Pitfalls and Sensitivities in Groundwater Modelling

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Groundwater models provide a scientific and predictive tool for determining appropriate solutions to water allocation, surface water-groundwater interaction, landscape management or impact of new development scenarios. However, if the modelling studies are not well designed from the outset, or the model does not adequately represent the natural system being modelled, the modelling effort may be largely wasted, or decisions may be based on flawed model results, and long term adverse consequences may result. This paper presents the common pitfalls and sensitivities which are normally encountered during groundwater modelling studies. It will help in improving the model conceptualisation and understanding the uncertainty in model results.

Keywords: Groundwater; Modelling; Conceptualization; Calibration; Prediction

INTRODUCTION

A groundwater model is a computer-based representation of the essential features of a natural hydrogeological system that uses the laws of science and mathematics. Its two key components are a conceptual model and a mathematical model. The conceptual model is an idealised representation (usually graphical) of one's hydrogeological understanding of the essential flow processes of the system. A mathematical model is a set of equations, which, subject to certain assumptions, quantifies the physical processes active in the aquifer system(s) being modelled.

While the model itself obviously lacks the detailed reality of the groundwater system, the behaviour of a valid model approximates that of the aquifer(s). A groundwater model provides a scientific means to synthesise the available data into a numerical characterisation of a groundwater system. The model represents the groundwater system to an adequate level of detail, and provides a predictive tool to quantify the effects on the system of specified hydrological, pumping or irrigation stresses.

Typical model purposes include improving hydrogeological understanding (synthesis of data); aquifer simulation (evaluation of aquifer behaviour); designing practical solutions to meet specified goals (engineering design); optimising designs for economic efficiency and account for environmental effects (optimisation); evaluating recharge, discharge and aquifer storage processes (water resources assessment); predicting impacts of alternative hydrological or development scenarios (to assist decision-making); quantifying the sustainable yield (economically and environmentally sound allocation policies); resource management (assessment of alternative policies); sensitivity and uncertainty analysis (to guide data collection and risk-based decision-making); and visualisation (to communicate aquifer behaviour).

There are very few published and accepted guidelines on groundwater flow modelling. The notable example is the suite of Standard Guides[1-5] from the American Society for Testing and Materials (ASTM), which are reasonably well-accepted standard practice guidelines. The groundwater modelling guideline documents are quite consistent in regard to the accepted general approach to groundwater modelling (with greater or lesser emphasis on certain aspects, depending on the application of the guideline) which may be summarised as:

- Define purpose of study and objectives;
- Develop conceptual model;
- Select model approach/code (analytical or numerical and software package);
- Develop and calibrate model;
- Assess parameter sensitivity and calibration uncertainty;
- Complete prediction scenarios and sensitivity/uncertainty analysis;
- Report; and
- Post-audit (at some time in future).

MODELLING OF GROUNDWATER FLOW

Groundwater modelling begins with a conceptual understanding of the physical problem. The next step in modelling is translating the physical system into mathematical terms. In general, the results are the familiar groundwater flow equation and transport equations. The governing flow equation for three-dimensional saturated flow in saturated porous media is:

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)-Q=S_s\frac{\partial h}{\partial t} \quad (1)$$

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where K_{xx} , K_{yy} , K_{zz} are hydraulic conductivity along the *x*, *y*, *z* axes which are assumed to be parallel to the major axes of hydraulic conductivity; *h*, the piezometric head; *Q*, volumetric flux per unit volume representing source/sink terms; and S_S , the specific storage coefficient defined as the volume of water released from storage per unit change in head per unit volume of porous material.

The transport of solutes in the saturated zone is governed by the advection-dispersion equation which for a porous medium with uniform porosity distribution is formulated as:

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial x_i}\left(cv_i\right) + \frac{\partial}{\partial x_i}\left(D_{ij}\,\frac{\partial c}{\partial x_j}\right) + R_c \qquad i, j = 1, 2, 3 \quad (2)$$

where *c* is the concentration of the solute; R_c , sources or sinks; D_{ij} , dispersion coefficient tensor; and v_i , the velocity tensor.

An understanding of these equations and their associated boundary and initial conditions is necessary before a modelling problem can be formulated. Basic processes, that are considered, include groundwater flow, solute transport and heat transport. Most groundwater modelling studies are conducted using either deterministic models, based on precise description of cause-and-effect or input-response relationships, or stochastic models reflecting the probabilistic nature of a groundwater system.

The governing equations for groundwater systems are usually solved either analytically or numerically. Analytical models contain analytical solution of the field equations, continuously in space and time. In numerical models, a discrete solution is obtained in both the space and time domains by using numerical approximations of the governing partial differential equation. Various numerical solution techniques are used in groundwater models. Among the most used approaches in groundwater modelling, three techniques can be distinguished: Finite Difference Method, Finite Element Method, and Analytical Element Method. All techniques have their own advantages and disadvantages with respect to availability, costs, user friendliness, applicability, and knowledge required of the user.

