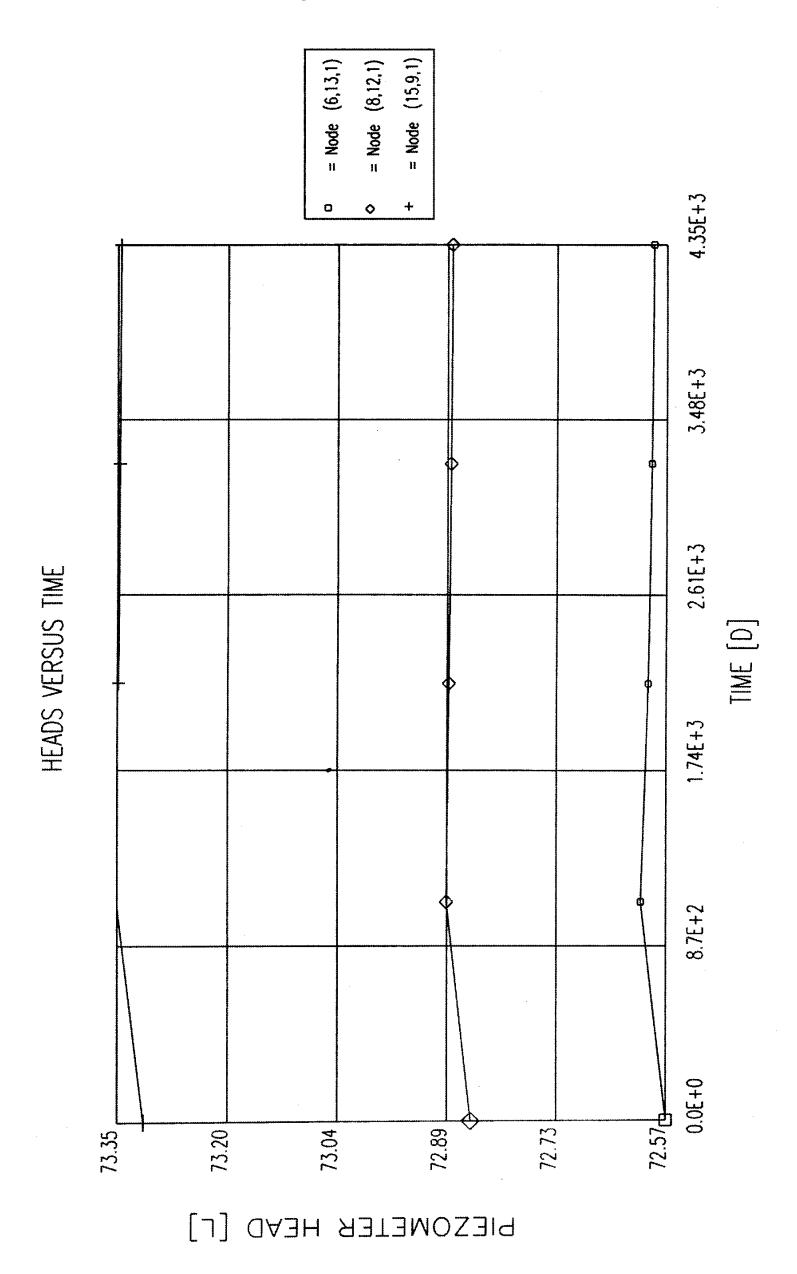


Figure 3- Head distribution for the three selected nodes.

