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Volume-based inverse model (VINMOD): innovative approach to quantify groundwater pollution in heterogeneous aquifers

Allelign Zeru and Gerhard Schäfer

ABSTRACT

The inversion method of pumped concentration can be used as an alternative or complementary method to the conventional methods for groundwater pollution evaluation and quantification. This method is useful even when the monitoring wells are few and also when the contamination source is unknown. In a homogeneous-isotropic case, with radially dominated groundwater flow field, this method of inversion can be performed analytically. However, in many cases, the real aquifer systems are heterogeneous. A novel volume-based inverse model (VINMOD) is developed for numerical inversion of pumped concentration under heterogeneous conditions. VINMOD helps us to determine the mean concentration and mass flow rate of an "undisturbed" contaminant plume at a predefined imaginary control plane (ICP). Model verification and preliminary tests are presented using a hypothetical single-layer aquifer. It is noticed that VINMOD is highly sensitive to the groundwater flow velocity and the well capture zone geometry, which in fact influences the determination of total mass flow rate of a pollutant in the groundwater.

Key words | control plane, groundwater pollution, heterogeneous, ICP, inversion, pumping test

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INTRODUCTION

Groundwater is the major source of water supply for domestic and industrial uses in many urban industrial areas. However, with ever-growing human activities such as industrialization and agriculture, groundwater reserves are threatened. Effluents from industrial areas as well as accidental spills and leaks are the main sources of groundwater contamination in many industrialized countries. For instance, among others, chlorinated solvents are toxic chemicals that are known to be the most common groundwater contaminants of industrial origin (Guillemin & Roux 1991; Beth & Cherry 1999). Exposure to these chemicals may cause serious health problems to humans and the natural environment (e.g. IARC 1995; Lee *et al.* 2002; Brown *et al.* 2003).

In the case when groundwater contamination is detected, it becomes essential to determine the extent, level and source of contamination. Conventionally, among many others, determination of the extent and level of contamination is undertaken by taking as many samples as possible from several points (Zhou 1996; Puls & Paul 1997). In general, this requires the installation of several observation wells. As a result, the cost of such operations can be very high, especially when high sampling resolution is required (Zeru 2004). Moreover, drilling of a large number of monitoring wells could also be constrained by geological and land-use factors. Other methods, such as forward mathematical models, require knowledge of source parameters. But in many cases, especially in complex industrial areas, the origin of the contamination is not known and determining it could require costly investigations.

Alternatively, groundwater pollution can be evaluated using concentration measurements during pumping tests through capturing and mathematically analyzing the pollution situation in the vicinity of the pumping well without requiring several monitoring wells. The recent approach for

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quantification of groundwater pollution is based on a concept involving the inversion of pumped concentration (Schwarz *et al.* 1998; Schwarz 2001). With this approach, the contaminated site can be screened out and hot spot zones can eventually be used to determine the extent and level of groundwater contamination by inverting the pumped concentration at the hot spot zone. The analytical solution provided by Schwarz (2001), which has been subsequently applied and reported (e.g. Holder *et al.* 1998; Schwarz *et al.* 1998; Bockelmann *et al.* 2001; Schäfer *et al.* 2001, 2004; Zeru & Schäfer 2002, 2003*a*,*b*,*c*, 2005; Alberti *et al.* 2003; Bockelmann *et al.* 2003; Zeru 2004), has been used for the inversion of pumped concentration under homogeneous, isotropic conditions with dominantly radial flow to the pumping well. However, in many cases, the real geo-hydrological systems are complex and, therefore, the aquifer media must be characterized by heterogeneous media. Depending on the local permeability values, the well capture zone geometry can vary from that of a circular capture zone (Franzetti & Guadagnini 1996; Riva *et al.* 1999). The total mass flow to be calculated from the inversion of pumped concentration in homogeneous and isotropic conditions can correspondingly differ from that of the heterogeneous formation (e.g. Elder 2002).

Several studies have been conducted and mathematical models have been developed for the use and applications of radial flow to a pumping well (e.g. Kaleris *et al.* 1995; Rayne *et al.* 2001; Fleming *et al.* 2002; Kamra *et al.* 2002; Peng *et al.* 2002; Rock & Kupfersberger 2002). But the applications of most of these studies have focused mainly on capture zone delineation for wellhead protection, aquifer parameter determination, groundwater pathline and travel time studies, point concentration profile studies, etc.

This paper presents the development of a volume-based inverse model (VINMOD), an innovative approach for groundwater pollution quantification through the inversion of pumped concentration. It takes into account the presence of local heterogeneity around the pumping well and the groundwater flow velocity profile at the ICP (Imaginary Control Plane). Although the method can be applied for multiple-well systems, we focused only on a single-well system here. The new inverse model is based on the relationships between the contaminant mass before and after pumping. VINMOD uses the flow velocity field obtained from the numerical groundwater flow code MODFLOW (McDonald & Harbaugh 1988). In addition, under heterogeneous conditions, VINMOD requires well capture zone information and streamlines to determine streamtube areas. A particle tracking code such as MODPATH (Pollock 1989, 1994) and PMPATH (Chiang & Kinzelbach 1998) can be used to get particle positions. The irregular streamtube areas are digitized and calculated using OS Digitizer (Zeru 2004). Verification of the mathematical model is made using a simplified homogeneous aquifer and the resulting inverted concentration is compared with that of the analytical solution (Schwarz *et al.* 1998). We further tested VINMOD for an irregular well capture zone by introducing local heterogeneities around the pumping well. The effect of local heterogeneity on the inverted concentration is demonstrated.