The data requirements for a groundwater model comprise hydrogeological framework data and hydrological stress data. The framework data describe the physical system (aquifer geometry, hydrological interaction processes), and parameters that do not change with time. The stress data describe the dynamic hydrological stresses on the system (initial conditions, time-varying data and the translation of management strategies into modelling scenarios). Compiling the data is not a simple task, and many diverse data sources need to be accessed.

Some of the frequently used groundwater modelling codes include MODFLOW, MT3D, MOC3D, AQUIFEM, FEMWATER, SUTRA, FEFLOW, PMWIN, Groundwater Vistas, Visual Modflow, Groundwater Modelling System etc. It is generally accepted that Modflow, originally developed by the US Geological Survey[6], is the industry-leading public domain numerical flow model, although it is not necessarily suitable for every modelling study. There are a number of graphical user interfaces for Modflow. There are also several text books that detail modelling methodologies with Modflow[7].

PITFALLS AND SENSITIVITIES

Pitfalls and sensitivities are often specific to a model[8]. However, an attempt has been made to sum up the frequently occurring problems. There are many model programs available for a numerical approach to the groundwater flow. These programs are based on the elementary conservation of equations (Darcy's law and the continuity equation). The differences are mainly found in the method of discretization (finite differentiations, finite elements and analytical elements) and the way in which the user can define the boundary conditions.

Two classes of model programs can be distinguished in the groundwater quality models. The first class comprises the 'lumped' model programs in which chemical aspects are defined by strongly simplified parameters (dispersion, sorption, retardation). Well-known model programs in this class are: MT3D, HST3D, RT3D, MODWALK. Just like the groundwater flow models, the differences between the various programs lie mainly in the method of discretization and the way in which the user can define the boundary conditions. The second class of model programs explicitly describes the chemical reactions. Representatives of this class are FREEQM and CHARON. This type of model program can not be used without considerable chemical expertise.

Model Setup

Conceptual Model

A conceptual model is constructed prior to numerical modelling. This conceptual model defines, among other things, the global structures of the subsoil and the substances found in it. The hydraulic properties play a particularly important role for the groundwater flow. The choices made in the conceptual model with regard to the limits of the model field, both horizontally and vertically, are generally not changed in the further course of the modelling process. The choice of the location and type of the boundary can greatly influence the model results and therefore requires effective underpinning.

The layers are often classified into aquifers and separating layers. The method of binding these layers greatly influences the simulated flow field, and thereby the model results. Another important aspect is the existence of hydraulic short circuits or blockages. These phenomena occur in separating layers, fracture systems (open or closed), sand and gravel banks and dams. Information on these phenomena is often not explicitly included or is insufficiently known.

Non-recognition of these structures can lead to incorrect interpretation of the results during the further course of the modelling process. Moreover, the negligence of density variation can lead to completely incorrect flow directions and calibrated constants. In the coastal areas in particular, the effects of density variation due to deviations in the salt content will have to be taken into account. This also applies at waste dump sites and other locations with strongly polluted groundwater.

For the total sediment discharge, it is particularly the estimation of local heterogeneity which is important. These help to determine the travelling times and breakthrough curves. Also vital is a good hypothesis of the geo-hydrochemical processes. Examples of important aspects are the sorption processes (balance or imbalance, linear or non-linear), the presence of decomposition, the geochemical conditions (for example rich or poor in oxygen), the presence of organic matter in the sediment, etc. The limited observation material is often not adequate to be able to distinguish between various processes in the calibration phase, so that the modelling is strongly dependent on the expertise in the conceptual phase.

Choice of Model Program

The choice of model program is not particularly critical for the final results of a model for groundwater flow. However, the modeller must be aware of the underlying assumptions and the usage limitations of the various model programs. The top system (small surface waters, drainage and unsaturated zone) may be defined in more detail in one model than in another, for example.

In the modelling of total sediment discharge, the differences between the various model programs may be very relevant, however. There is numerical dispersion in most of the model programs based on finite elements and finite differentials. The mass balance is often not guaranteed in model programs based on the finite elements approach. This may result in major errors, particularly when there are strong gradients in the concentration, due to the model incorrectly distributing the flux and the concentration over a large surface area.

Besides physical and chemical considerations, practical considerations also play a role in the choice of model program. The more organised the input of parameters and options, the less the chance of practical usage errors. Moreover, the calculating time and the memory required may also play a role in the more complex (unsteady) problems.

