

Groundwater Modeling and Its Role in Aquifer Storage Management

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Groundwater Flow Modeling

Groundwater flow modeling implies performing numerical experiments on a groundwater flow model. The objective of such an experimentation for practicing engineers, is usually to check the feasibility of any human intervention into the groundwater system, e.g., pumpage, recharge etc. For groundwater academics, the objective could be to understand various processes involved in the groundwater system.

Groundwater Flow Model

A groundwater flow model is essentially a tool to project the State variables of the groundwater system for an assigned pattern of forcing function, and known initial and boundary conditions and parameters.

A brief description of various terms appearing in this definition is included in the following paragraphs.

State Variables

The state variables are essentially the variables that describe the “state” of a system. These variables may be divided in two categories viz. Mandatory and Problem-specific. The mandatory state variable is: Piezometric head or Water table elevation. This variable is henceforth termed as “head”. The Problem specific state variables are essentially derived from the head distribution in space and time. These could include, depending upon the problem at hand, depth to water table, static storage, influent/effluent seepage, outflow to sea, sea water intrusion etc.

Forcing Function

The forcing function may comprise among others the following constituents:

- Withdrawals (i.e., pumpage)
- Recharge (derived from- rainfall, applied irrigation, seepage from surface water bodies etc.)
- Evapotranspiration from the saturated zone

Initial and Boundary Conditions

Initial conditions: Initial conditions, as the name implies comprise of the spatial distribution of the head at the instance when the assigned excitation commences to act. There are two possible interpretations of the Initial conditions. Mathematically, they are necessary for arriving at a unique solution of a differential equation. Conceptually, they can be visualized as the

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influence of the hydraulic conditions occurring prior to the activation of the assigned forcing function.

Boundary conditions: Here too there are two possible interpretations. Mathematically, they are necessary for arriving at a unique solution of a differential equation. Conceptually, they can be visualized as the influence of the hydraulic conditions occurring across the boundary of the domain, of the solution. Thus, to obtain a unique solution of the differential equation, it is necessary to define boundary conditions all along domain boundary. The boundary condition may either be a known head (head assigned) or a known flow rate (flow assigned) across the boundary. It can be thus concluded that for obtaining a unique solution it is necessary to know either the head or normal flows all along the boundary.

Boundary heads are assigned wherever an aquifer is terminating into a water body. At the interface between the two, the head may be assumed to be equal to the water elevation in the water body.

Normal flows need to be known for the part (s) of the domain boundary not interfacing with water bodies. These flows are more difficult to estimate (unless they are known to be zero i.e., an impervious boundary) and would usually require water balance of the adjoining areas.

Out of the two types of boundary conditions, the head assigned boundaries are more suitable for forecasting since the water elevations in the hydraulically connected water bodies may generally not be significantly influenced by the pumping/recharge pattern in the aquifer. Thus, the known prevalent water elevations may be assumed to hold good under the projected conditions (i.e., the pumping/recharge rates different from the prevalent ones). On the other hand, the lateral inflows across the boundary are very sensitive to any change in pumping/recharge. Thus, the inflow rates under the projected conditions may vary significantly from the prevailing ones. In other words the known prevalent inflow rates may not provide the necessary boundary conditions.

Model Parameters

The spatial distribution of the appropriate (that is, depending upon the type of aquifer) aquifer parameters need to be assigned for computing the head distributions corresponding to the assigned forcing function. The data from pumping tests shall rarely be adequate to meet this input requirement. The spatial distribution is usually obtained from a solution of *Inverse problem*. The solution requires the historical data of forcing function, heads, initial and boundary conditions. It aims at evolving such distribution of the aquifer parameters, which lead to a closest match between the observed, and the model-computed heads. Typically this requires repeated *direct* modeling corresponding to a selected historical period, with varying values of aquifer parameters, and finally arriving at the *best possible* match.

Components of a GW Flow Model

Typically a groundwater flow model comprises of the following components:

1. An equation (algebraic or differential) governing the flow

2. An algorithm to solve the chosen equation numerically to compute the time and space distribution of the head
3. A set of algorithms to compute the problem- specific state variables from the pre- computed head distributions
4. Computer codes to implement the selected algorithms

A brief description of these components is incorporated in the following paragraphs.

