Multi-compartmental modelling for aquifer parameter estimation using natural tracers in non-steady flow

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A method is developed for aquifer parameter estimation incorporating dissolved hydrochemical constituents and environmental isotopes. This model is developed for basins with lack of hydrological information but with enough wells to allow for hydraulic head measurements and water sampling for chemical and isotoic analyses. It was developed for aquifer systems with observed hydraulic head fluctuations. The model is based on a distributed parameter approach in which the aquifer is represented by a finte number of cells. Inflows through external aquifer boundaries and internal fluxes are evaluated by optimizing a set of mass balance equations expressing the conservation of water, isotopes and dissolved chemicals. Storativity and transmissivity coefficients are then evaluated by the previously calculated flow components and the periodic changes in hydraulic heads. This paper presents a methodology to enhance the accuracy of estimated physical parameters in heterogeneous and anisotropic aquifers by adding chemical and isotopic information.

Key Words: Aquifer parameter estimation; compartmental modelling of non-steady flow; environmental tracers; isotopes; hydrochemistry.

INTRODUCTION

Aquifers in many basins have been heavily exploited for many years without complete information about the hydrological characteristics of the groundwater system. To properly manage groundwater resources, there is a need for accurate information about inflows (recharge), outflows (discharge) and physical characteristics of the aquifer. Usually the aquifer's physical parameters such as transmissivities and storativities are poorly known. Experience has shown that evaluating discharge (pumpage and natural outflows) is often technically easier than estimating recharge, transmissivities and storativities. Quantitative flow models aimed at estimating the hydraulic head potential usually suffer from lack of information about the spatial distribution of transmissivities and storativities. In fact, the largest uncertainty in calculating the water budget of a groundwater basin often stems from the hydrologist's inability to reliably estimate the distribution of physical parameters.

Numerical models in hydrology can be solved for flow components (magnitude and velocity) and for the aquifer's parameters (i.e. storativity and transmissivity) providing that the flow system is relatively simple and that the initial head and/or fluxes are known all over the flow domain as well as at the boundaries. The methods for aquifer parameter estimation, the so-called inverse method of groundwater hydrology, are introduced via various approaches into the flow equation as exemplified by recent works of Carrera and Neuman[1,2]. These methods, however, encounter difficulties, especially in heterogeneous and anisotropic aquifers, where the aquifer geometry and the hydrogeological systems are not well defined.

In many undeveloped or remote basins, however, where aquifer parameters are not available, water samples are relatively easy to obtain and can be analyzed for dissolved constituents and environmental isotopes.

In the past, hydrologists have used chemical and isotopic data primarily in a qualitative sense. Several attempts have been presented in evaluation of one or two flow components, namely recharge[3–7]. In recent years attempts have been carried out to extract quantitative information about various sources of inflows from hydrochemical and isotopic data. Lawrence and Upchurch[8] used statistical analysis on spatially distributed dissolved ions. Adar[9] and Adar *et al.*[10,11] used quadratic programming for least error estimation for a set of water, ions and isotopic mass balance expressions in a compartmental aquifer system. The latter is an attempt to solve the aquifer flow components, where the physical aquifer parameters are unknown. Gorelick *et al.*[12] used least squares and least absolute error multiple regressions combined with a numerical model of flow (required for transport) and transport of conservative and decaying substances. Wagner and Gorelick[13,14] demonstrate parameter estimation for transport and flow plus transport, respectively, in one- and two-dimensions with real data and realistic situations. Their approach is

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applicable 'to groundwater systems that are well defined ... and for which parameters regarding hydraulic behavior and solute transport have been determined', and not for aquifer parameter estimation.

In all the aforementioned papers, dissolved constituents and environmental isotopes were combined with a flow equation system in order to obtain a better estimation of groundwater inflows. This paper deals with the incorporation of dissolved chemicals and isotopes in a novel mathematical approach for the estimation of flow components and aquifer's physical parameters in a lumped system. This method can be used in aquifers in which periodic changes in hydraulic head are observed. In other words, it may suit a flow system which reflects seasonal variations influxes and/or pumpage enabling the hydraulic heads at the end of a specific season to return more or less to their original position.

