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5 Application of Particle Tracking Models to Aquifer Contamination Assessment

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Abstract

Particle tracking models are very useful tools in aquifer contamination assessment and management. They help acquiring better insight into the physical, environmental and economical aspects of water quality problems. This paper describes the application of particle tracking models in the assessment and management of contaminant transport in aquifer system.The potential bacteriological contamination of Seiy'un wellfield due to the migration of contamination from the cesspools and sewage disposal pits is assessed using the United States Geological Survey (USGS) particle- tracking code MODPATH in conjuction with the USGS flow model MODFLOW. The developed model is used to assess the potential contamination of the wellfield, by identifying the flow pattern in the wellfield aquifer and the capture zones of individual wellfield boreholes and estimating contaminant travel times from sources to boreholes.

Keywords: particle tracking, groundwater, contaminant transport, aquifer system

الملخص

تعتبر نماذج تتبع الجزيئات أدوات مفيدة جداً في تقدير و إدارة تلوث الخزانات الجوفية. فهي تساعد في الحصول على فهم أفضل للجوانب القيزيائية واالبيئية والاقتصادية لمسائل نوعية المياه. هذه الورقة تقدم وصفاً لتطبيق نماذج تتبع الجزيئآت في مجال تقدير وإدارة إنتقال الملوثات قي أنظمة الخزانات الجوفية. تم استخدام برنامج تتبع الجزيئآت الذي طورته هيئة المساحة الجيولوجية الأمريكية لتقدير التلوث البكتيريولوجي الممكن لحقل آبار مدينة سيئون نتيجة لهجرة الملوثات من البيارات والحفر الراشحة وذلك عن طريق تحديد نسق الجريان في الخزان الجوفي للحقل ومناطق التغذية Capture Zones الخاصة لكل بئر وكذلك تحديد أزمنة السريان من مصادر التلوث إلى الآبار.

1. INTRODUCTION

Particle tracking models are very useful tools in the assessment of well capture. They can be used to identify potentially responsible parties for contamination of drinking water well as well as to identify regions for well head protections. In many contaminated sites, multiple possible sources or responsible parties could cause the pollution. The need to identify the responsible party or parties results in litigation and

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assessment of groundwater flow patterns [Harr, 1996]. Models are used to simulate the groundwater flow and to see whether groundwater underneath potential sources is eventually captured by the pumping well. To further assess the feasibility of a potential source, the travel time of contaminants from the source to the well is estimated to see if the timing fits with possible releases from the site. Numerical Particle tracking models in conjunction with numerical flow models can be used to evaluate the capture zone and travel times.

In wellhead protection, the headwaters of the well or regions which supply water to the well are identified. The community councils and the regulatory authorities decide on appropriate land use for these regions which will have minimal impact on the subsurface groundwater.

2. MATHEMATICAL GROUNDWATER QUALITY MODEL

Mathematical model of solute transport in groundwater simulates the movement of solute in groundwater by solving the general governing equation represinting the physical process that occur in the system togather with the boundary and initial conditions applicable to the domain of solution.

The governing equation of three dimensional solute transport in groundwater is given by:

$$\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial h}{\partial x_j}\right)+W^{*}=S_S\frac{\partial h}{\partial t}, \qquad i,j=1,2,3 \tag{1}$$

where

K_{ij} = hydraulic conductivity tensor [LT^{-1}];
h = hydraulic head [L];
S_S = specific storage [L^{-1}];
W^* = $W^*(x,y,z,t)$ = the volume flux per unit volume[T^{-1}];
x_i,x_j = Cartesian co-ordinates[L];and
t = time[T].

and transport equation

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c}{\partial x_j}\right)-\frac{\partial}{\partial x_i}\left(cV_i\right)+\frac{W^{*}}{\theta}c'+\sum_{k=1}^{N}R_k=\frac{\partial c}{\partial t}, \qquad i,j=1,2,3 \tag{2}$$

where $\sum_{k=1}^{N}R_k$ is the chemical sink/source term given by

$$\sum_{k=1}^{N}R_k=-\frac{\rho_b}{\theta}\frac{\partial\bar{c}}{\partial t} \qquad \text{for equilibrium-controlled sorption.}$$

$$\sum_{k=1}^{N}R_k=-\lambda\left(c+\frac{\rho_b}{\theta}\bar{c}\right) \quad \text{for first order irreversible rate reactions.}$$

where

c is the solute concentration, [ML^{-3}];