CONCEPT OF THE INVERSION OF PUMPED CONCENTRATION

In order to know the total mass flow rate of contaminated groundwater crossing a given section, we will be interested to know the concentration information along that section, i.e. the concentration distribution perpendicular to the mean flow direction of groundwater. At field conditions, we may require to have several monitoring wells along that section to know the concentration distribution. Alternatively, we employ a mathematical approach to determine the concentration distribution based on, among other parameters, the pumped concentration without using concentration data from several monitoring wells. In this case, contaminants that are intercepted during pumping of polluted groundwater and corresponding values that are recorded at some time intervals are referred as concentration–time series data. However, since the concentration–time series data are obtained from the radially intercepted groundwater, these values do not represent the concentration distribution of the undisturbed plume across a given section of a plume. The undisturbed concentration of a plume refers to the concentration distribution before pumping groundwater.

Thus, a mathematical approach that is used to get back the concentration distribution of the undisturbed plume based on the radially intercepted concentration is called Inversion of Pumped Concentration. The resulting concentration distribution at a predefined imaginary control plane (ICP), a plane which can arbitrarily be defined perpendicular to the mean flow direction of groundwater, is referred to as the inverted concentration distribution. Figure 1 shows a simplified schematic representation for pumping well positions and concentration–time series as well as inverted concentration curves for multiple pumping tests along an ICP. Each concentration value in the concentration–time series data represents the concentration between two isochrones corresponding to a given time interval.

The inverted concentration distribution is used to calculate the mean concentration and total mass flow rate of the contaminant plume. In addition, the concentration–time series curves from multiple pumping tests help to provide information on the most probable position of the plume with respect to the transversal direction at the ICP. For instance, the concentration–time series curve from the second well P2 shows elevated values compared to the other two wells, P1 and P3. Since the concentration–time series data from P3 is very small compared to P1, one can infer that the major part of the plume passes between pumping well P2 and pumping well P1.

For a radial flow towards the pumping well, Schwarz (2001) provided a recursive analytical solution for the inversion of pumped concentration under homogeneous conditions as

$$C_{\mathrm{inv}_j} = \frac{\pi C p_j - 2\sum_{k=1}^{j-1} C_{\mathrm{inv}_k}\left[\arccos\left(\frac{r(t_{k-1})}{r(t_j)}\right) - \arccos\left(\frac{r(t_k)}{r(t_j)}\right)\right]}{2\arccos\left(\frac{r(t_{j-1})}{r(t_j)}\right)} \tag{1}$$

where C_{inv} [ML^{-3}] is the inverted concentration along the transverse direction where the ICP is positioned, C_{p} [ML^{-3}] is the pumped concentration, r [L] is the radius of influence, t [T] is the pumping time in the concentration–time series and j is the streamtube index ($j = 1, 2, 3, \ldots, n$) which corresponds to a concentration–time series with n data points. A streamtube is defined as tubular surface formed by two adjacent streamlines along which the fluid flows. The radius of influence in a radially symmetric flow field is determined from

$$r_j = \sqrt{\frac{Qt_j}{\pi b \phi}} \tag{2}$$

where r[L] is the radius of influence, Q[L^{3}T^{-1}] is the pumping rate, t[T] is the time since the start of pumping, ϕ[$-$] is the porosity and b[L] is the thickness of the aquifer. Some of the main assumptions in the solution of Equation (1) include: (1) the flow towards the pumping well is radial and the aquifer is confined, homogeneous and isotropic with constant thickness (Figure 2), (2) the contaminant plume can be represented by piston type flow stripped with streamlines of the natural groundwater flow and (3) the concentration in a given streamtube is constant.

The following sections present the concept, development and numerical implementation of a mathematical model for the inversion of pumped concentration under heterogeneous conditions and when the natural flow is not neglected.

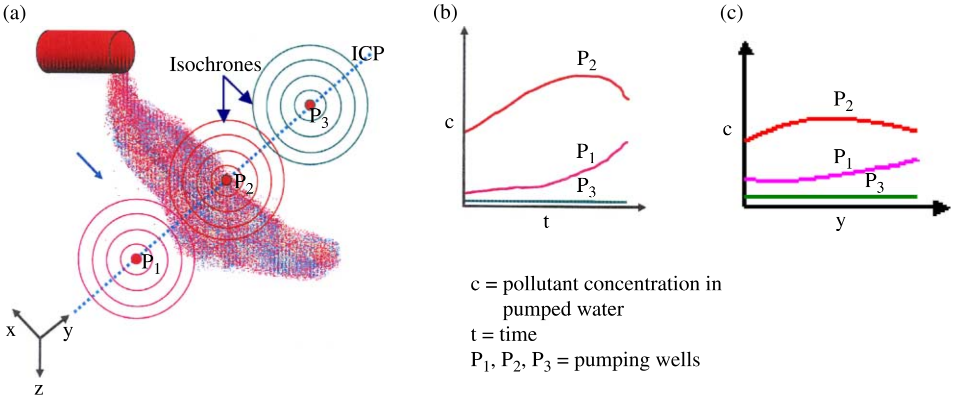

Figure 1 | Schematic representation of integral pumping test for the inversion of pumped concentration (after Bockelmann *et al.* 2001).