THEORY

The model presented below relies basically on three types of conceptual models applied in hydrology (and in hydrodynamics): (a) evaluation of the motion of water and solutes with a multi-compartmental mixing cell model as suggested by Rasmussen[15] and Campana and Simpson[16]; (b) solution of a set of water and dissolved constituents mass balance equations via a quadratic programming optimization scheme exemplified by works carried out by Woolhiser *et al.*[17], Adar[9] and Adar *et al.*[10,11]; and (c) a mathematical model combining an inverse process to estimate compartmental conductances, storage coefficients, and for evaluation of the resulting pressure distribution in a multi-compartmental model for a non-steady flow as described by Sorek *et al.*[18,19,20]

The model is based on accounting for natural available tracers such as dissolved chemicals, stable isotope ratios and electrical conductivity measurements that are relatively easily obtained and measured in an aquifer and in potential recharge sources. It conceptualizes an aquifer that is discretized into finite cells such that the spatial distribution of tracers and heads are approximated by unique values for each tracer and head assuming a complete dilution within each cell (the mixing cell principle). The following assumptions are considered to be true in the aquifer:

1. Tracers are conservative; all reactions, dissolution and/or precipitation are negligible. The spatial change in the concentration of the solute is solely due to dilution. In principle, non-conservative tracers can be utilized as long as the rate of change due to subsurface water–mineral interaction or rate of decay functions are known.
2. Seasonal pulsations of fluxes for each cell can be represented by mean values spanning over a time interval in which the hydraulic head may be regarded as a constant value or as an average value of cyclic process in time. Pulsation of hydraulic heads throughout observation points in the aquifer may change in amplitude, yet their period phases remain alike.
3. Transport of dissolved constituents are dominated by advection process (i.e. compartmental Peclet number is infinite).

Further practical assumptions are embedded in the model: (a) concentrations of solutes, which are constant within each cell for specific time step, are measurable and known together with the concentrations of the same tracers in the inflow and outflow components; (b) all of the flows entering or leaving the aquifer system are known qualitatively, yet most of the source-sink and discharge flow components are known quantitatively, including the concentration of the dissolved constituents.

Being aware of the fact that in groundwater flow, solutes and isotope concentrations change in space and time, we discretize the aquifer into finite cells assuming that within each cell (for a specific time step) solutes and isotopes are fully mixed, yet their concentrations may differ from one cell to another. Thus, it is justified to measure for each cell a mean indicative set of solutes and/or isotopes. With respect to the second assumption one can identify each potential recharge source and represent a potential water source that can contribute to the system via the set of tracers.

With regard to the above ideas, we will now write a set of balance equations for the flux and solutes within a given time period Δt and for each cell (n) separately.

For a fluid with constant density, ρ, the mass balance for the (n)th compartment is expressed by the following equation.

$$Q_n - W_n + \sum_{i=1}^{In} q_{in} - \sum_{j=1}^{Jn} q_{nj} = S_n^* \frac{dh_n}{dt} \qquad (1a)$$

where In and Jn denote the number of sources and/or compartments from which flow enters the (n)th compartment, and leaves it, respectively; q_{in} and q_{nj} denote the fluxes from the (i)th source or compartment into the (n)th one, and from the (n)th one into the (j)th one, respectively; Q_n and W_n denote the fluid sources and sinks, respectively, in the (n)th compartment; S_n^* represents the storage capacity within cell n; and h_n denotes the hydraulic head associated with that compartment. Figure 1 illustrates the aforementioned flow parameters in a schematic compartmental system.

As the head (h_n) for each compartment varies, we may identify points in time, say t_1 and t_2 ($t_2 > t_1$), at which the hydraulic heads are the same (e.g. at the beginning and at the end of a specific season). This means that over that time interval $\tau = t_2 - t_1$ (regardless of the sequence of changes in heads during this time interval), the total

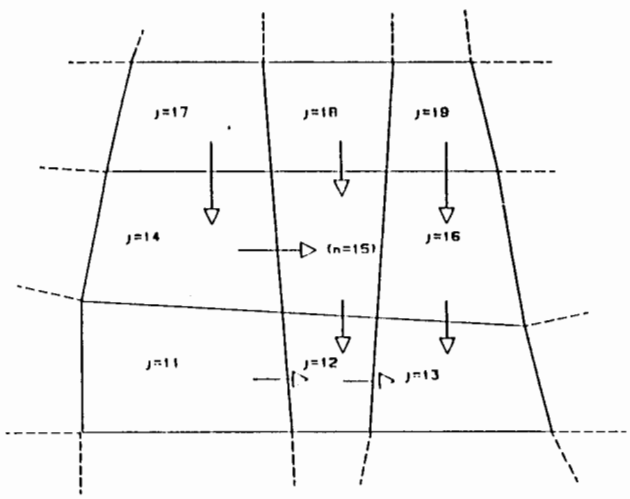

Fig. 1. Schematic flow configuration between cells designating flow (through permeable boundaries) with arrows