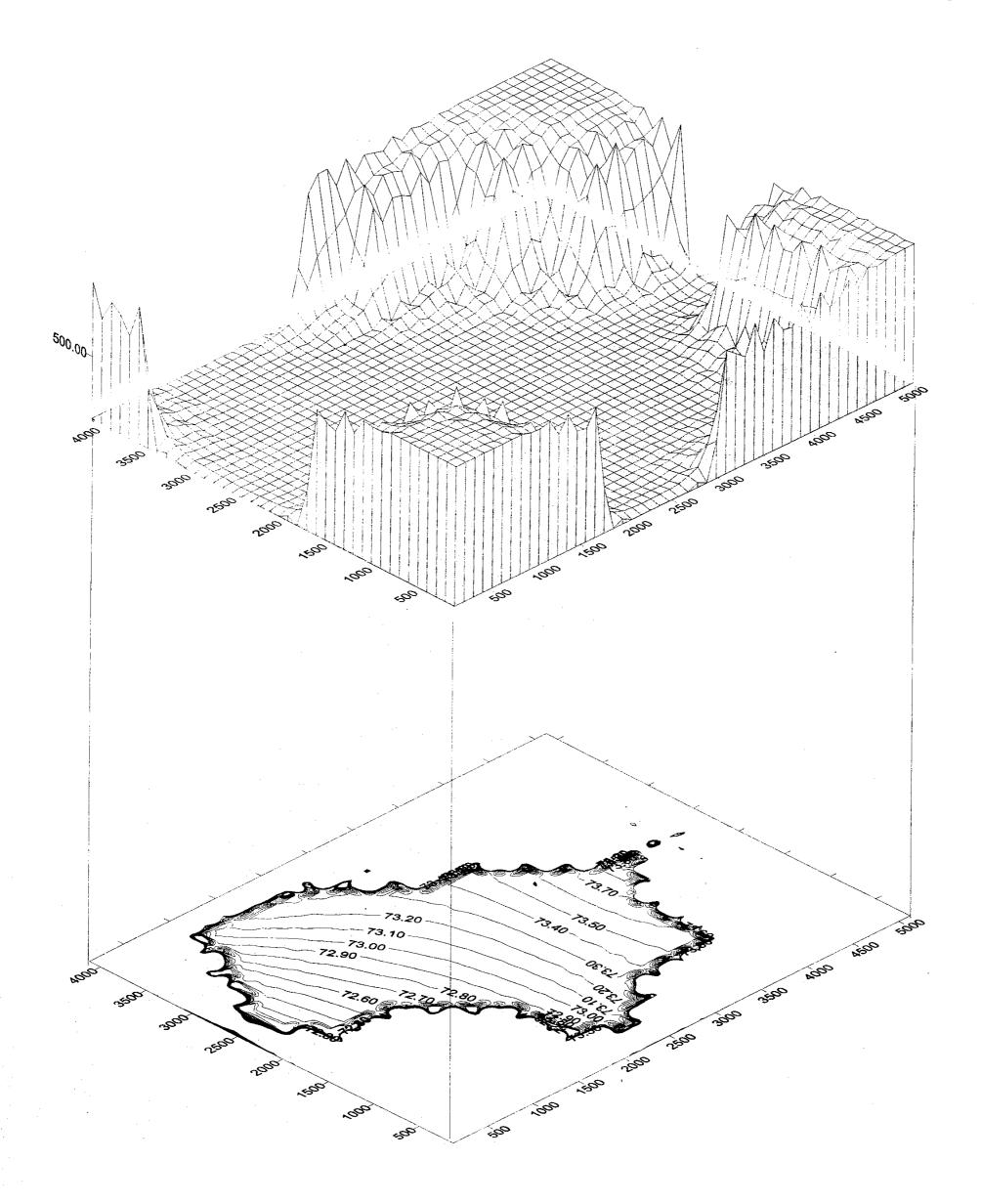


Figure 4- Steady state ground water flow model (Layer 1).

NORTH

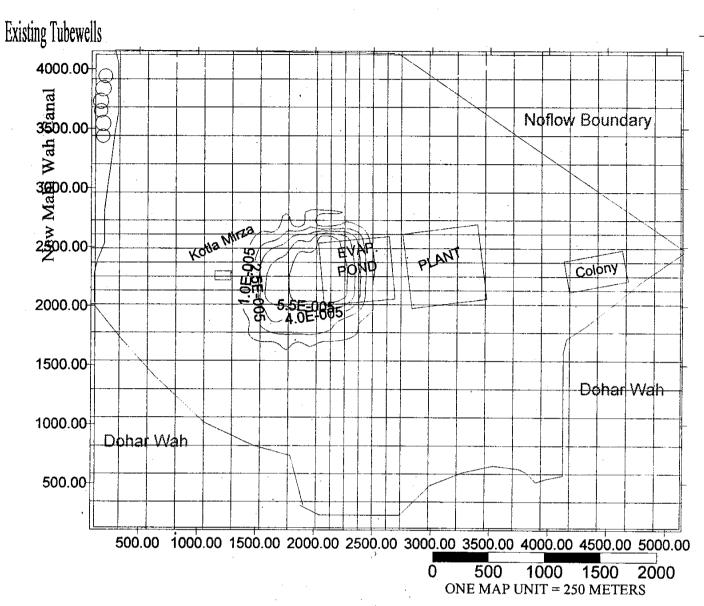


Figure 5- Development of chromium plume from continuous source since 1972 (Layer 1).

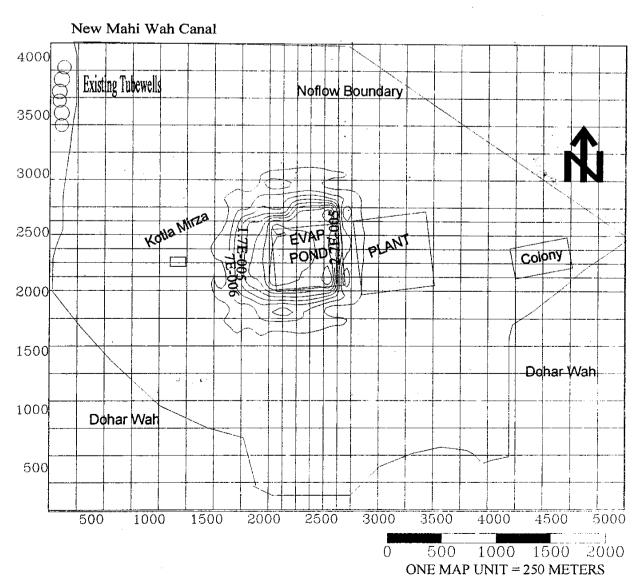


Figure 6- Development of chromium plume from continuous source (transient simulation: Layer 1).