$\bar{c}$ is the sorbed concentration [MM^{-1}], a function of the dissolved concentration, *c*, as defined by a sorption isotherm

D_{ij} is the hydrodynamic dispersion coefficient tensor [L^2T^{-1}];

R_k is the rate of change in solute mass in reaction *k* of *N* different reactions; [$ML^{-3}T^{-1}$]

c' is the concentration of solute in source or sink fluid [ML^{-3}];

ρ_b is the bulk mass density of solid (mass of solid/volume of sediments) [ML^{-3}];

λ is the first order decay rate (equal to ln2/half life) [T^{-1}];

θ is the porosity, [dimensionless]; and

x_i, x_j are the Cartesian co-ordinates, [L].

3. PARTICLE TRACKING VERSUS ADVECTION-DISPERSION MODELS

General Contaminant transport simulation comprises simulating both the advective and the dispersive transport components. As seen from the general equation of solute transport that the dispersive part is a second order partial derivative function while the advective part is of first order. This creates numerical difficulties in solving this elliptical differential equation. Most numerical methods for solving the advection-dispersion equation can be classified as *Eulerian*, *Langrangian* or *mixed Eulerian Langrangian*. Eulerian methods solve the transport equation using a fixed spatial grid. The finite difference and finite element methods are primary examples of the Eulerian methods. Eulerian methods, which work well in solving the groundwater flow equation, were among the earliest methods applied to the transport equation, and they are still the more commonly used methods today. Eulerian methods are efficient and accurate in solving problems which are not advection-dominated, but they are susceptible to numerical dispersion and oscillation in solving advection-dominated problems. A sufficiently fine grid must be used to overcome these numerical difficulties.

Lagrangian methods use a deformed grid or a moving coordinate system with fixed grid in solving the transport equation. They provide an accurate and efficient solution to advection-dominated problems, but they have serious problems in dispersion-dominated problems. The lack of a fixed grid or fixed coordinate system may lead to numerical instability and computational difficulties, particularly in non-uniform media with multiple sources/sinks and complex boundary conditions [*Yeh*, 1990]. The random walk method [*e.g. Hockney and Eastwood*, 1981; *Ahlstrom et al.*, 1977; *Prickett et al.*, 1981] is a typical example of the Langrangian approach.

Mixed Eulerian-Langrangian methods solve the advection term of the transport equation with a Langrangian approach and the dispersion and the reaction terms with an Eulerian approach. The method of characteristics [*e.g. Konikow and Bredehoeft*, 1978; *Zheng*, 1993] is an example of the mixed Eulerian-Langrangian approach. Although the characteristics approach is successful in eliminating the numerical dispersion, and is simple in concept, the method is cumbersome to program and execute [*Pinder*, 1973], since it gives solutions at irregular points in space and time which may not be commensurate with points of interest.

Based on [Kenzelbach, 1987, Moltyaner et al., 1993 and Zheng and Bennet, 1995], the strength and limitations associated with various solution methods can be summarised as:

- Eulerian approach is to be preferred over other approaches when sufficient spatial discretization is feasible.
- Langrangian or mixed Eulerian-Langrangian methods may be preferred to Eulerian methods when the discretization requirement for the Eulerian methods are too stringent, or when the transport model is to be build on an existing flow model where it becomes difficult to change the grid spacing.
- When the grid is highly irregular, the accuracy of the Langrangian methods suffers.
- Langrangian methods encounters serious numerical difficulties when many stagnation zones are present in the flow domain.
- Langrangian methods can result in simulated concentration distributions that are highly irregular and sensitive to the number of particles used in the solution.

Considering the numerical difficulties and the incertainities associated with evaluating the dispersion coefficient involved in the dispersive term of the solute transport equation, it becomes convenient in many situation not to use a full solute transport model (advection-dispersion model), but rather an advective transport model would be sufficient to produce acceptable results. Particle tracking models are of this type. They are used to trace out flow paths or pathlines of infinitely small imaginary particles placed in the flow field. Particle tracking codes are post processors to flow models because they accept the head distribution from a flow model use it to obtain a velocity distribution which is used to trace out pathlines in space and time. Particle tracking analysis should be used routinely with flow modelling to detect conceptual errors that can not be identified solely by examining the head distribution [Anderson and Woessner, 1992].