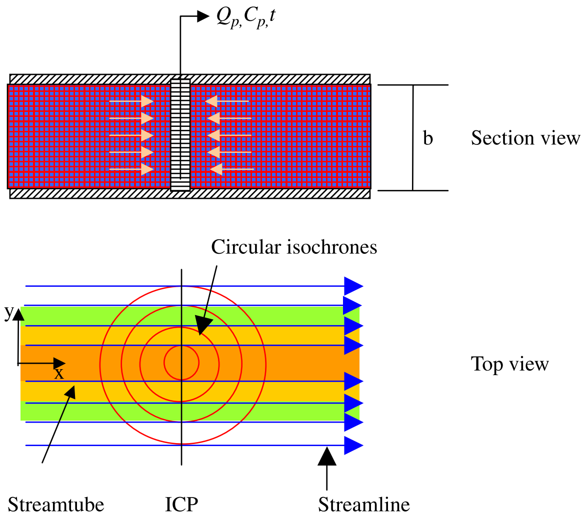

Figure 2 | Schematic representation of well capture zones from a hypothetical single-layered confined homogeneous aquifer with a fully penetrating screened well and a constant discharge Q_p.

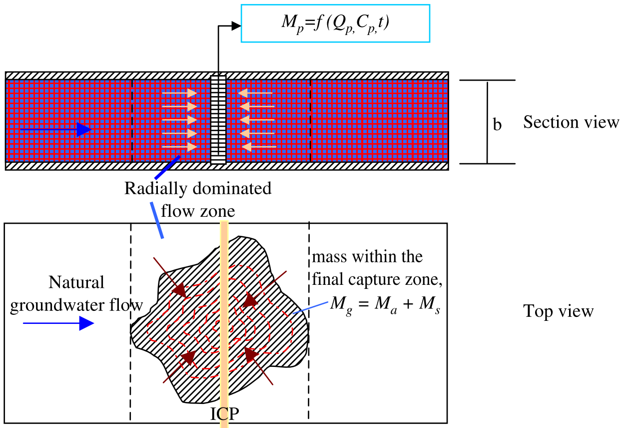

Figure 3 | Schematic representation of a well capture zone from a hypothetical single-layered confined heterogeneous aquifer with a fully screened pumping well and a constant discharge Q_p.

DEVELOPMENT OF INVERSION MODEL FOR HETEROGENEOUS MEDIA

Concept of VINMOD

Under homogeneous-isotropic aquifer conditions, the geometry of the well capture zone can be simplified and represented by a circular surface (e.g. Bennett *et al.* 1990) and, in steady-state flow conditions, the streamlines representing the natural groundwater can be schematically represented by straight lines. However, in the case of heterogeneous aquifer formations, depending on the local permeability values, the well capture zone geometry varies from that of a circular capture zone (Bair *et al.* 1990, 1991) and the water particles follow preferential paths having relatively higher permeability. As a result, the streamlines of groundwater flow in a heterogeneous aquifer can diverge or converge.

Thus, in order to implement the concept of the inversion of pumped concentration from a heterogeneous media, a single fully penetrating pumping well with a constant discharge Q_p of contaminated groundwater is considered (Figure 3). In this case, the contaminant mass M_p that can be calculated from the pumped water depends on the contaminant concentration C_p in the pumped water, the well discharge Q_p and the duration of the pumping period t. For a given pumping time interval, the pumped contaminant mass M_p corresponds to the contaminant mass in the groundwater M_g within the capture zone. The contaminant mass present in the groundwater, M_g, is assumed to be equal to the sum of the aqueous phase mass M_a and the sorbed mass M_s.

The pumped concentration, however, is attributed to the undisturbed contaminant plume partitioned with streamlines that form streamtubes of the natural groundwater flow. In order to determine the total contaminant mass flow rate at the ICP, the concentration distribution at the transversal axis of the undisturbed plume along the ICP has to be determined.

Mathematical model

In order to obtain the concentration distribution of the undisturbed plume by numerical inversion of pumped concentration, the following assumptions are made: (1) the contaminant plume is symmetrical relative to the longitudinal

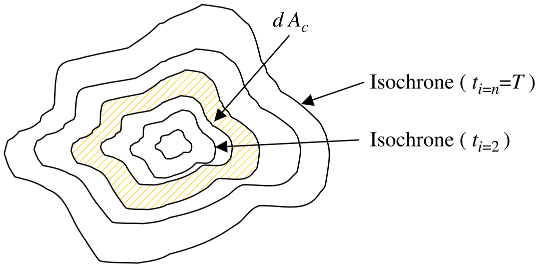

Figure 4 | Schematic representation of consecutive capture zones (dA_c = the area element of the capture zone increased during the time interval dt).