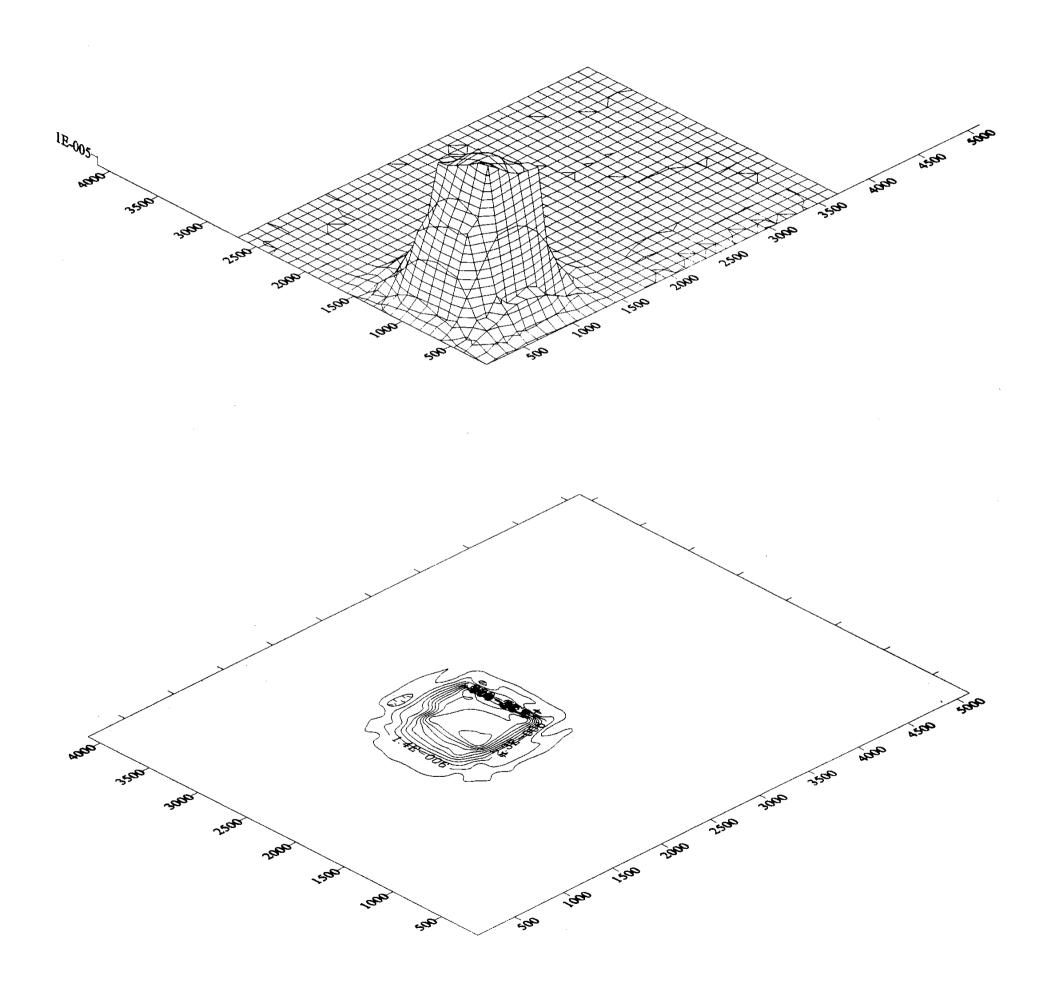


Figure 7- Development of chromium plume with 4 stress periods (transient simulation: Layer 2).