Governing Equations

Any equation governing the groundwater flow is essentially an expression of the continuity equation which, in the context of groundwater flow, can be heuristically stated as follows:

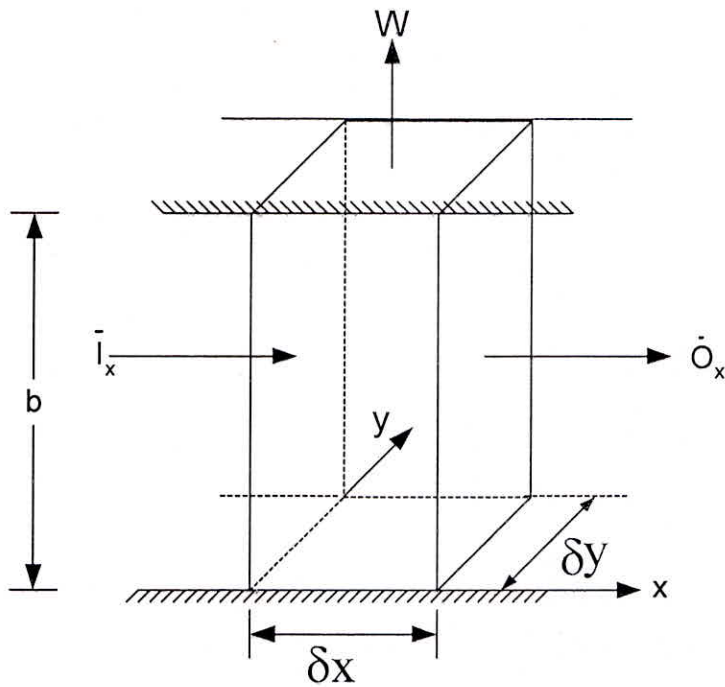
Across any selected domain of saturated flow, the difference between the inflow and the outflow rates equals the rate of change of the storage of water in that domain.

The selected domain is usually an infinitesimally small element. Thus, in case of a general three dimensional flow it is an infinitesimally small volume. However, if the flow occurs predominantly in two orthogonal directions with very little or no flow in the third orthogonal direction (e.g., two- dimensional horizontal flow), the domain could be infinitesimally small area with a unit/ physical dimension in the no- flow direction. Further, if the flow occurs predominantly only in one direction, the domain is an infinitesimally small length with unit/ physical dimensions in other two no- flow directions.

Two types of inflows/ outflows are considered while writing the continuity equation for groundwater flow. First type comprises the ones occurring on account of the prevalent hydraulic gradients. The second type comprises *external* inflow or outflow (also termed as Source or Sink terms), i.e., driven by the forcing function. The gradient driven inflow and the outflow rates are expressed in terms of the space derivatives of the head (viz., piezometric head/ water table elevation) and a flow parameter (Hydraulic conductivity in general or Transmissivity in case of one/ two- dimensional horizontal flow) by invoking Darcy's law. The rate of change of the storage is expressed in terms of the time derivative of the head, this time invoking an appropriate storage parameter (Specific storage in general or Storage coefficient in case of one/ two- dimensional horizontal flow).

Plugging in the expressions for the gradient driven inflow and outflow rates and the rate of change of storage in the continuity equation, leads a differential equation comprising the spatial and temporal derivatives of the primary state variable, flow and storage parameters, and the forcing function.

The procedure described above is illustrated by deriving a differential equation governing two- dimensional horizontal flow in a confined aquifer. The derivation essentially involves writing down the continuity equation for an element having infinitesimally small dimensions (δx and δy) in lateral directions x and y , and extending over the entire thickness in the vertical direction (see the following figure).



Gradient driven flow rates in x- direction:

$$\begin{aligned} \dot{I}_x &= -K_{xx} \frac{\partial h}{\partial x} b \delta y \\ &= -T_{xx} \frac{\partial h}{\partial x} \delta y \\ \dot{O}_x &= -\left[T_{xx} \frac{\partial h}{\partial x} + \frac{\partial}{\partial x} \left(T_{xx} \frac{\partial h}{\partial x} \right) \delta x \right] \delta y \end{aligned}$$

$$\dot{I}_x - \dot{O}_x = \frac{\partial}{\partial x} \left(T_{xx} \frac{\partial h}{\partial x} \right) \delta x \delta y$$

$$\text{Similarly } \dot{I}_y - \dot{O}_y = \frac{\partial}{\partial y} \left(T_{yy} \frac{\partial h}{\partial y} \right) \delta x \delta y$$