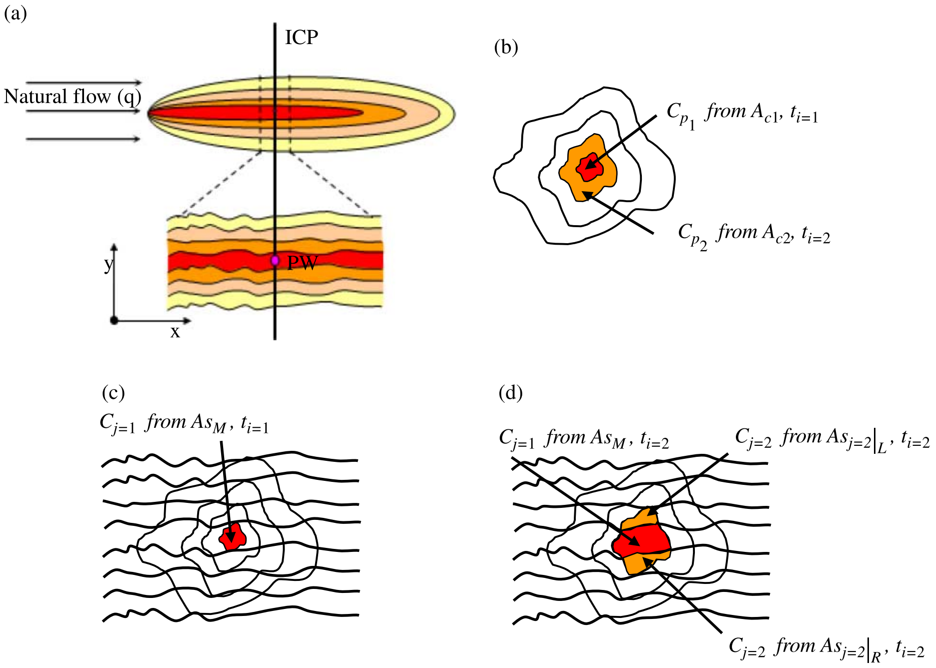

Figure 5 | Example of superimposition of the streamlines in a contaminant plume and the well capture zones. (a) Contaminant plume representation with streamlines that form streamtubes, (b) zonal concentration that can be obtained during pumping, (c) concentration in the middle streamtube area As_M by superimposing the first capture zone and the middle streamtube, (d) concentration in the middle (or first) and neighboring (or second) streamtubes areas, As_M, $As_{j=2}|_L$ and $As_{j=2}|_R$ by superimposing the second capture zone and the three streamtubes (left, right, and middle).

axis of the plume itself, in which the longitudinal axis of the plume is assumed to pass through the pumping well position, (2) the variation of layer thickness within the well capture zone is negligible and, therefore, a constant layer thickness can be considered, (3) neglecting sorbed mass, the well pumps only the dissolved contaminant mass in a given capture zone that corresponds to a given pumping time interval t, (4) the pumping well is screened throughout the layer thickness and the contaminant concentrations are mixed uniformly along the layer thickness, (5) the pumped concentration in a given time interval represents the mean concentration of the capture zone in that time interval and (6) the concentration within a given streamtube of a contaminant plume is assumed to be constant.

From the third assumption, the total contaminant mass in the groundwater is equal to the aqueous phase contaminant mass, the dissolved contaminant mass that is assumed to be equal to the pumped contaminant mass:

$$M_g = M_p \tag{3}$$

where M_p[M] is the pumped contaminant mass. The total contaminant mass in the groundwater in a given volume of the capture zone at the end of the pumping period can be expressed as

$$M_g = \phi \int_{V(T)} c(t) \mathrm{d}v \tag{4}$$

where $V(T)[\mathrm{L}^3]$ is the total volume of the saturated soil within a capture zone at the end of the pumping time T[T], $c(t)$ is the mean concentration for the isochrone corresponding to pumping time t and $\phi[-]$ is the porosity. For the total pumping period, with a constant layer thickness and a capture zone shown in Figure 4, Equation (4) can be rewritten as

$$M_g(T) = \phi b \int_{A_c(T)} c(t) \mathrm{d}A_c \tag{5}$$

where $\mathrm{d}A_c[\mathrm{L}^2]$ is the area element of the capture zone corresponding to the time interval $\mathrm{d}t$ and b[L] is a constant aquifer thickness. The areas As_j that are common to both the capture zones and the corresponding streamtubes can be obtained by superimposing the streamlines (Figure 5(a))

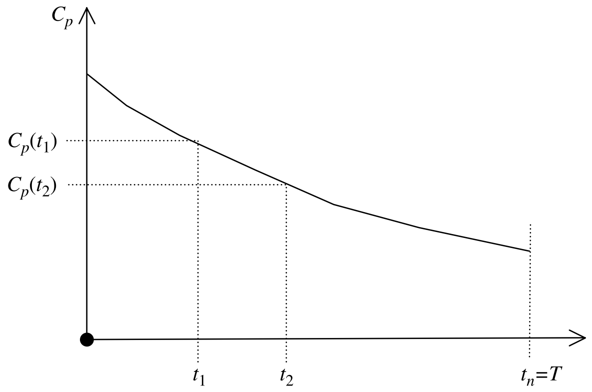

Figure 6 | Example of pumped concentration C_p as a function of the pumping time t.

and the well capture zones obtained during pumping (Figures 5(c–d)). The value of the concentration in a given streamtube C_j, after superimposition, is in fact attributed to the concentration of the undisturbed plume (Figure 5(a)).

For the first pumping time t_1, the concentration $C_{j=1}$ from the middle stream area $As_{j=1} = As_{\mathrm{M}}$ corresponds to the concentration of the first capture zone. The concentration in the immediate neighboring streamtubes relative to the middle streamtube, $C_{j=2}$, corresponds to the concentration of the left and the right streamtubes. Similarly, the concentration of any of the outer streamtube areas on the respective sides corresponds to the concentration of the respective streamtubes. For instance, taking the first two isochrones of the superimposed capture zones and streamtubes (Figure 5(d)), the sum of the contaminant mass at time t_2 can be expressed as

$$M_{\mathrm{g}}(t_{i=2}) = \phi b[C_{j=1}As_{j=1}|_{\mathrm{M}} + C_{j=2}As_{j=2}|_{\mathrm{L}} + C_{j=2}As_{j=2}|_{\mathrm{R}}] \qquad (6)$$

where $C_j[\mathrm{ML}^{-3}]$ is the concentration in a given streamtube, $As[\mathrm{L}^2]$ is the superimposed streamtube area within the capture zone under consideration, and M, L and R are indices for the middle, left and right streamtubes, respectively, relative to the pumping well position, assuming that the groundwater flow direction is in the x direction.