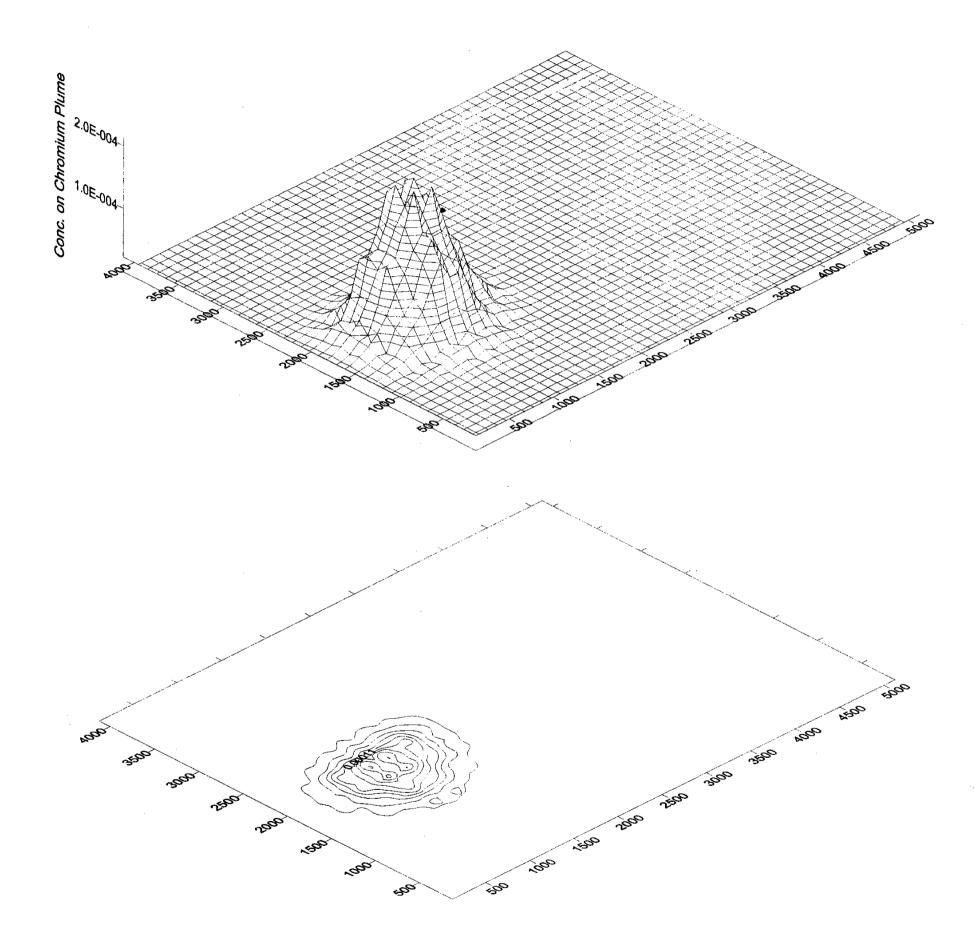


Figure 8- Development of chromium plume after 60 years (transient simulation: Layer 1).

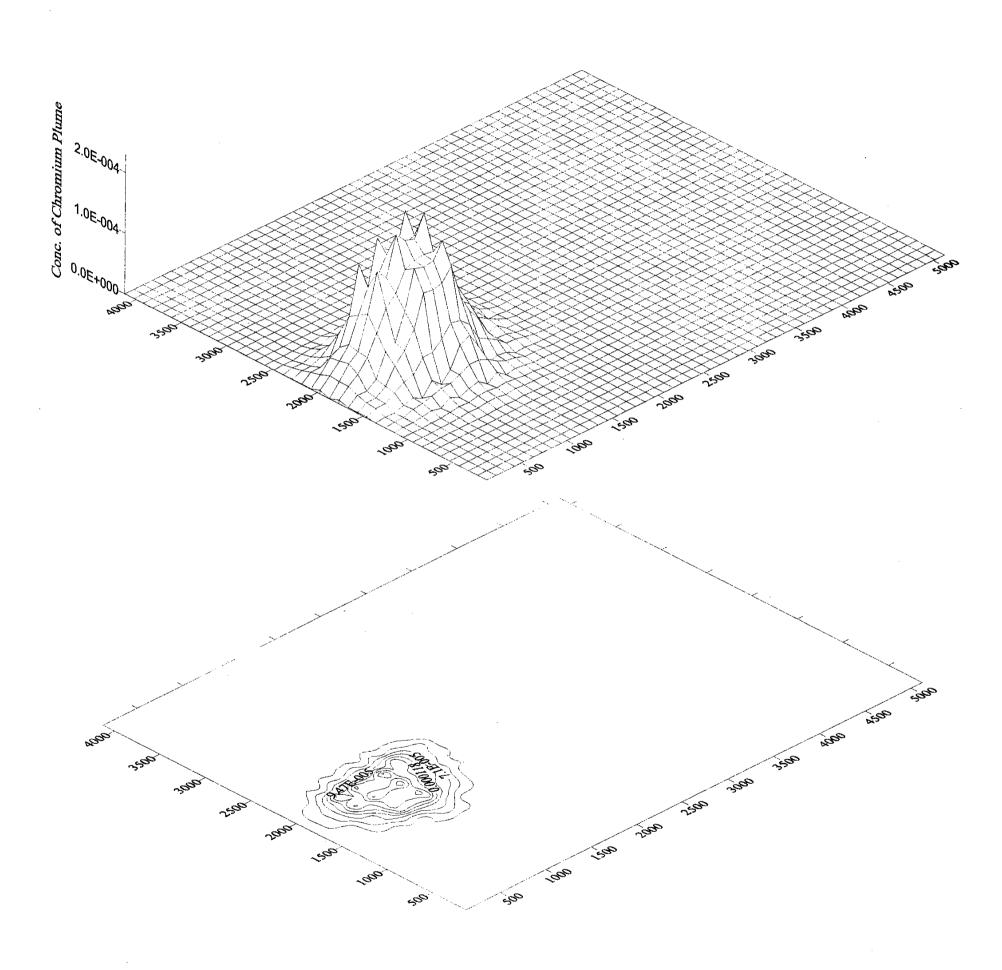


Figure 9- Development of chromium plume after 75 years (transient simulation: Layer 1).