Analysis of the Model

Sensitive Parameters

In groundwater flow models, the sensitive factors often depend on the objective of the model. For many models, the degrees of resistance of separating layers are sensitive parameters as they are more difficult to estimate (variation of 10 or 100) than, for example, the permeability of aquifers (variation of 2). Local holes in separating layers have much larger regional effects than local areas with high permeability. Conversely, areas with a much higher local resistance in the separating layer, hardly have any influence at all, while local areas with high resistance in aquifers are generally relevant.

The lack of flow over a separating layer means that the value of the resistance is not important, but does make it almost impossible to determine the resistance. Once flow has been applied over this layer in a scenario (through extraction, for example), the resistance may well be a dominating factor (if it is relatively great, for instance).

The most sensitive parameters for total sediment discharge models depend on the type of substance being described and on the local situation. For those substances which absorb to organic matter, the retardation factor and the organic matter content can often be noted as being sensitive parameters.

Discretization

The spatial and temporal discretization must be small enough to minimise numerical errors. Generally speaking, this means that smaller steps must be taken when the gradients become steeper. The steepness of the gradients is partly determined by the hydraulic properties of the system and can often be characterised by the composite leakage factor. Elements must generally be smaller than this leakage factor. This, therefore, also applies to surface waters where there are hardly any resistance layers at all. The errors made in such cases can lead to both incorrect flows in the model and to incorrect hydraulic parameters in the calibration.

Many total sediment transport models are very sensitive to the grid size in terms of the numerical dispersion. The discretization suitable for a flow model is not automatically also suitable for a total sediment discharge model based on the velocity field of the flow model in question. The time step and grid distances can be chosen independently of one another. Some model programs automatically determine the (maximum) time step. If this is not the case, major numerical errors may occur.

Reduction of the grid distances and the time steps will not automatically produce better model results. A very fine grid may give the impression of a very detailed and therefore accurate model. Unless information is added on the right scale however, the only added value of a finer grid is its ability to prevent numerical errors. In combination with overly detailed parameterization, a finer grid may even provide less information. Conversely, too coarse an elements network can lead to 'stable' calibration results, which are incorrect due to insufficient possibilities for simulation of variations in hydraulic head and flux.

One of the main pitfalls in the modelling of boundaries is the definition of a closed boundary or fixed hydraulic head at the location of a catchment boundary under an infiltration area. That boundary and therefore, the flow and the hydraulic head, change as the circumstances change. The same applies in modelling a freshwater-salt water boundary area. This can not be seen as a closed boundary either if the circumstances in its vicinity change.

Special attention is required for the discretization in the vertical. A quasi 3D approach is effective for modelling for regional flow. Quasi 3D means that the vertical differences in the hydraulic head within an aquifer are neglected in the calculations. This does not mean that there can be no vertical flow component within the aquifer. In such cases, great care must be exercised with the schematization in aquifers and separating layers, as incorrect connections can lead to major errors in the model. Moreover, in local problems and in flows in heterogenic packages, this approach may lead to relevant errors, particularly in the calculated flow distribution and the total sediment discharge.

Parameterization

A numerical groundwater flow model or a groundwater transport model comprises many spatially distinguishable units (blocks, elements). In principle, each unit is attributed a value for the parameters (permeability, storage coefficient, dispersion coefficient, sorption etc). This results in many (often tens of thousands of) degrees of freedom. Given the limited availability of information, both in terms of the geological definition as the observations of the dynamics (hydraulic head and concentration measurements), it is essential that the number of degrees of freedom be reduced. This takes place through a certain form of processing of the parameter values. Common methods include zoning, whereby a certain zone is attributed the same value and a geostatistic interpolation.

A pitfall of parameterization is that structures which are modelled are too detailed and can not be adjusted in the course of the modelling, due to a lack of field observations, so that they in fact begin to lead a life of their own. Another important point is that the scale on which information on the parameter values is available is not always in keeping with the model discretization. This applies to geological information from drilling, for example, and to geohydrological information from pumping tests. The parameters in the grid blocks must become 'block effective' values. The point observations therefore need to be scaled up. The method of scaling may be very sensitive, particularly when there is great heterogeneity. If a 'simple' mathematical average or a linear interpolation of the point values is used in such cases, major errors may be the result, particularly with regard to the breakthrough curves and residence times. It is difficult to determine beforehand which method should be used, but there must in any case be careful verification in relation to observations from the field.

Boundary Conditions

An important component of the modelling process is formulation of the boundary conditions. These are not only the conditions concerning the physical external boundaries of the model, but also the conditions concerning the so-called interior boundaries (extraction points, drains etc). It is essential to include as many observations of fluxes (discharges) alongside the potentials (measured or estimated hydraulic heads and groundwater levels). Hydraulic parameters in a model without given fluxes can not, in principle, be defined as these may otherwise be attributed any possible value (and therefore also useless ones) in a calibration procedure.