magnitude of the head derivatives (dh_n/dt) in each compartment has not changed. Hence, since $S_n^* \neq S_n^*(t)$, we obtain

$$\frac{1}{\tau}\int_{t_1}^{t_2} S_n^* \frac{dh_n}{dt}\,dt = 0; \qquad h_n|_{t_1} = h_n|_{t_2} \tag{1b}$$

Thus, by integrating equation (1a) over a time period $\tau = t_2 - t_1$ and dividing by τ, we obtain accordingly

$$\bar{Q}_n - \bar{W}_n + \sum_{i=1}^{In} \bar{q}_{in} - \sum_{j=1}^{Jn} \bar{q}_{nj} = 0 \tag{1c}$$

where $\bar{q}_{in}$ and $\bar{q}_{nj}$ denote the average values of q_{in} and q_{nj}, respectively, e.g.

$$\bar{q}_{in} = \frac{1}{\tau}\int_{t_1}^{t_2} q_{in}\,dt \tag{1d}$$

Likewise, the time averaged values of the source and sink fluxes in cell n are $\bar{Q}_n$ and $\bar{W}_n$, respectively. Note that equation (1c) expresses a quasi-steady state situation resulting from the time averaging process.

For quasi-steady state variations of concentrations, when mixing cell concept is applied, and in view of assumption 1 and equation (1c), we write a mass balance expression for a dissolved constituent k, in cell n.

$$\bar{C}_{nk}\bar{Q}_n - C_{nk}\left[\bar{W}_n + \sum_{j}^{Jn} \bar{q}_{nj}\right] + \sum_{i}^{In} \bar{q}_{in} C_{ink} = 0; \qquad k = 1, 2, \ldots, K \tag{2}$$

where C_{ink} is the average concentration of solute k entering cell n together with the flux coming from cell i; C_{nk} denotes average concentration of the (k)th constituent within cell n; and $\bar{C}_{nk}$ is the average concentration of k associated with source $\bar{Q}_n$. However, when constructing balance equations from field measurements, equations (1c) and (2) should account for various errors. Water balance (equation (1c)) may not hold because of an error in measurements of the identified fluxes. Mass balance of solutes (equation (2)) may be affected by analytical errors in measuring concentrations, especially in quantifying cell concentrations. To reflect the above mentioned inconsistencies, we introduce an error term into equation (1c) and (2) respectively.

$$\bar{Q}_n - \bar{W}_n + \sum_{i}^{In} \bar{q}_{in} - \sum_{j}^{Jn} \bar{q}_{nj} = e_n \tag{3}$$

$$\bar{C}_{nk}\bar{Q}_n - C_{nk}\left[\bar{W}_n + \sum_{j}^{Jn} \bar{q}_{nj}\right] + \sum_{i}^{In} \bar{q}_{in} C_{ink} = e_{nk} \tag{4}$$

where e_n and e_{nk} are the deviations from flux and solute balance in cell n, respectively. Upon combining equations (3) and (4) to a matrix form for each compartment, n, we obtain:

$$\underline{C}_n \underline{q}_n + \underline{D}_n = \underline{E}_n \tag{5}$$

where $\underline{C}_n$ is a matrix with known concentrations in cell n of the form

$$\underline{C}_n = \begin{bmatrix} 1 & 1 & \ldots & 1 & -1 & \ldots & -1 \\ C_{1n1} & C_{2n1} & \ldots & C_{I_n n1} & -C_{n1} & \ldots & -C_{n1} \\ C_{1n2} & C_{2n2} & \ldots & C_{I_n n2} & -C_{n2} & \ldots & -C_{n2} \\ \vdots & \vdots & & \vdots & \vdots & & \vdots \\ C_{1nK} & C_{2nK} & \ldots & C_{I_n nK} & -C_{nK} & \ldots & -C_{nK} \end{bmatrix}_{(K+1)*(I_n+J_n)} \tag{6a}$$

where the first row accounts for water balance, and the other K rows express solute mass balance where K is the total number of tracers used in the analysis. Negative sign denotes coefficients which are associated with outgoing fluxes. q_n is a vector of the unknown fluxes through the boundaries of cell n, described by

$$\underline{q}_n = [\bar{q}_{1n}, \bar{q}_{2n}, \ldots, \bar{q}_{I_n n}, \bar{q}_{n1}, \bar{q}_{n2}, \ldots, \bar{q}_{nJn}]_{(I_n+J_n)*1} \tag{6b}$$