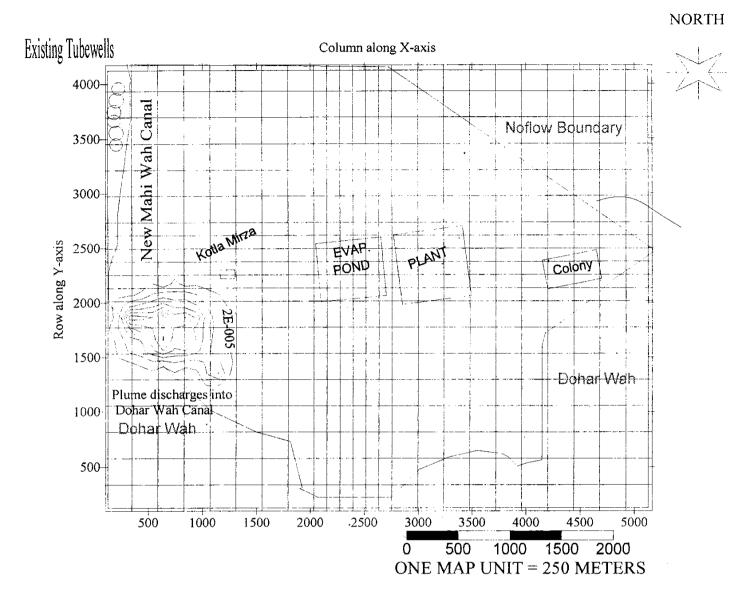


Figure 10- Development of chromium plume w.r. to surface features after 105 years.

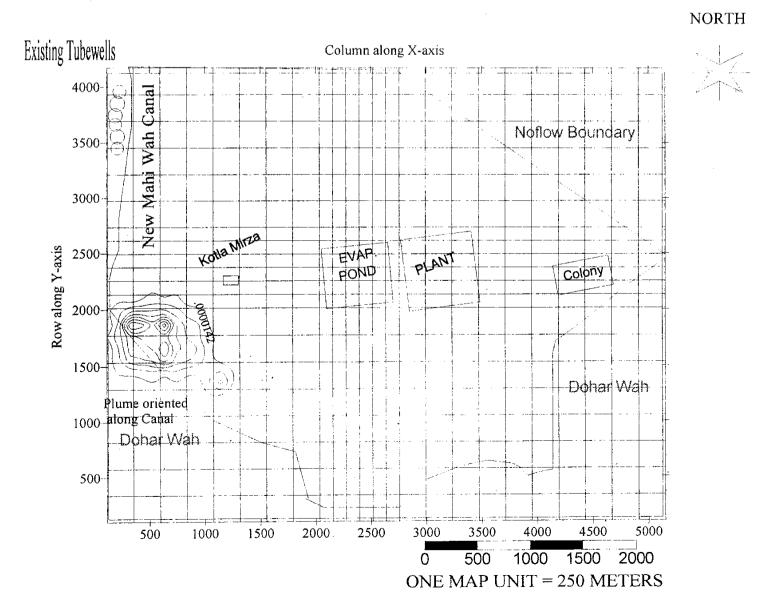


Figure 11- Development of chromium plume w.r. to surface features after 120 years (transient simulation: Layer 1).

MONITORING PLAN

Monitoring Wells

The hydraulic heads derived when the model was run under steady state (1972-1992 period) conditions were used in the modeling of the transient condition to simulate the most recent position of the dispersion plume (1992-1998). The most recent position of plume is shown in figure 13 on the finite-difference grid. On the basis of this estimated current position, six monitoring well sites were selected. They are marked in figure 13 as nodes (1,8,6), (1,8,8), (1,8,13), (1,7,12), (1,11,6) and (1,11,13). Monitoring wells should be drilled up to a depth of 10 m and 20 m for layer 1 and layer 2 respectively. These wells should be used for periodic water sampling.

Solute Concentrations in the Observation Wells

'Observation wells' were assumed at nodes (1,11,6), (2,11,6), (1,7,6), (1,5,11 Kotla Mirza) and (1,5,14)----- in the path of the expected plume passage)----to project the changes in concentration during different time intervals. The results of these simulations are shown in figure 14, figure 15, and figure 16.

In figure 14, the level of solute concentration begins to rise after 35 years; it attains a near equilibrium condition after 65 years. Almost no level of concentration was received by the observation wells at nodes (1,7,6) and (2,7,6).

In another experiment, the simulation time was increased from 80 to 140 years and this time observation wells were located at nodes (1,5,11) and (1,5,14). In figure 15 and figure 16, the level of concentration tends to increase after 45 years reaching its maximum value after 80 and 90 years respectively for layer 1 and layer 2. The concentration is relatively lower in layer 1. As figure 16 shows, the chromium concentration tends to drop after 80 years at (1,5,11) and after 100 years at (1,5,14).