On the other hand, taking the volume of the pumped water for the defined pumping period with two isochrones (see Figure 5(b)), the pumped contaminant mass M_{p} is expressed as

$$M_{\mathrm{p}} = Q_{\mathrm{p}} \int_t c_{\mathrm{p}}(t)\mathrm{d}t \qquad (7)$$

where $Q_{\mathrm{p}}[\mathrm{L}^3\mathrm{T}^{-1}]$ is a constant pumping rate and $c_{\mathrm{p}}[\mathrm{ML}^{-3}]$ is the concentration in the pumped water at the pumping time t. Figure 6 shows an example for the pumped concentration as a function of time. It should be noted here that a pumped concentration at a given time in the concentration time series with n data points represents the average zonal concentration between two isochrones. Thus, for instance, $c_{\mathrm{p}}(t_1)$ corresponds to the first capture zone associated with the first time interval and $c_{\mathrm{p}}(t_2)$ corresponds to the zone between the first and the second capture zones, associated with the second time interval.

The contaminant mass in the groundwater, Equation (6), can be generalized as

$$\begin{aligned} &M_{\mathrm{g}}(t_{i=j}) = \phi b C_j As_{M}; t_{i=1} \\ &M_{\mathrm{g}}(t_{i=j}) = \phi b\left[C_j\left(As_j\big|_{\mathrm{L}} + As_j\big|_{\mathrm{R}}\right) + \sum_{k=1}^{j-1} C_k(As_k|_{\mathrm{L}} + As_k|_{\mathrm{R}})\right]; \; t_{i>1} \end{aligned} \qquad (8)$$

where $As_{\mathrm{M}}[\mathrm{L}^2]$ is the streamtube area that is equal to the well capture zone at the first pumping period. For a symmetrical plume, the concentrations for mirror image streamtubes relative to the pumping well position are equal. In this case, the concentrations in the left and right streamtubes are equal but also unknown. However, the value of the concentration in the middle streamtube is assumed to be equal to the pumped concentration recorded during the first time interval, i.e. corresponding to the first well capture zone. Since the pumped concentration is known, the concentration in the middle streamtube at the first pumping time is thus known. Rearranging the known and unknown terms, and from Equations (3), (7) and (8), the inverted concentration at the ICP can be defined and expressed as

$$\begin{aligned} &C_{inv_1} = \frac{Q_p C_{p_1} \triangle t_1}{b\phi As_{M}}; t_{i=1} \\ &C_{\mathrm{inv}_j} = \frac{Q_p \sum_{k=1}^{j} C_{p_k} \Delta t_k - b\phi \sum_{k=1}^{j-1} C_{\mathrm{inv}_k}(As_k|_{\mathrm{L}} + As_k|_{\mathrm{R}})}{(As_j\big|_{\mathrm{L}} + As_j\big|_{\mathrm{R}})b\phi}; \; t_{i>1} \end{aligned} \qquad (9)$$

where C_{inv_1} [ML^{-3}] is the inverted concentration at the first time $t_{i=1}$, C_{inv_j}[ML^{-3}] is the inverted concentration for the streamtube j at time $t_{i>1}$, j is the streamtube index ($j = 1, 2, \ldots, n$), i is the time index in the concentration–time series data ($i = 1, 2, \ldots, n$), and M, L and R are the indices for the middle, left and right streamtubes. Unlike the homogeneous aquifer configuration, the groundwater flow velocity profile at the ICP in a heterogeneous aquifer can vary from one streamtube to the other. Thus, the total mass flow rate passing through the ICP can be calculated from the sum of individual mass flow rates of each streamtube as

$$m_j = C_{\mathrm{inv}_j} q_j \tag{10}$$

where m_j[MT^{-1}] is the mass flow rate, C_{inv_j}[ML^{-3}] is the inverted concentration and q_j[L^{3}T^{-1}] is the flow rate in a given streamtube of contaminant plume.

Numerical implementation

Based on the equations provided in the previous section (see Equations (9) and (10)), a volume-based inverse model (VINMOD) is developed for the numerical inversion of pumped concentration at a predefined ICP. The total mass flow rate and the inverted concentration distribution that can be calculated with VINMOD represent the mass flow rate and the natural concentration distribution of the undisturbed contaminant plume. VINMOD requires principal input parameters such as concentration–time series data, groundwater flow velocity field, aquifer thickness, porosity of the aquifer material and areas of streamtubes. Figure 7 shows the flowchart of VINMOD.

The concentration–time series data can be obtained through simultaneous recording of the contaminant concentration in the pumped water as a function of the time during the pumping test. The velocity field is calculated using the groundwater flow model MODFLOW (McDonald & Harbaugh 1988). The ICP, where the inverted concentration distribution and the total mass flow rate are calculated, is defined perpendicular to the mean groundwater flow direction.

The well capture zones, for the eventual determination of streamtube areas, are determined from the velocity field of the transient flow period. The well capture zones are then delineated using the backward particle tracking method. A particle tracking code MODPATH (Pollock 1989, 1994) is used to calculate the mean pore velocity and provide particle positions backwards in time. Once well capture zones are delineated and streamlines are superimposed, the graphical tool OS Digitizer (Zeru 2004) is used for on-screen digitizing and calculating the streamtube areas within the irregular capture zone. The advanced on-screen digitizing tool EDigitizer (Zeru 2006*b*) can also be used in digitizing and calculating streamtube areas.