Total gradient driven (Inflow - Outflow) rate

$$= \frac{\partial}{\partial x} \left(T_{xx} \frac{\partial h}{\partial x} \right) \delta x \delta y + \frac{\partial}{\partial y} \left(T_{yy} \frac{\partial h}{\partial y} \right) \delta x \delta y$$

Where x, y are the coordinates along two principal permeability directions, t is the time coordinate, $h(x, y, t)$ is the head, I and O dots represent the inflow and outflow rates, K is hydraulic conductivity, T is Transmissivity, and suffixes denote the directions.

Forcing function driven out flow rate = $W \delta x \delta y$

Where W is the net abstraction per unit area per unit time (LT^{-1}).

$$\text{Total } (\dot{i} - \dot{O}) = \frac{\partial}{\partial x} \left(T_{xx} \frac{\partial h}{\partial x} \right) \delta x \delta y + \frac{\partial}{\partial y} \left(T_{yy} \frac{\partial h}{\partial y} \right) \delta x \delta y - W \delta x \delta y$$

$$\text{Rate of change of storage} = \frac{\partial h}{\partial t} S \delta x \delta y$$

Resulting governing differential equation:

$$\frac{\partial}{\partial x} \left(T_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(T_{yy} \frac{\partial h}{\partial y} \right) - W = S \frac{\partial h}{\partial t}$$

Where W is the forcing function (net external abstraction rate LT^{-1}) and S is storage coefficient.

Solution Algorithms

The differential equation governing the flow can be solved to obtain the spatial distribution of the head at pre-selected successively advancing discrete times. A realistic solution that accounts for the heterogeneity, anisotropy, and time and space variation of the forcing function, would have to be necessarily numerical in nature. A variety of numerical algorithms are available for solving the differential equations governing the groundwater flow. The easiest among them is the Finite difference method (FDM). A brief description of this method follows in the next paragraph.

Finite Difference Method

This method essentially involves the following steps:

Discretization of space and time

This is the first step of the modeling. Space, i.e., the area over which the system response is to be simulated, is discretized by a finite number of points- usually known as *nodes*. Typically the nodes may lie at the intersections of rows and columns superposed over the space. Similarly the time domain, i.e., the period over which the response is to be simulated, is discretized by a finite number of *discrete times*. Thus, a spatial distribution of any variable (say Storage coefficient) implies data comprising the values of the variable at each node. Similarly a spatial and temporal distribution of any variable (say, piezometric head) implies data comprising nodal values of the variable at the selected discrete times.

Marching in time domain

A strategy of “marching in time domain” is adopted for computing the nodal values of the head at successively advancing discrete times. This essentially involves: knowing the nodal heads at the beginning of a time step and computing the heads at the end of the time step. These computed heads form the “known heads” in the subsequent time step, and thus, the solution commences from the Initial condition and “marches” in the time domain.

Computation of the nodal heads at the end of a time step is accomplished as follows:

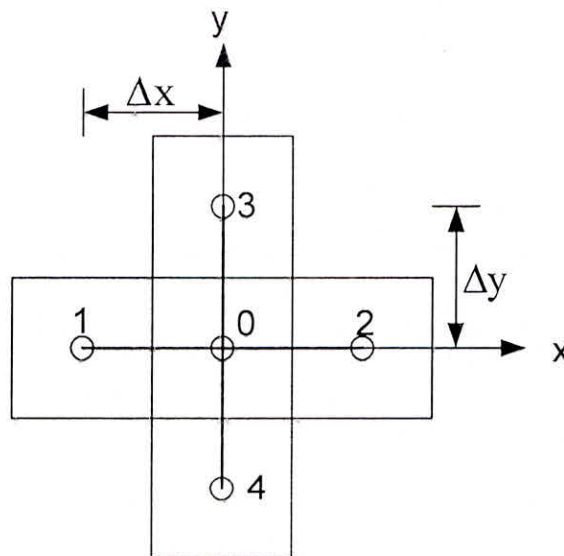
Formulation of linear algebraic equations

FDM essentially involves transforming the problem of solving the governing differential equation into a problem of solving a determinate system of linear equations. Formulation of the system of equations is discussed in the following paragraphs.