Calibration and Scaling up

Measurements with which a model is calibrated (hydraulic head, fluxes and concentrations) are often point observations in relation to the 'block effective' values which the model calculates. When, there is great small-scale variability in particular, it is very questionable to what extent a calculated head or concentration in a grid block or element must meet the measured point value. The trend must generally be in keeping, though even this need not always be the case. Prior effective (geostatistic) analysis of the representativeness of the measuring points is therefore always recommendable.

Calibration and Minimization Criteria

Calibration (both manually and using calibration programs) is carried out by changing parameter values in order to gear the model results to observations. A squares sum or a variance is often used as a measure for calibration. A large number of calibration procedures is based on unweighted criteria. In other words, all measurements are attributed equal importance. This can lead to imbalance calibration, for example in areas where there are clusters of observations with a great deal of superfluous information. The cluster then weighs disproportionately heavy in relation to a single measuring point at a different location. If the scope of the variables' values is very diverse (in concentration measurements, for example), there is a risk that a peak in the observations will be disproportionately weighted.

Steady models are commonly used in the geohydrological practice. These models neglect the effect of storage and can only describe an 'average' flow, and are, therefore, usually only applied for modelling of the quantity. The principle behind steady models is that a balanced situation is described, *ie,* a situation in which the effects of changes in time can be neglected with regard to the effects to be calculated. There are a number of pitfalls here, particularly for the description of the groundwater flow (flow direction and residence times). There is often less sensitivity for the effects in terms of groundwater levels or hydraulic head.

The observations used in the calibration come from a dynamic system. Observations from a so-called 'average hydrological year' are often applied, and this can lead to serious errors (also in terms of hydraulic head) in systems with a long-term 'memory' (great inertia). For calibration of the hydraulic parameters of the quantity, it is often more advisable to look for an almost steady state, (*ie,* a state in which the storage variation is negligible) such as that found at the end of the rainy season, and also to take the average of this over a number of years.

In order to calibrate a steady model effectively, (*ie*, usable for calculation of an average flow situation), the steady values must be calculated for the observations from the dynamic system (hydraulic head, concentrations, precipitation, surface water levels etc). A rule of thumb in this is to take the average over approximately four times the correlation length (the period within which the variables to be modelled still show cohesion).

If there is little dynamics in the calibration phase, it is difficult to determine the parameters which influence time-dependent behaviour (storage). If possible (in groundwater decontamination for example), great dynamic variation should be applied to the starting state, for the benefit of calibration of the model.

Use of the Model

In the user phase (forecasting), the model results are often sensitive to different parameters when compared with the calibration phase (present state). A well-known example is that a model calibrated for an average state can not effectively be applied to a dry or wet state. Another example is that the groundwater flow is often strongly dependent on the feed from the top system. Due to the complexity of the top system, many model studies invest a great deal of energy in its calibration. However, if the model is intended for analysis of the effects of a change in deep groundwater reclamation, the separating layers between the aquifers may be equally important.

One of the best-known pitfalls in separating layers is that the calibration phase is generally dominated by a small hydraulic gradient, to the extent that its resistance can not be calibrated, while that resistance may be a deciding factor when reclamation is increased in the new situation. Measures in the top system often lead to a change in the representative resistance of that top system. It also occurs that a change in the flow (direction and volume) alters the hydraulic properties of layers.

For total sediment discharge models too, the conditions (in terms of flow and discharge) may be quite different in the user phase than in the calibration phase. Diffusion and decomposition may have an important effect on the total sediment discharge in the calibration phase for example, while convective transport is much more important in the user phase. What is needed in that case is modelling outside of the scope of the calibration. Generally speaking, the dynamic variation is different and more limited in the starting state than in the user phase. A change in the direction of flow (horizontal and/or vertical) can have major consequences for the parameter values determined by the calibration (for example those for retardation and sorption).

CONCLUDING REMARKS

The modelling studies in India have so far been confined to academic and research organisations. The practising professionals mostly still prefer to employ lumped models for planning of groundwater development and recharge. Such models completely ignore the distributed character of the groundwater regime. Thus, they are based upon rather conservative concepts like safe yields and are incapable of accounting for the stream-aquifer interaction and the dependence of lateral recharge on the water table pattern. Consequently, permissible mining, (*ie,* withdrawals in excess of vertical recharge) and perennial yield can not be arrived at. The objectives of modelling studies in India have been mainly (i) groundwater recharge; (ii) dynamic behaviour of the water table; (iii) stream-aquifer interaction; and (iv) sea-water intrusion etc. It is important to understand general aspects of groundwater flow models so that application or evaluation of these models may be performed correctly.

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