CONCLUSIONS

Findings

Based on the modeling results for the present and future situation, it is concluded that:

At this stage, the dispersion plume has neither **expanded** nor moved considerably; it is less than 700 m **beyond the** pond boundary. The level of concentration found at the monitoring wells is well below the WHO permissible maximum limit of 0.05 ppm for chromium in groundwater.

There is no much difference in the expected level of chromium concentration in layer 1 and layer 2.

At its existing dispersion rate of 17 m/year, the plume would arrive at Kotla Mirza in 2020.

Recommendations

Based on the recent trends in plume dispersion, it is suggested that monitoring wells be drilled at six proposed sites for the purposes of periodic water sampling. The proposed well sites are nodes (1,8,6), (1,8,8), (1,8,13), (1,7,12), (1,11,6) and (1,11,13). The wells should be 10 m deep for layer 1 and 20 m deep for layer 2 (Figure 14).

Flushing by natural recharge in the area of contamination will take about 100 years depending upon the potential of recharge. However, it could also be accomplished by artificially injecting water in the aquifer to flush out chromium concentration rapidly. Suitable sites for flushing the aquifer artificially are the proposed monitoring well locations at nodes (1,11,6) and (1,11,13) at the upward hydraulic gradient.

Monitoring should be performed at wells that exist at the downward hydraulic gradient and a record of the continuous changes in the concentration level should be kept.

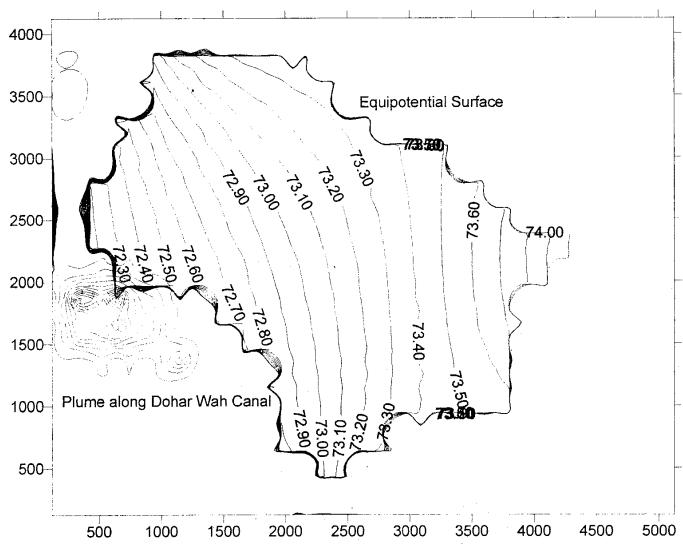


Figure 12- Location of chromium plume with respect of equipotential surface after 120 years (transient simulation: Layer 1).

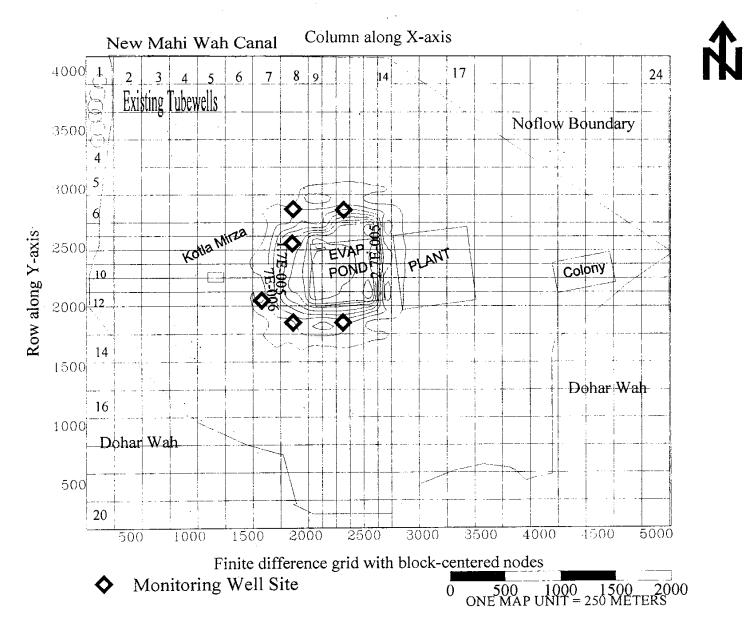


Figure 13- Location of monitoring well site for periodic water sampling.