Interior Nodes: At each interior node, the space and time derivatives of the head appearing in the governing differential equations are approximated by corresponding finite differences. (This leads to inevitable truncation errors. However, these errors may be controlled by having not-so-large space and time steps.) This provides one linear equation for each node.

The procedure is illustrated below by writing down the finite difference form of the governing differential equation derived earlier.

Consider an interior node “0” surrounded by four nodes “1”, “2”, “3” and “4” as shown below.



Interior Node

The space and time derivatives of “h” at node “0” are expressed in terms of the respective finite differences as follows:

$$\frac{\partial}{\partial x} \left(T_{xx} \frac{\partial h}{\partial x} \right) = \frac{1}{\Delta x} \left[\frac{h_2 - h_0}{\Delta x} \left(\frac{T_0 + T_2}{2} \right) - \frac{h_0 - h_1}{\Delta x} \left(\frac{T_0 + T_1}{2} \right) \right]$$

$$\frac{\partial}{\partial y} \left(T_{yy} \frac{\partial h}{\partial y} \right) = \frac{1}{\Delta y} \left[\frac{h_3 - h_0}{\Delta y} \left(\frac{T_0 + T_3}{2} \right) - \frac{h_0 - h_4}{\Delta y} \left(\frac{T_0 + T_4}{2} \right) \right]$$

$$S \frac{\partial h}{\partial t} = S_0 \frac{h_0 - h_0^i}{\Delta t}$$

Where (h) are the unknown nodal heads at the end of the time- step, S is the Storage coefficient, h^i is the known head at the beginning of the time- step, Δt , Δx and Δy are the time and space steps, and the subscripts denote the node numbers.

Substitution of these finite- differences in the governing equations leads to the following form of a linear equation in terms of five unknown heads.

$$A(h_0) + B(h_1) + C(h_2) + D(h_3) + E(h_4) = F$$

Boundary nodes: An additional linear equation is obtained for each boundary node by invoking the respective known boundary condition.

Thus, as many equations are available as the number of the unknowns, viz., the nodal heads at the end of the time step.

Solution of linear algebraic equations

Theoretically the determinate system of equation can be solved by any standard numerical algorithm e.g., Gauss elimination, Gauss Seidel etc. However, the total memory requirement can be prohibitively large even for moderately sized domains. Consider this: if there are 1000 nodes (not an unusually large number), the memory required for storing the coefficient matrix alone would be one million words! However, the memory requirement can be significantly reduced by utilizing the “sparseness” of the coefficient matrix. Many specific algorithms like IADIE, LSOR, SIP etc. have been devised on these lines. These algorithms, apart from reducing the memory requirement, also reduce the round-off errors.

Problem- Specific State Variables

The end product from the solution of the governing differential equation comprises the mandatory state variable, i.e., nodal heads at successive discrete times. Other state variables which may be derived from these distributions may include among others, nodal depths to water table, influent/ effluent seepage, static storage, sea water intrusion etc.

Feasibility Checks

The feasibility of a trial pumping/ recharge pattern can be checked through groundwater flow modeling by broadly implementing the following steps:

1. Identify the aquifer system (spatial extent, boundary/ initial conditions, parameters etc.)
2. Quantify the proposed pumping/ recharge pattern
3. Identify the constraints and the corresponding state variables of the groundwater system
4. Formulate the nodal forcing functions by adding algebraically the proposed pumping/ recharge and other “natural” source/ sink terms
5. Project the nodal heads and hence the relevant state variables
6. Check feasibility

The constraints may be derived from technical, social, socio-economic considerations. It is apparent that there can not be any universal constraints. The constraints essentially represent the local concerns. For example, in coastal aquifers, certain outflow to sea is necessary for restricting the sea water intrusion to an *acceptable* level. Thus, the minimum permissible outflow to sea may be derived from the maximum acceptable extent of the sea water intrusion. Then, the feasibility of any proposed pumping pattern may be checked by comparing the projected outflow with the pre-stipulated minimum permissible outflow. If the projected outflow is found to be smaller, the proposed pumping pattern may be moderated iteratively until the projected outflow gets equal to the minimum permissible limit.