$\underline{D}_n$ is a vector containing elements that are measured and known quantitatively in cell n (such as known fluxes of pumpage), described by

$$\underline{D}_n = [(\bar{Q}_n - \bar{W}_n), (\bar{C}_{n1}\bar{Q}_n - C_{n1}\bar{W}_n), (\bar{C}_{n2}\bar{Q}_n - C_{n2}\bar{W}_n), \ldots, \bar{C}_{nK}\bar{Q}_n - C_{nK}\bar{W}_n)]_{(K+1)*1} \tag{6c}$$

$\underline{E}$ is the error vector in cell n, described by

$$\underline{E} = [e_n, e_{n1}, e_{n2}, \ldots, e_{nK}]_{(K+1)*1} \tag{6d}$$

The total flux components in the aquifer can now be estimated by a minimization of the square error sums J. Similar to a procedure suggested by Woolhiser *et al.*[17], by virtue of equation (5) and by assembling the square error terms over all cells we obtain

$$J = \sum_{n=1}^{N} [\underline{E}_n^T \underline{\underline{W}} \underline{E}_n] = \sum_{n=1}^{N} (\underline{C}_n \underline{q}_n + \underline{D})^T \underline{\underline{W}} (\underline{C}_n \underline{q}_n + \underline{D}_n) \tag{7}$$

where $(\,)^T$ denotes transpose and $\underline{\underline{W}}$ represents a diagnonal matrix comprised of weighting values about estimated errors (independent of each other) expected for each of the terms building the mass balance for the fluid and the constituents. The weighting matrix, $\underline{\underline{W}}$, also reflects the degree of confidence to which the tracers are assumed conservative and the degree of accuracy of the chemical and isotope analyses. The solution of equation (7) for q_n is decomposed into linear and non-linear parts and J can be minimized to evaluate q_n by an algorithm developed, for example, by Wolf[21].

The solved time averaged fluxes are now used to estimate conductances to cell boundaries. The flux through a common permeable boundary, is proportional to the hydraulic head difference across this boundary. Integrating Darcy's linear momentum expression for any time interval over a control volume surrounding such a boundary for inflow from cell i into cell n, yields:

$$\bar{q}_{in} = T_{in}^*(\bar{h}_i - \bar{h}_n) \tag{8}$$

where T_{ij}^* ($= T_{ji}^*$) denotes conductance at the common boundary between cells i and j, and $\bar{h}$ denotes the time averaged measured hydraulic head. Similarly, the outflow from cell n to cell j, reads

$$\bar{q}_{nj} = T_{nj}^*(\bar{h}_n - \bar{h}_j) \tag{9}$$

Writing equations (8) and (9) for all permeable boundaries of the multicompartmental system, we obtain a global set of the form

$$q = \underline{\underline{h}}\,\underline{T}^* \tag{10}$$

where $\underline{\underline{h}}$ is a diagonal matrix given by

$$h_{\xi\eta} = \delta_{\xi\eta}(\bar{h}_i - \bar{h}_j); \qquad \xi, \eta = 1, 2, \ldots, N_b \tag{11a}$$

Here, N_b denotes the number of permeable boundaries in the aquifer cell system. $\delta_{\xi\eta}$ is the Kronecker delta, where $\xi = \eta$ for permeable (active) boundary. $(\bar{h}_i - \bar{h}_j)$ represents the averaged head difference governing outflow from cell i into cell j. The vector of conductances, $\underline{T}^*$, is given by

$$\underline{T}^* = [T_1^*, T_2^*, \ldots, T_{Nb}^*]_{Nb*1} \tag{11b}$$

and q denotes the vector of solved (see equation (7)) averaged fluxes across permeable boundaries, given by

$$q=[\bar{q}_1,\bar{q}_2,\ldots,\bar{q}_N,]_{N,*1} \tag{11c}$$

Hence, conductances in the aquifer cell system T^*, are solved using the set of equations as described in equation (10).