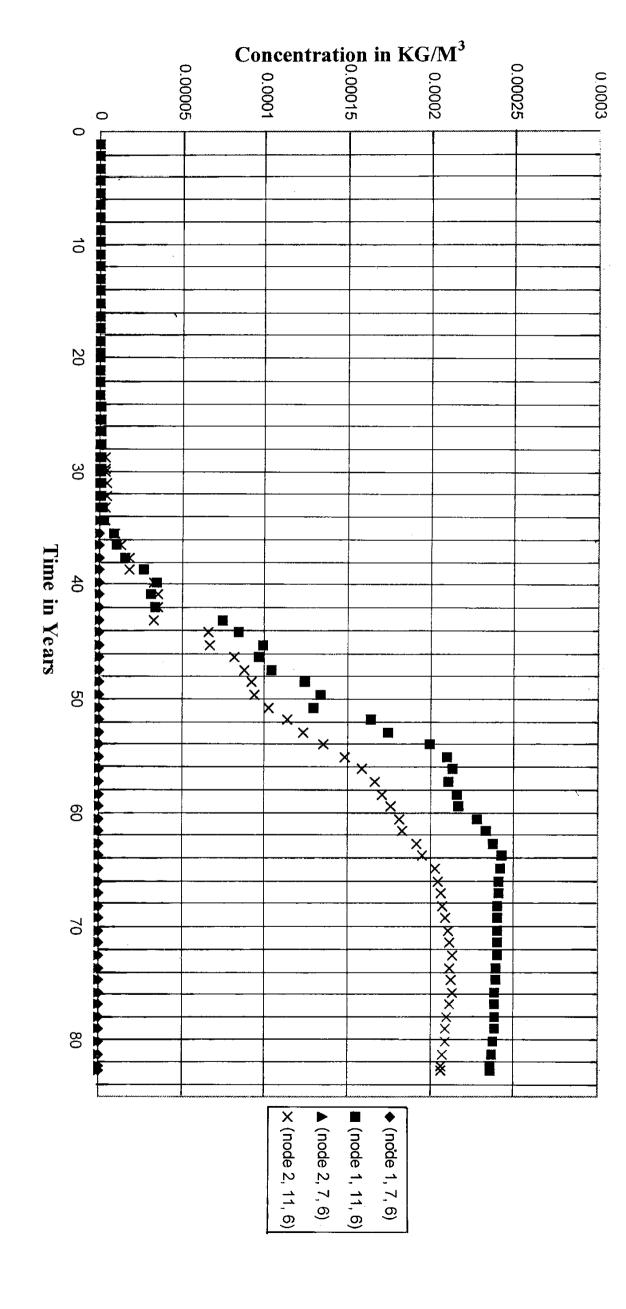


Figure 14- Concentrations of chromate for 80-year simulation period at nodes in Layer 1 and 2.

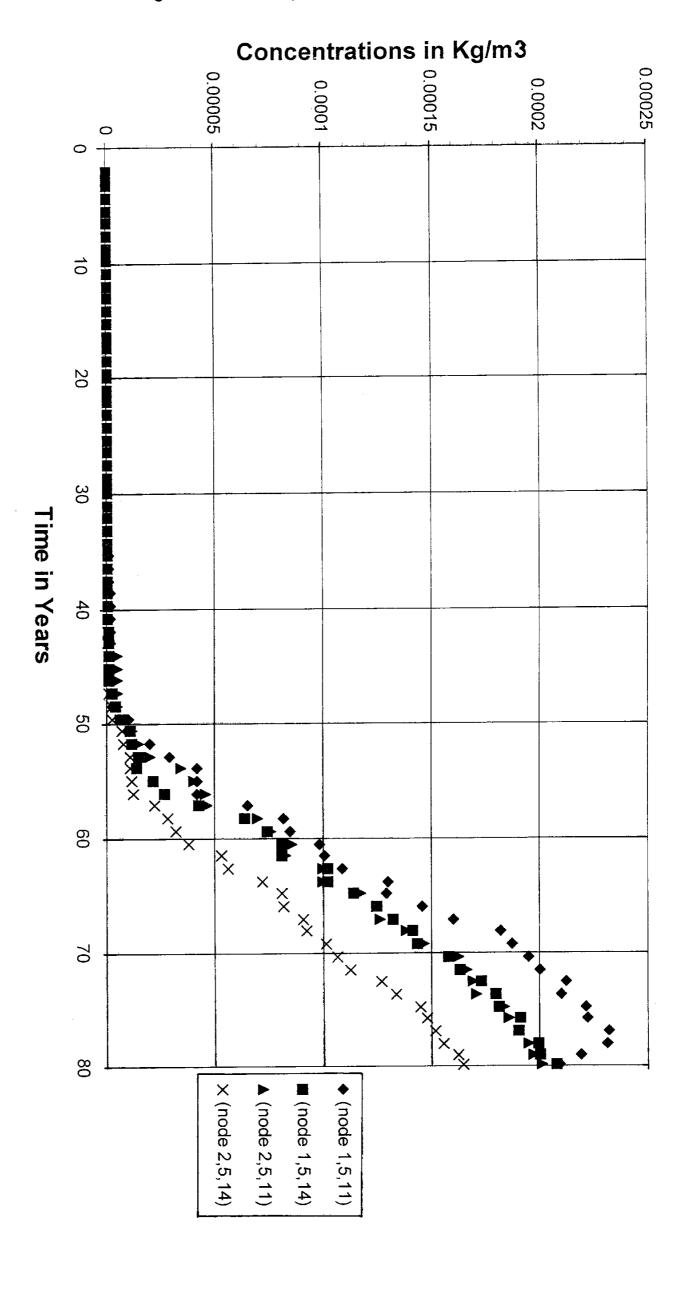


Figure 15- Concentrations of chromate for 80-year simulation period at nodes in Layer 1 and 2.