Uncertainty in Projections

The governing differential equation imbibed in a model may be based upon a few assumptions e.g., horizontality of the flow, uniqueness of the parameters, linearity of flow. Further additional assumptions may have to be made while implementing the model e.g., principal permeability directions, boundary conditions, spatial distribution of the aquifer parameters, time and space distributions of the forcing function etc. These assumptions, necessitated by a gap between the data requirement (which is always huge) and the data availability (which alas is always limited), may not always hold. Further, there are inevitable numerical errors! All this introduces an uncertainty in the model projections.

The uncertainty level may be controlled to an extent, by choosing a model with an appropriate differential equation, and then subsequently using hydrologic/ geohydrologic “sixth sense” to bridge the data gap while formulating the data base for the model. The latter obviously would come with experience. This makes groundwater modeling as much an art as science. Finally it is good to remember that a model is at its best a simplistic version of the system and needs to be evolved as the understanding of the system improves and additional data become available. As such, the worst thing any modeler (and more so a groundwater modeler) can do is to forsake the common sense and have a blind faith in his model.

Optimality

It is apparent that an array of feasible pumping patterns may be arrived at by simulation as described in the preceding section. The next step towards the planning is to pick up the *most rewarding* (or *least penalizing*) optimal pattern from the array of the evolved feasible patterns. This would require specifying quantitatively objective function(s) that relate the *reward /penalty* to the pumping pattern. Apparently the objective function would be derived from the *intended* objective(s) of the pumping activity. Typically the functions may comprise among others one or more of the following expectations.

- i) Maximizing the water production under specified constraints like: limiting the drawdowns/ water table depths/ sea water intrusion/ stream-aquifer interflows etc.
- ii) Maximizing the net benefit from water production i.e., benefit from the pumping minus the cost of pumpage or water production per unit cost, under specified constraints discussed above. The cost of pumpage may be expressed in terms of the pumping pattern and unit pumping cost. The latter may be assumed to be constant or lift-dependent.
- iii) Minimizing the maximum drawdown/ maximum water table depth/ pumping cost for a specified water production.
- iv) Minimizing the pumpage from a prevalent well network for a specified level of aquifer remediation (i.e., attenuation of concentration of stipulated species in the groundwater)
- v) Minimizing cost of pumping from a prevalent well network for a specified level of aquifer remediation
- vi) Maximizing the aquifer remediation by pumping from a prevalent well network subject to the constraints described in (i).
- vii) Maximizing the aquifer remediation for a specified financial allocation
- viii) Maximizing the net benefits/calorific value of the cropping pattern that can be irrigated by the pumpage or conjunctively by pumpage and the available canal supplies

It is apparent that except for a few rather simplistic objective functions [like (i), ii) with constant pumping cost, (iv)], computation of all other functions described above for a given pumping pattern would require operation of a simulation model. The maximization/ minimization of the objective function is accomplished by invoking an *optimizer*. The optimizer could be a *hard* optimizer (i.e., based upon traditional gradient based algorithms) or a soft optimizer like *genetic algorithm*. The hard optimizer depending upon the nature of objective function could be based upon linear programming, quadratic programming, non-linear programming or dynamic programming. A linking of the simulation model with an optimizer leads to what is usually termed as a *linked simulation optimization model*.

Approximated-Simulation Optimization Models

The main problem encountered in implementing a linked simulation optimization model is the prohibitive computational effort required for repeated runs of the computationally expensive simulation model. This problem can be overcome by replacing the computationally expensive physically based simulation model by a black box type model (i.e., devoid of any science) that is computationally inexpensive. Classical regression technique may be invoked to model the flow and transport processes

in groundwater aquifers. A regression model may be generally developed in the following steps.

- i) Invoking past experience or professional knowledge/intuition, stipulate a list of forcing functions (i.e., inputs into the model) that may lead to the desired state variable (i.e., output from the model).
- ii) Organize an adequate data base comprising the relevant forcing functions and the corresponding state variables. The data may be historical/ experimental, or in the present context may be generated by multiple runs of the physically based simulation model.
- iii) Again, invoking past experience or professional knowledge/intuition, assume a trial functional relation between the forcing functions and the state variable. The trial function may comprise apart from the forcing functions and the state variable, a few unknown fitting parameters.
- iv) Estimate the fitting parameters by the least squares approach.
- v) Validate the parameter estimation, and compute the “goodness” statistics.
- vi) Revise the functional relation if necessary and repeat.