In compartmental simulation of an aquifer, conductance coefficient (T^*) replaces transmissivity term (T) used in a continuum approach. In view of equation (8), e.g. for inflow boundaries, we may write the relation between T^* and T in the following form:

$$\bar{q}_{in}=T^*_{in}(\bar{h}_i-\bar{h}_n)=T_{in}\frac{l_{in}}{b_{in}}\frac{\bar{h}_i-\bar{h}_n}{} \tag{12}$$

where T_{in} denotes the transmissivity between observation wells i and n at the boundary in between the same cells respectively, l_{in} denotes the length of the (in) boundary between those cells and b_{in} represents the distance between observation wells i and n, normal to the boundary (in) as depicted in Fig. 2.

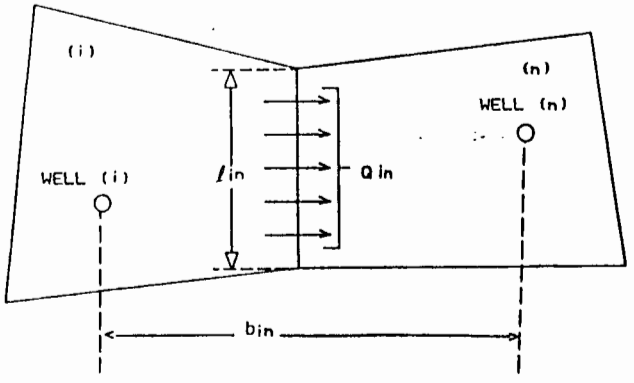

Fig. 2. Scheme of flow between two compartments (i) *and* (n) *and description of dimensions* l *and* b

Thus far, fluxes and conductances were evaluated based on time average compartmental heads and concentrations obtained for time interval τ. Estimated transmissivities for every active boundary can then be calculated by equation (12).

For evaluating compartmental storage coefficients, one may use the information about temporary head variations in the flow domain during (or within) the time period τ. Suppose one assigns M specific observations for compartmental head $h_n^{(m)}$ during time period τ; $(m=1,2,\ldots,M)$ where $h_n^{(m)}$ denotes the head in cell n at time m as illustrated in Fig. 3.

In view of equations (8) and (9), and since conductances were already solved, we write the temporal values of boundary inflow/outflow ($q_{in}^{(m)}$ and $q_{nj}^{(m)}$, respectively) fluxes for each observation time m in the following manner:

$$q_{in}^{(m)}=T^*_{in}(h_i^{(m)}-h_n^{(m)}) \tag{13a}$$

$$q_{nj}^{(m)}=T^*_{nj}(h_n^{(m)}-h_j^{(m)}) \tag{13b}$$

Substituting equation (13) into equation (1a) and assembling for all N aquifer compartments, we obtain a global set of linear ordinary equations at observation time (m) of the form

$$\underline{S}^*\frac{d\underline{h}^{(m)}}{dt}+\underline{T}^*\underline{h}^{(m)}=\underline{R}^{(m)} \tag{14}$$

where $\underline{S}^*$ denotes a diagonal matrix of compartmental storage capacity coefficients; $\underline{T}^*$ denotes the matrix of conductances in which the two terms T_{in}^* and T_{nj}^* are associated with permeable boundaries (inflow and outflow, respectively, and no-flow boundary is expressed by zero term); $\underline{h}^{(m)}$ is a vector of compartmental head terms measured at time observation m; and $R^{(m)}=(Q^{(m)}-W^{(m)})$ is a vector of the known compartmental source and sink flux terms.