The graphical interface for VINMOD, software also called VINMOD for MS Windows (Zeru 2006 *a*), consists of

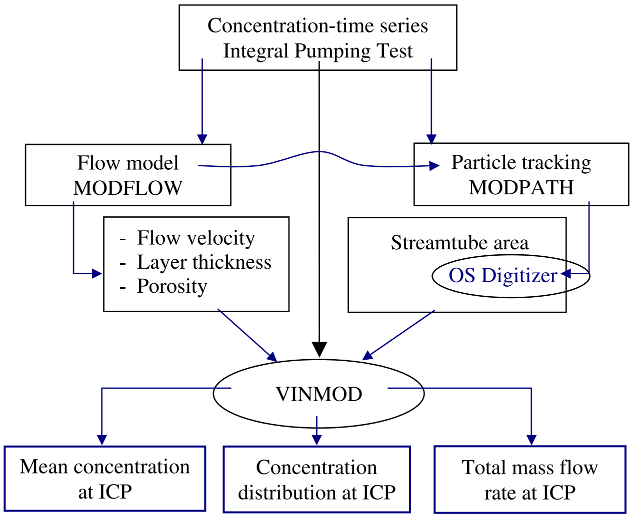

Figure 7 | Simplified flowchart of VINMOD.

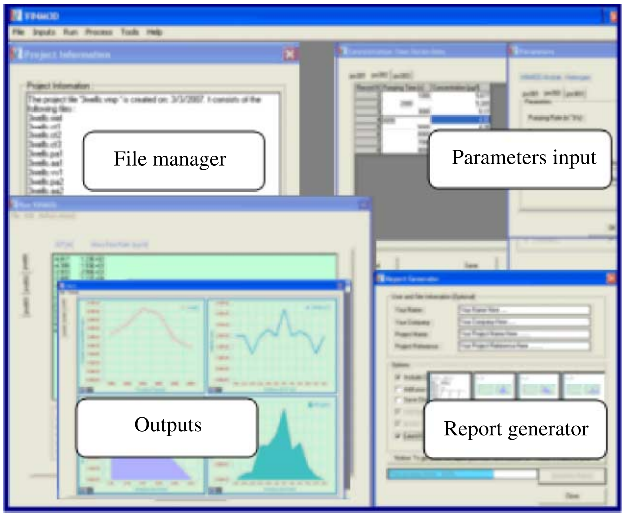

Figure 8 | A screenshot of the software VINMOD for MS Windows (Zeru 2006).

Table 1 | Main variables or parameters used in the numerical model

Variable or parameter	Value
Model area	500 m × 500 m
Grid size	5 m × 5 m (1 m × 1 m around the well)
Layer thickness	35 m
Hydraulic conductivity	0.001 m/s
Hydraulic gradient	0.002
Porosity	0.17
Hydraulic conductivity	$K = 0.001$ m/s
Longitudinal dispersivity	$\alpha_L = 10$ m
Dispersivity ratio (α_T/α_L)	0.1
Source concentration	12.5 μg/l
Source-to-pump distance	150 m
Pumping rate	250 m^3/h
Stress period I (T) (steady state period)	1095 d (3 yr)
Stress period II (transient period)	3 d

four main units: File Manager, Parameters Input, Simulator and Outputs unit, and Report Generator. It also has options for the aquifer type to be used in the simulation. Input data such as concentration–time series, flow velocity profile, streamtube areas and other input parameters, such as aquifer porosity and thickness, hydraulic gradient, etc., are read in ASCII format. The time intervals used for the concentration–times series data serve to determine the backtracked particle positions using a particle tracing code such as MODPATH (Pollock 1989) or PMPATH (Chiang & Kinzelbach 1998). Simulation outputs include inverted concentration distribution and corresponding mass flow rates at the ICP, mean concentration and total mass flow rate at the ICP. Graphical plots for concentration–time series, inverted concentration distribution, velocity profile and mass flow rate at the ICP can be viewed and exported in image (bitmap) format. All input information and simulation results, including the graphs and user remarks, can be generated in one PDF file using the Report Generator unit of the VINMOD software. Figure 8 shows a screenshot of the VINMOD software.

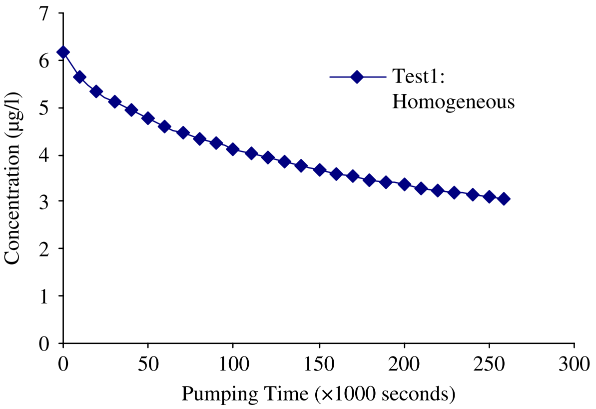

Figure 9 | Concentration–time series data from MT3D simulation output under homogeneous conditions.

MODEL VERIFICATION

Homogeneous aquifer scenario

VINMOD is first tested under homogeneous conditions by comparing the volume-based inverted concentration distribution with the analytically inverted concentration distribution. A stationary plume relative to the pumping well is used for the test. In this case, the concentration gradient in the plume is neglected. A known source with a fixed concentration of 12.5 μg/l was injected and positioned at about 150 m upstream of the ICP position. Both the steady state and transient flow regimes are considered. For the transient period, a single pumping well was set to pump contaminated groundwater at a rate of 250 m^3/h for three consecutive days. Thus, a single-layered numerical flow and transport model is set up with an ideal representation of a homogeneous-confined aquifer. The numerical codes MODFLOW (McDonald & Harbaugh 1988) and MT3D (Zheng 1990) are used for the flow and transport simulation, respectively. In addition, the particle tracking code PMPATH (Chiang & Kinzelbach 1998), which uses a semi-analytical particle tracking scheme of MODPATH (Pollock 1989), is used in delineating the well capture zones. The detail of the numerical model parameters are presented in Table 1.