4. APPLICATION TO SEIY'UN WELLFIELD CASE

The groundwater flow system in the Jethma wellfield area was simulated using the well-known USGS MODFLOW code [McDonald & Harbaugh, 1988] assuming steady state conditions. Particle tracking code USGS MODPATH [Pollock, 1998] was used to compute flow path lines and travel times. In most field situations, the advective transport term is much larger than the dispersive term. Hence purely advective simulation of contaminant transport using particle-tracking methods provides a good first estimate of solute movement. More over a full solute transport model requires data on dispersion, adsorption and chemical reactions parameters, which are difficult to measure and are seldom available for most groundwater aquifers. Furthermore, dispersion and chemical reaction in the subsurface are not yet fully understood. Particle-tracking models of advective transport offer an attractive alternative as the complicating effects and uncertainties associated with full solute transport models are minimized.

The present model grid has a nodal spacing of 30 m around the wellfield increasing to 100 m elsewhere as shown in Fig. 1.

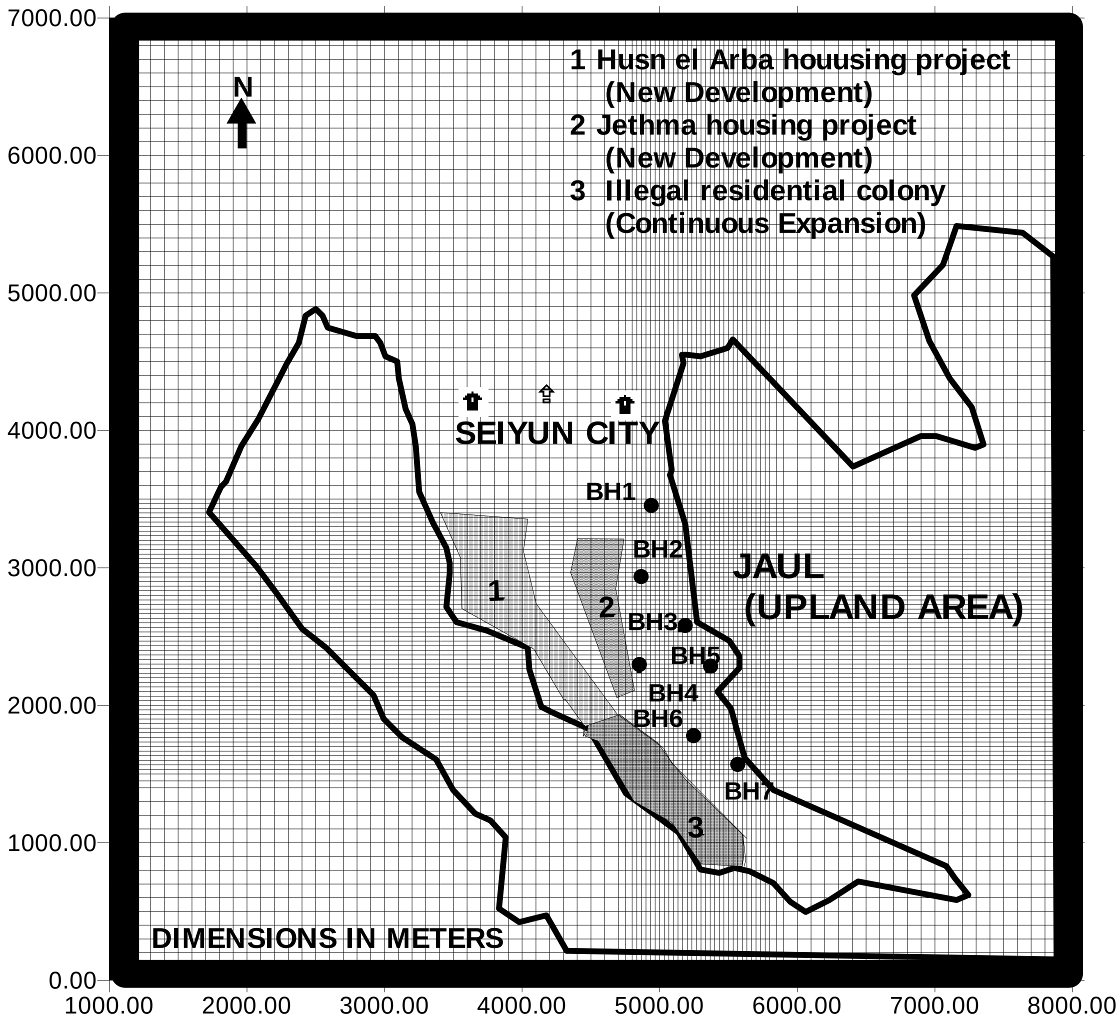

Fig. 1. Finite difference grid of simulated aquifer area

The model lateral boundaries were set sufficiently far away from the well field area to minimize their effect on the simulation result. The model boundaries were set from regional groundwater contour map of Wadi Hadhramaut prepared recently by the National Water Resources Authority [NWRA, 2002] based on water well survey and logs.