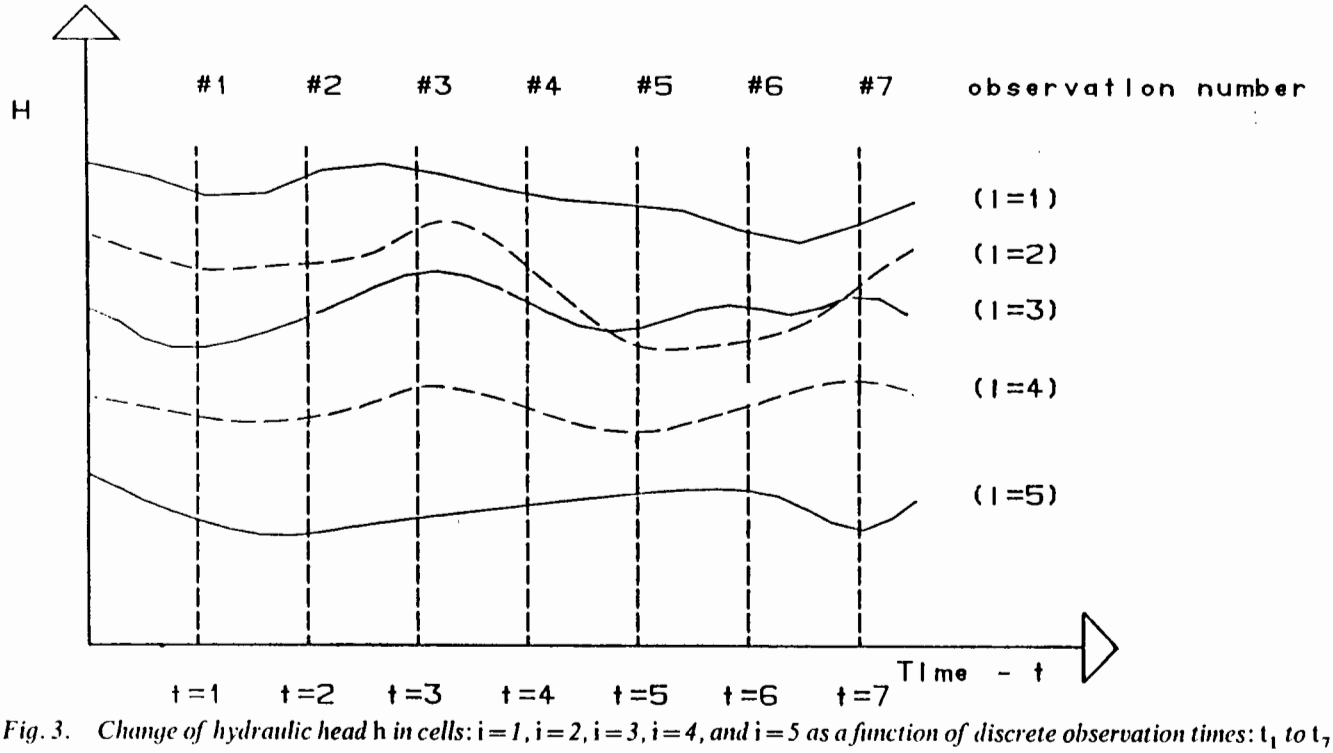

Fig. 3. Change of hydraulic head h *in cells*: i = 1, i = 2, i = 3, i = 4, *and* i = 5 *as a function of discrete observation times*: t_1 *to* t_7

Our goal is to solve the S_n^* storage capacities, for each compartment in the aquifer, given that $h_n^{(m)}$, $R_n^{(m)}$ and T_{in}^* (or T_{nj}^*) values are known. To do that we rewrite equation (14) to the form

$$\underline{\underline{x}}^{(m)}\underline{S}^* = \underline{y}^{(m)} \tag{15}$$

where $\underline{\underline{x}}^{(m)}$ is a diagonal matrix of known head rates for all aquifer compartments at observation (m)

$$x_{ij}^{(m)} = \delta_{ij}\frac{\mathrm{d}h_i^{(m)}}{\mathrm{d}t} \qquad i,j = 1, 2, \ldots, N \tag{16}$$

$\underline{y}^{(m)}$ is a vector of known terms at observation time (m),

$$\underline{y}^{(m)} = [R^{(m)} - \underline{\underline{T}}^* h^{(m)}]_{N*1} \tag{16b}$$

and S^* is the vector of storage capacities for all compartments at observation (m).