The corresponding concentration–time series data observed from MT3D simulation output is in turn used in VINMOD and the analytical solution for the inversion of pumped concentration. The MT3D simulated concentration distribution at the same ICP, referred to here as the "real"

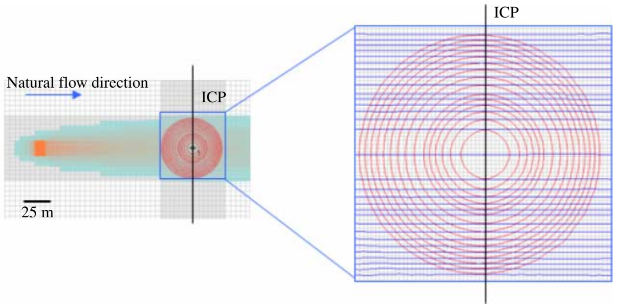

Figure 10 | Superimposition of well capture zones and streamlines of a contaminant plume under homogeneous conditions.

concentration distribution, is also used for further comparison. Figure 9 shows an example of the concentration–time series data obtained from the MT3D simulation. Figure 10 shows the superimposition of the well capture zone and the streamlines. The well capture zones and the streamlines of the natural groundwater flow are considered here as circular and straight lines, respectively.

Figure 11 shows the inverted concentration distribution using VINMOD compared with the concentration distributions from the analytical inversion and the "real" concentration distribution. It can be noticed that the trend of the inverted concentration distribution with VINMOD shows a similar trend as that of the analytically inverted concentration and the "real" concentration distribution from the MT3D simulation. The gap between the curves of the inverted concentration distribution and the "real" concentration distribution is due to the presence of dispersion during pumping (Zeru & Schäfer 2005). However, the general trend of the inverted concentration distribution with VINMOD indicates that the model works well and confirms its validity for the inversion of pumped concentration with a similar degree of certainty as the analytical inverse model for a radially dominated flow field.

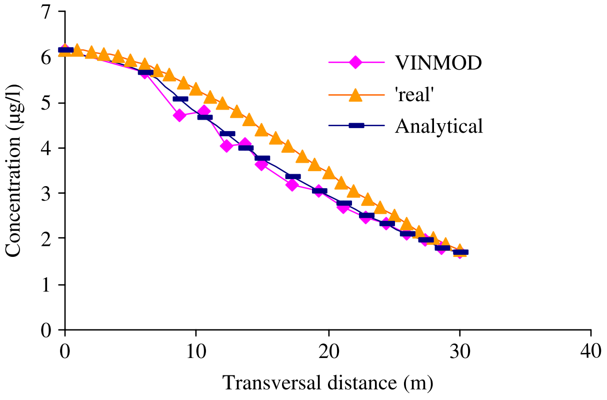

Figure 11 | Comparison of inverted and "real" concentration distributions.

Heterogeneous aquifer scenario

In order to test VINMOD under heterogeneous condition, the hydraulic conductivity around the pumping well is modified (Figure 12) while keeping all other parameters presented in Table 1. The resulting well capture zone is no longer circular and, after superimposition with the corresponding streamlines, the streamtube areas for the mirror image streamtube indices are not necessarily equal (Figure 13).

Figure 14 shows both the inverted concentration distribution obtained with VINMOD and the "real" concentration distribution. It can be noticed that the inverted concentration distribution shows some oscillation effect compared to the "real" concentration distribution (Figure 14(a)). Since the inversion of pumped concentration with VINMOD depends on the volume of the capture zone and the inversion method is recursive, any irregularities in the shape of the capture zone can cause oscillation of the inverted concentration distribution. However, the general trend of the inverted concentration distribution follows the trend of the "real" concentration distribution. In this case, taking the area under the two distribution curves, the values of the inverted concentration

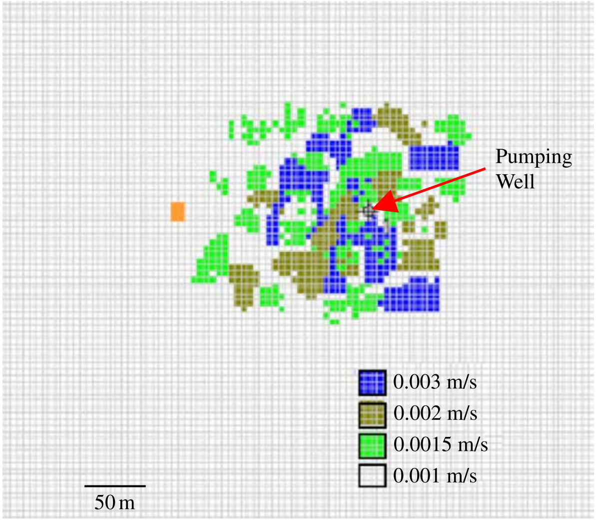

Figure 12 | Randomly assigned local heterogeneity with highly permeable zones in the vicinity of the pumping well.