The developed model was intended to assess the potential contamination of the wellfield, by identifying the flow pattern in the wellfield aquifer and the capture zones of individual wellfield boreholes and estimating contaminant travel times from sources to boreholes.

The groundwater table contours obtained from the flow model for the aquifer area around the wellfield is shown in Fig. 2. The pattern of groundwater flow, as obtained from the particle-tracking model by setting particles around the perimeter of the model boundary and tracking their path lines forward in time, is shown in Fig. 3.

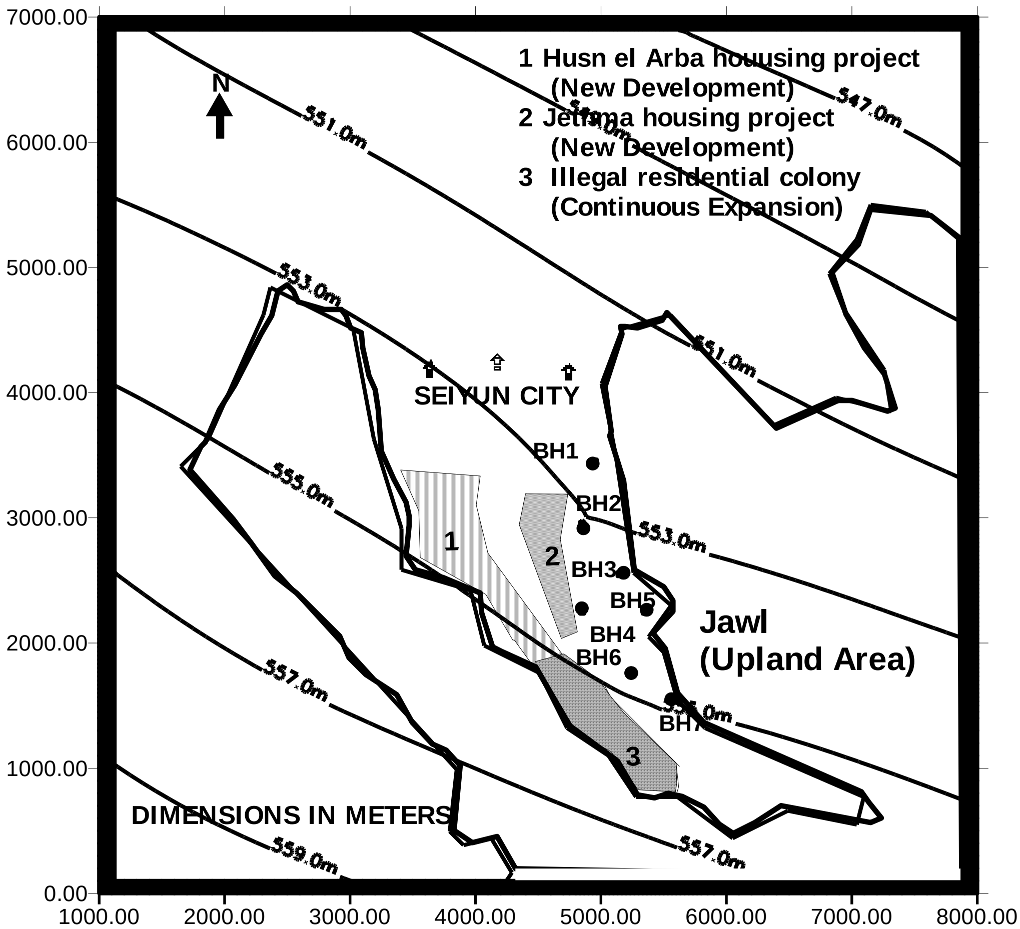

Fig. 2. Water table contours in the simulation area obtained from ground water flow model.