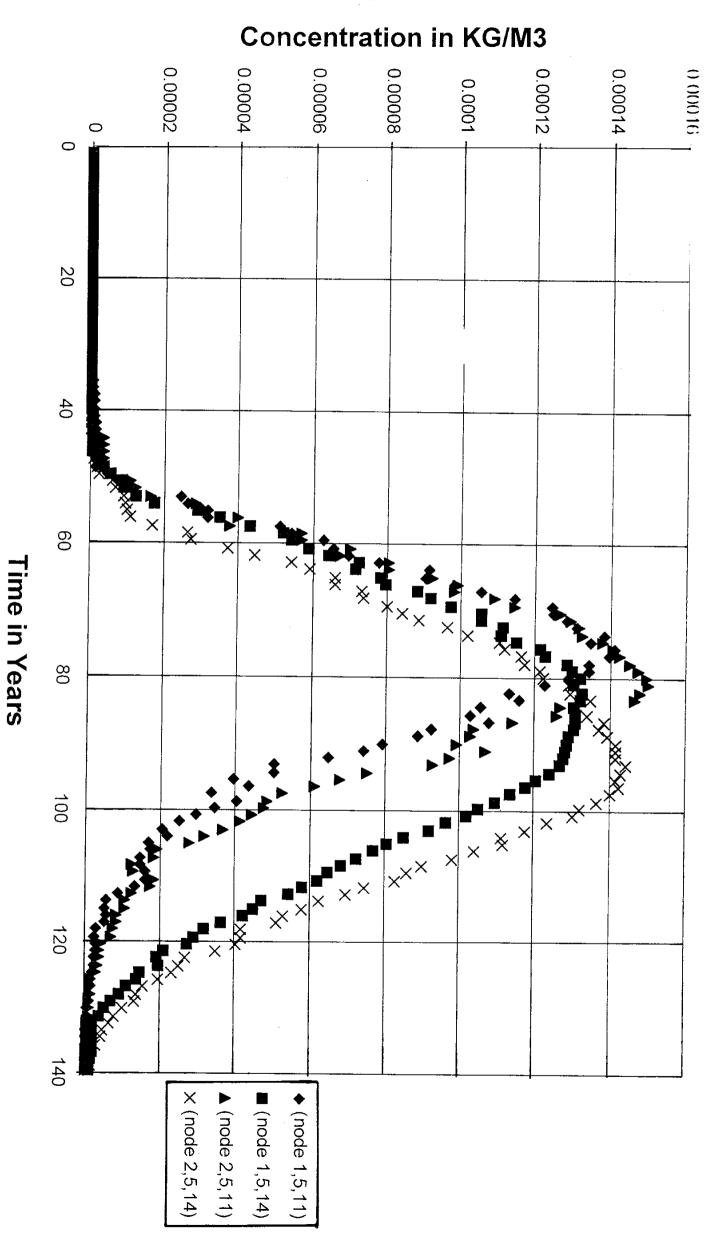


Figure 16- Concentr ations of chromate for 140-year simulation period at nodes in Layer 1 and 2.

REFERENCES

- Konikow, L. F., and J. D. Bredehoeft, 1978, Computer model of two-dimensional solute transport and dispersion in groundwater: U.S. Geol. Surv., Tech. of Water-Resources Invest, Book 7, Chap. C2, 90p.
- McDonald, M. C. and A. W. Harbaugh, 1988, MODFLOW, A modular three-dimensional finite difference ground-water flow model: U.S. Geological Survey, Open-file report 83-875, Chapter A1, Washington, DC.

Pinder, G. and W.G. Gray, 1977. Finite element simulation in surface and subsurface hydrology: Academic press, 295p.

Pollock D. W., 1989. Documentation of a computer programs to compute and display pathlines using results from the U.S. Geological Survey modular three-dimensional finite-difference groundwater flow model: U.S. Geological Survey, Open-file report 89-381, Dever.

- Solving Ground Water Problems with Models, 1992, Proc.: Fifth International Conference on the use of models to analyze and find working solutions to ground water problems, Feb. 11-13, The Grand Kempinski Hotel, Dallas, Texas. 714p.
- Strazimiri D. L., and Motz L. H, 1997, Groundwater flow model of the northern part of the Lushnja aquifer in Albania: Hydrological Sciences Journal, v.42, p. 679-691.
- Wang, H.F. and M.P. Anderson, 1982, Introduction to groundwater modeling finite difference and finite element methods: W. H. Feeman and Co., 237p.
- Zheng, C., 1990, MT3D, a modular three-dimensional transport model: S.S. Papadopulos & Associates, Inc., Rockville, Maryland.