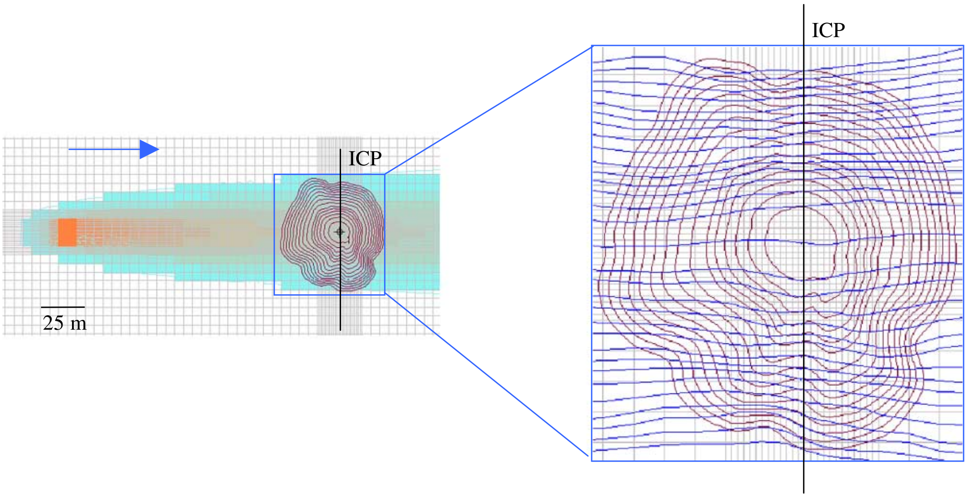

Figure 13 | Superimposed well capture zones and streamlines of a contaminant plume with randomly distributed hydraulic conductivity in the well capture zones.

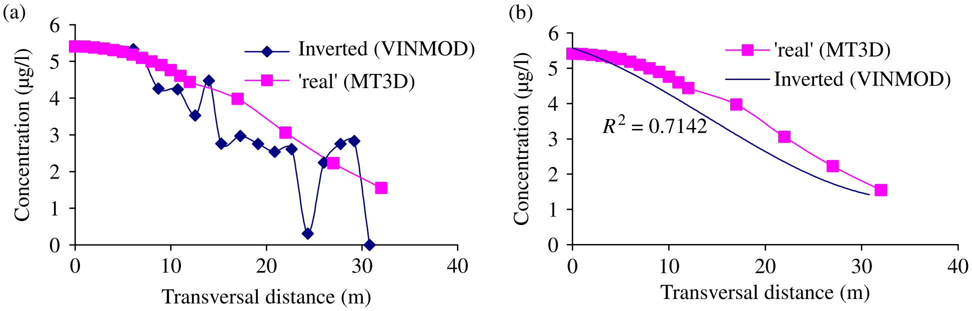

Figure 14 | Inverted concentration distribution compared with the "real" concentration distribution at the predefined ICP: (a) inverted concentration distribution, (b) trend-line of inverted concentration distribution.

distribution with VINMOD is less than that of the "real" concentration distributions by about 11%. Although this margin of error cannot be taken as conclusive, as results from a single simulation may not be adequate, the use of VINMOD under heterogeneous conditions can, however, provide reasonably acceptable results. It is noticed that analyzing the concentration–time series using a "homogeneous aquifer approach" leads to an underestimation of the concentration distribution by about 4% (Figure 15).

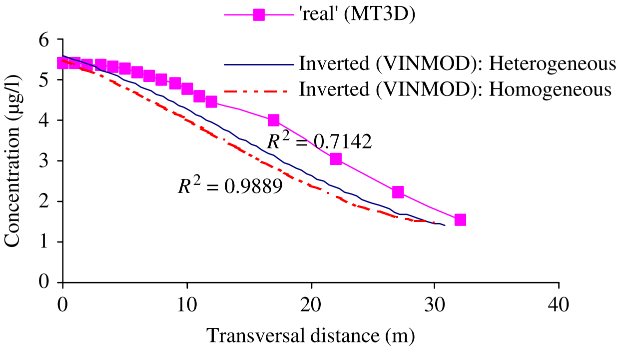

Figure 15 | Inverted concentration distributions under heterogeneous and simplified homogeneous cases compared with the "real" concentration distribution.

Thus, the change of both the groundwater flow velocity as well as the well capture zone, caused by the presence of local heterogeneity around the pumping well, can significantly alter the magnitude of the total mass flow rate at the ICP.

CONCLUSIONS

With a small number of monitoring wells, the inversion of pumped concentration can be used as an alternative, or supplementary, method to other conventional methods such as point measurements, interpolation and geophysical methods for determining the extent and level of groundwater pollution.

In the case of homogeneous-isotropic media, where radial flow is dominant and the effect of the natural flow is negligible, the method of inversion of pumped concentration can be performed analytically. However, in many cases, the real geohydrological systems are complex and, therefore, the aquifer must be considered as heterogeneous. In this case, the method of inversion of pumped concentration needs to be approached numerically. A volume-based inverse model (VINMOD) is developed and used for the numerical inversion of pumped concentration. VINMOD calculates the mean concentration, the concentration distribution and the corresponding mass flow rate of the "undisturbed" plume for groundwater pollution quantification, taking a predefined imaginary control section (ICP) as a reference.

It has been noticed that, in the given heterogeneous case, VINMOD is very sensitive to the groundwater flow velocity variations within the streamtubes. The groundwater velocity profile at the ICP can strongly influence the calculated total mass flow rate. In addition, the geometry of the well capture zone is also an important parameter for the inversion of pumped concentration. Thus, the presence of local heterogeneity can significantly affect the inverted concentration and corresponding mass flow rate while quantifying groundwater pollution with the method of the inversion of pumped concentration.

Because of its flexibility in handling irregular well capture zones, VINMOD can thus further be applied for both heterogeneous and homogeneous conditions where uniform groundwater flow is no longer negligible.

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