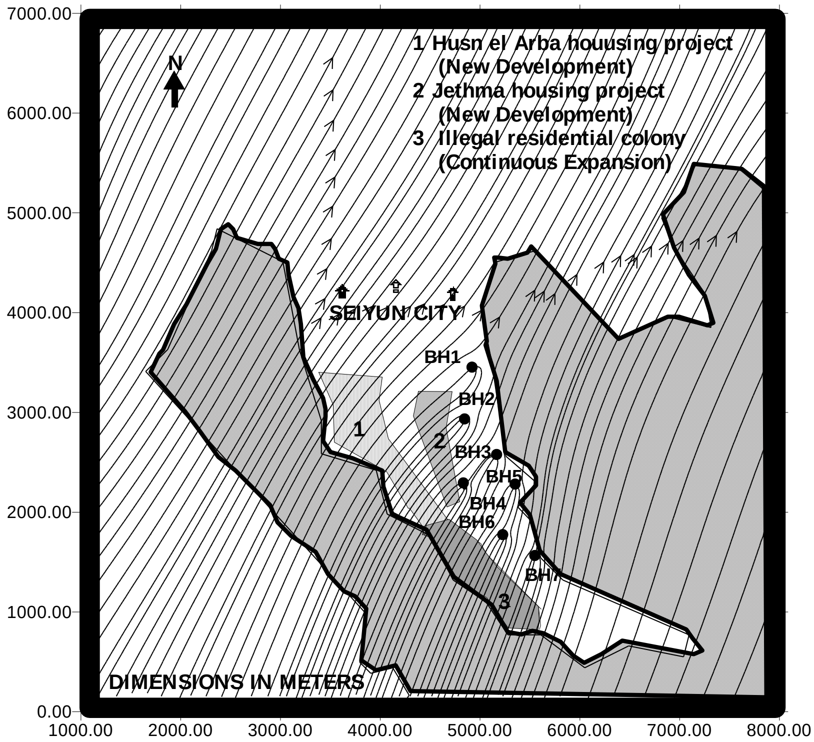

Fig. 3. Path lines as obtained by forward tracking of particles set along the perimeter of model area.

The capture zones for individual boreholes of the wellfield were delineated by setting particles at each borehole. Particles were then tracked backward in time. These capture zones are shown in Fig. 4.

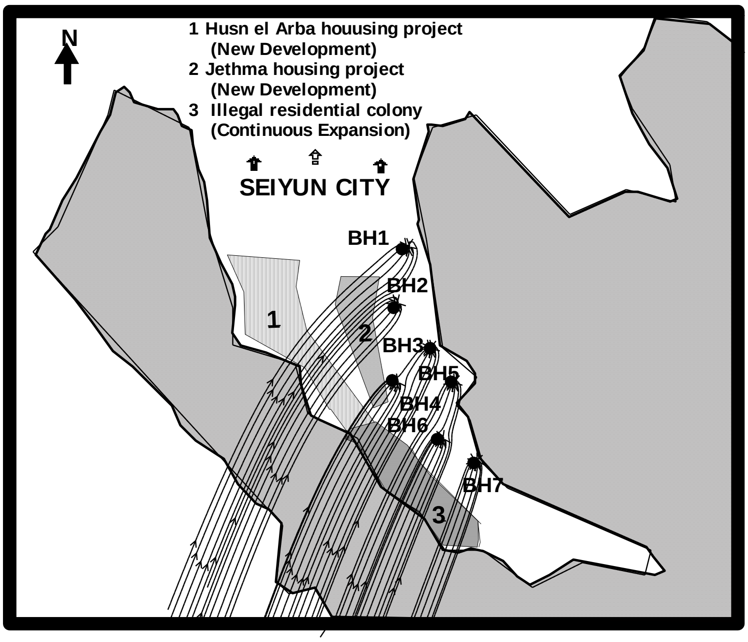

Fig. 4. Capture zones of wellfield boreholes delineated by backward particle tracking.

From Figs. 3 and 4 it is clear that fortunately only a small part of the city lies in on the aquifer area from which the flow is towards the wellfield. This part of the city forms the recent unplanned expansion that has to be addressed in order to protect the wellfield from potential pollution. The city zones that lie in the capture zones of the wellfield boreholes can be easily identified from the Fig. 5.

The contaminant fronts corresponding to certain travel times obtained by backward tracking particles located at the bore holes are presented in Fig. 5.