It is easy to see that a proper choice of the functional relation is very crucial towards credibility of the regression model. Further, the computational efforts required for generating the data base could be large. However, this may be considered as a good investment in the sense that once the regression model is developed the subsequent simulation of the state variables would be computationally inexpensive.

ANN Methodology

Artificial neural network (ANN) methodology is being increasingly employed to simulate the aquifer response to a variety of inputs including pumping pattern and weather and for addressing complex groundwater management problems. The methodology although inspired by the working of human brain and bearing a somewhat exotic name, is essentially a specialized regression strategy. However, unlike the general regression the function relating inputs to the outputs is rather regimented. The function comprises an input layer, hidden layers and an output layer. The input layer contains the input variables (termed as input nodes) that comprise the physical inputs and a bias term assigned a constant value of 1.0. Similarly the output layer has the output variables (again termed as output nodes). There may be several hidden layers containing several nodes, their number not being known a priori. Nodes are connected in the forward direction (i.e., commencing from the input layer and terminating at the output layer) across the layers by transfer functions correlating input (say X_{ij}) into and output (say Y_{ij}) from j^{th} node of i^{th} hidden layer. The most widely non-linear transfer function is as follows.

$$Y_{ij} = \frac{1}{1 + e^{-X_{ij}}}$$

The input (X_{ij}) is deemed to be a weighted mean of outputs from all the nodes of the preceding (i.e., $i-1$) layer, the weights being unknown a priori. Thus, X_{ij} is written in terms of outputs ($Y_{i-1,k}$, $k=1,2,\dots$) from all the nodes of the layer ($i-1$).

$$X_{ij} = \sum_k w_{i-1,j,k} Y_{i-1,k}$$

Where $w_{i-1,j,k}$ is the weight assigned to the link joining the k^{th} node of the layer (i-1) to the j^{th} node of i^{th} layer. The outputs ($Y_{0,k}$) from the input layer are deemed to be the values assigned to the input variables and the constant bias term. Thus, the computations commence from the input layer, proceed in the forward direction, and terminate at the output layer. The outputs from the nodes of the output layer are deemed to be the estimates of the corresponding output variables. The weights are estimated by the least squares criterion. The necessary number of hidden layers and the nodes therein are determined by a trial procedure honoring the requirement of *parsimony*, i.e., keeping the number of hidden layers and the nodes to a minimum without sacrificing the predictive capability of the ANN model. Theoretically the bare minimum ANN model may have only one hidden layer with number of nodes two in excess of the number of input nodes. The computational procedure aimed at determining the optimal number of hidden layers and the nodes therein, and estimating the corresponding weights is termed as *training* of the ANN network. It is easy to see that these are respectively analogous to steps (iii) and (iv) of the general regression procedure described earlier.

It is easy to see that generating a regression or ANN model of the aquifer response may be an elaborate and computationally expensive procedure involving several runs on the physically based simulation models, followed by parameter estimation/training. However once such an approximated-simulation model is generated, it would be a computationally inexpensive numerical tool. Being inexpensive it could be linked to an optimization model leading to an approximated-simulation optimization model that may not be prohibitively computationally expensive.

Indian Scene

In India the groundwater development is planned by conducting lumped water balance studies on historical data. Government of India set up a committee in 1996 to standardize the procedure for implementing this approach. The committee finalized its recommendations in 1997. The recommendations, usually termed as GEC-97 norms are widely invoked to estimate the ground water resource in the country. The norms essentially comprise two steps towards the resource estimation. The first step involves an estimation of the recharge from rainfall in monsoon season by conducting a lumped water balance study invoking the historical data of water table elevations, draft, recharge etc. Subsequently in the second step the annual utilizable recharge is estimated rather empirically as a fraction of the estimated recharge allowing for the *losses* comprising evapotranspiration and lateral outflows to drains. Whereas the first step involving estimation of recharge is quite rational (being based upon the well known continuity equation), the second step aimed at estimating the utilizable recharge is rather arbitrary. As such not surprisingly application of the norms in many studies is known to have led to a variety of anomalous results.

Conclusion

Groundwater modeling essentially involves projection of the problem-specific state variables of the groundwater system for a given forcing function, invoking the continuity equation at a micro level

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