$$\underline{S}^* = [S_1^*, S_2^*, \ldots, S_N^*]_{N*1} \tag{16c}$$

Next, upon implementing the Gauss–Markov (in Bard[22]) method in equation (15) through all M time observations, we obtain an optimal solution for $\underline{S}^*$, of the form

$$S^* = [\underline{X}^T\underline{X}]^{-1}\underline{X}^T\underline{Y} \tag{17}$$

where

$$\underline{X} = \begin{bmatrix} \underline{\underline{x}}^{(1)} \\ \underline{\underline{x}}^{(2)} \\ \underline{\underline{x}}^{(M)} \end{bmatrix}_{(N*M)*N} \tag{18a}$$

$$\underline{Y} = [[R^{(1)} - \underline{\underline{T}}^* h^{(1)}], [R^{(2)} - \underline{\underline{T}}^* h^{(2)}], \ldots, [R^{(M)} - \underline{\underline{T}}^* h^{(M)}]]_{(N*M)*1} \tag{18b}$$

Since $x^{(m)}$ is a diagonalized matrix, we can write an explicit expression for S_n^* commencing from equation (17).

$$S_n^* = \frac{\sum_{m=1}^{M} \frac{\mathrm{d}h_n^{(m)}}{\mathrm{d}t}\left[R_n^{(m)} - \sum_{\eta=1}^{N} T_{n\eta}^* h_\eta^{(m)}\right]}{\sum_{m=1}^{M}\left[\frac{\mathrm{d}h_n^{(m)}}{\mathrm{d}t}\right]^2} \tag{19}$$

where $\eta = 1, 2, \ldots, N$ denotes numbers of active boundaries.

The $h_n^{(m)}$ and $\mathrm{d}h_n^{(m)}/\mathrm{d}t$ values are at discrete time observations ($m = 1, 2, \ldots, M$) for each cell n. Figure 3 illustrates a typical log of hydraulic heads versus time for several aquifer cells.

Compartmental storage capcity S_n^* is related to the storativity S_{sn} and to the specific yield S_{yn} for confined and water table aquifers, respectively, by the following expressions

$$S_n^* = \phi_n V_n S_{sn} \tag{20a}$$

$$S_n^* = A_n S_{yn} \tag{20b}$$

where A_n is the area of cell n, V_n is its saturated volume, and ϕ_n is the porosity.

DISCUSSION

A novel methodology for estimating aquifer parameters is presented. The methodology is based on a multi-compartmental model incorporating measured concentrations of dissolved conservative constituents and hydraulic heads at discrete time observations.

The proposed method estimates aquifer parameters for non-steady flow regimes, such that through a seasonal time period the same head values are identified. Time averaging over such a time interval yields a quasi-steady flow equation and mass balance expressions for each of the sampled natural tracers.

First, inflows through external aquifer boundaries and fluxes crossing the common boundaries of the compartments are evaluated. The number of unknown fluxes is equal to the number of permeable boundaries of the compartments simulating the aquifer. The number of balance equations for water, isotopes and some of the dissolved chemicals (ions) must always exceed that of the unknown fluxes. The solution for the fluxes is expected to enhance accuracy being based on an optimization scheme of mass balance expressions to a variety of natural tracers.

Next, transmissivity and storativity coefficients are evaluated based on previously calculated fluxes and the variations in time of the measured hydraulic head. Transmissivities are estimated by using the time averaged fluxes calculated previously. Storativities are estimated on the basis of the evaluated transmissivities and an optimization procedure accounting for the temporal measured hydraulic head data.

Physical dispersion is not included explicitly in the mass balance equations. However, it is accounted for, implicitly, by varying the cell size and configuration. The maximum number of cells can not exceed the number of observation wells. Hence, the spatial distribution of observation wells influences the extent to which steep gradients of concentration and physical dispersion, in general, can be detected and accounted for in the model. This spatial distribution also effects the numerical error associated with the final solution, as in other existing inverse schemes. However, the developed method is advantageous in incorporating measured concentrations of natural tracers which is believed to improve the estimation of flow parameters especially in heterogeneous and anisotropic aquifers.

The proposed method enables the determination flows across external and internal boundaries alike. In addition, multi-compartmental modelling, inherently suits the mathematical description of a 3-D configuration by a relatively simple formulation.

The developed model is especially attractive for basins with a lack of hydrological information but with enough wells to allow temporal hydraulic head measurements and water sampling for natural tracer analyses. This type of information is relatively easy to obtain and inexpensive in comparison to pumping tests performance.

This paper is devoted to presenting a novel method for aquifer parameter estimation with input of additional, non-conventional, measured data. It presents a methodology whereby easy, accessible water sampling analyses may be incorporated in a rigorous formulation, which in itself is worthwhile presenting. The stage of numerical implementation will be recorded in the near future.

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