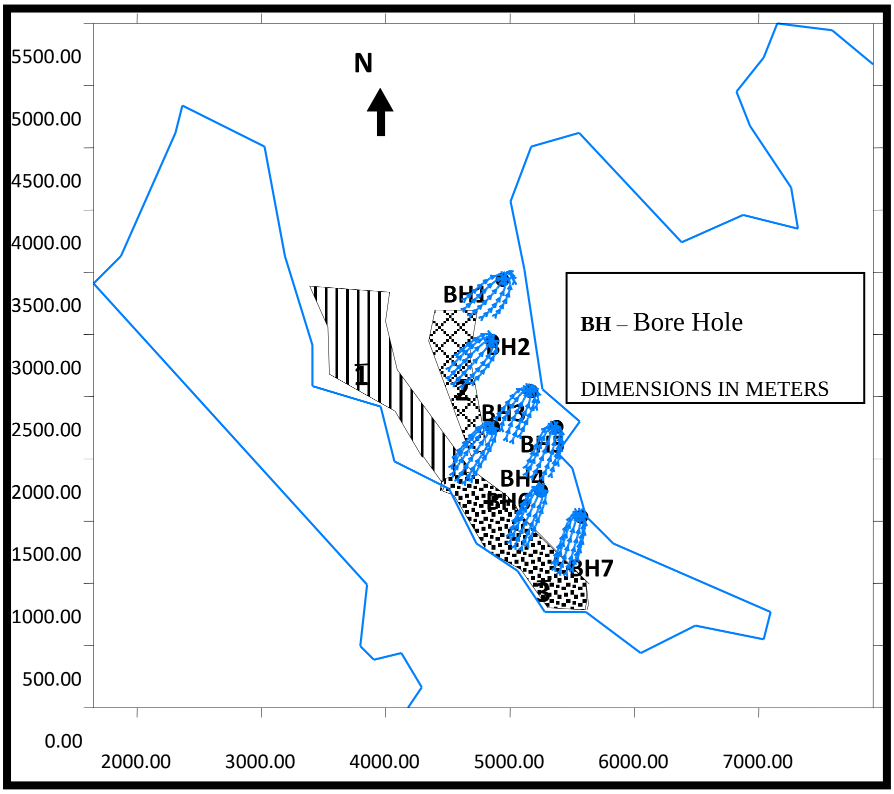

Fig. 5. Particles travel times to well field boreholes.
Time marks on the lines are at 100 days intervals.

It is evident from the Fig., that borehole 4 is the first well at which contaminants arrive. Next are boreholes 2 and 1. This is validated by the results obtained from the wellfield monitoring reports of NWSA, where early indications of bacteriological contamination were detected in boreholes 1, 2 and 4 in samples taken on May 1997. The model results indicated that it is only a matter of time before the contamination front will reach all the boreholes of the well field if the present sanitary situation in those areas remains unchanged. This is also validated by the NWSA monitoring reports 1998 that shows indications of bacteriological contaminations have been detected in the other four boreholes, i.e. boreholes 3, 5, 6 and 7 of the wellfield. This reports indicated unacceptable level of bacteriological contamination in borehole 4. While other boreholes show good results after chlorination, borehole 4 shows consistent unacceptable levels of typical coliform bacteria even after repeated borehole chlorination. This indicated that advective front of contamination from substantial source areas has reached the borehole and is advancing towards other wells.

The travel times to the various boreholes 1 through 7 are indicated in Fig. 5. The location of the advective front for certain travel times of some significance are useful in deciding about the extent of sanitized area for wellhead protection from various categories of contaminants. For example, it is believed that pathogenic bacteria have a life span of only 50 days in subsurface water. This means a *cordonne sanitaire* outside the 50-day front line ensures protection from pathogenic bacteria.

It should be born in mind that these times are only first estimates of the actual travel, as the advancement due to dispersion and the retardation due to adsorption or chemical reaction are not accounted for in advective transport modelling. But these travel times are very good estimates of the actual travel times. Multiplying these travel times by some safety factor ensures that no contaminant can travel across the sanitized zone set using these factored travel times, towards the boreholes in shorter time. The required safety factor can be assessed by the concerned water supply and sanitation authority or by the environmental protection councel based on the reliability of the data used and on the land use constrains as well as the unaccounted for dispersion effect.

4. CONCLUSIONS

The role of water quality models in investigating or evaluating various contaminated aquifer management and restoration policies has been stressed. The various numerical techniques employed by various water quality models were reviewed for their merits and shortcomings. The application of the water quality models in the assessment and management of contaminant transport in aquifer systems was demonstrated.

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