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Modelling of Groundwater Flow and Data Requirements

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Abstract

Groundwater is used for a variety of purposes, including irrigation, drinking and manufacturing. Groundwater is also the source of a large percentage of surface water. Accurate and reliable groundwater resource information (including quality) is critical to planners and decision-makers. Huge investment in the areas of groundwater exploration, development and management at state and national levels aims to meet the groundwater requirement for drinking and irrigation and generates enormous amount of data. We need to focus on improved data management, precise analysis and effective dissemination of data. Numerical models are capable of solving large and complex groundwater problems varying widely in size, nature and real life situations. With the advent of high speed computers, spatial heterogeneities, anisotropy and uncertainties can be tackled easily. However, the success of any modelling study, to a large measure depends upon the availability and accuracy of measured/recorded data required for that study. Therefore, identifying the data needs of a particular modelling study and collection/monitoring of required data form an integral part of any groundwater modelling exercise. This paper presents groundwater modelling process, basic data requirements for groundwater modelling and commonly used groundwater modelling software.

Keywords: *Groundwater, Numerical Model, MODFLOW, Calibration.*

1. INTRODUCTION

A groundwater model is any computational method that represents an approximation of an underground water system (modified after Anderson and Woessner 1992). While groundwater models are, by definition, a simplification of a more complex reality, they have proven to be useful tools over several decades for addressing a range of groundwater problems and supporting the decision-making process.

Groundwater systems are affected by natural processes and human activity, and require targeted and ongoing management to maintain the condition of groundwater resources within acceptable limits, while providing desired economic and social benefits. Groundwater management and policy decisions must be based on knowledge of the past and present behaviour of the groundwater system, the likely response to future changes and the understanding of the uncertainty in those responses.

The location, timing and magnitude of hydrologic responses to natural or human-induced events depend on a wide range of factors - for example, the nature and duration of the event that is impacting groundwater, the subsurface properties and the connection with surface water features such as rivers and oceans. Through observation of these characteristics a conceptual understanding of the system can be developed, but often observational data is scarce (both in space and time), so our understanding of the system remains limited and uncertain.

Groundwater models provide additional insight into the complex system behaviour and (when appropriately designed) can assist in developing conceptual understanding. Furthermore, once they have been demonstrated to reasonably reproduce past behaviour, they can forecast the outcome of future groundwater behaviour, support decision-making and allow the exploration of alternative management approaches. However, there should be no expectation of a single 'true' model, and model outputs will always be uncertain. As such, all model outputs presented to decision-makers benefit from the inclusion of some estimate of how good or uncertain the modeller considers the results.

A *groundwater flow model* simulates hydraulic heads (and watertable elevations in the case of unconfined aquifers) and groundwater flow rates within and across the boundaries of the system under consideration. It can provide estimates of water balance and travel times along flow paths. A *solute transport model* simulates the concentrations of substances dissolved in groundwater. These models can simulate the migration of solutes (or heat) through the subsurface and the boundaries of the system. Groundwater models can be used to calculate water and solute fluxes between the groundwater system under consideration and connected source and sink features such as surface water bodies (rivers, lakes), pumping bores and adjacent groundwater reservoirs.

2. MODELLING OF GROUNDWATER FLOW AND MASS TRANSPORT

A groundwater model is a simplified representation of a groundwater system. Groundwater models can be classified as physical or mathematical. A *physical model* (e.g. a sand tank) replicates physical processes, usually on a smaller scale than encountered in the field.

A *mathematical model* describes the physical processes and boundaries of a groundwater system using one or more governing equations. An *analytical model* makes simplifying assumptions (e.g. properties of the aquifer are considered to be constant in space and time) to enable solution of a given problem. Analytical models are usually solved rapidly, sometimes using a computer, but sometimes by hand.

A *numerical model* divides space and/or time into discrete pieces. Features of the governing equations and boundary conditions (e.g. aquifer geometry, hydrogeological properties, pumping rates or sources of solute) can be specified as varying over space and time. This enables more complex, and potentially more realistic, representation of a groundwater system than could be achieved with an analytical model. Numerical models are usually solved by a computer and are usually more computationally demanding than analytical models.

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:

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

where,

K_{xx}, K_{yy}, K_{zz}	=	hydraulic conductivity along the x,y,z axes which are assumed to be parallel to the major axes of hydraulic conductivity;
h	=	piezometric head;
Q	=	volumetric flux per unit volume representing source/sink terms;
S_s	=	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 follows:

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

where,

c	=	concentration of the solute;
R_c	=	sources or sinks;
D_{ij}	=	dispersion coefficient tensor;
v_i	=	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 required knowledge of the user.

3. GROUNDWATER MODELLING PROCESS

The groundwater modelling process has a number of stages. As a result, the modelling team needs to have a combination of skills and at least a broad or general knowledge of: hydrogeology; the processes of groundwater flow; the mathematical equations that describe groundwater flow and solute movement; analytical and numerical techniques for solving these equations; and the methods for checking and testing the reliability of models.

The modeller’s task is to make use of these skills, provide advice on the appropriate modelling approach and to blend each discipline into a product that makes the best use of the available data, time and budget. In practice, the adequacy of a groundwater model is best judged by the ability of the model to meet the agreed modelling objectives with the required level of confidence. The modelling process can be subdivided into seven stages (shown schematically in Figure 1) with three hold points where outputs are documented and reviewed.

The process starts with *planning*, which focuses on gaining clarity on the intended use of the model, the questions at hand, the modelling objectives and the type of model needed to meet the project objectives. The next stage involves using all available data and knowledge of the region of interest to develop the conceptual model *(conceptualisation)*, which is a description of the known physical features and the groundwater flow processes within the area of interest. The next stage is *design*, which is the process of deciding how to best represent the conceptual model in a mathematical model. It is recommended to produce a report at this point in the process and have it reviewed. *Model* *construction* is the implementation of model design by defining the inputs for the selected modelling tool.

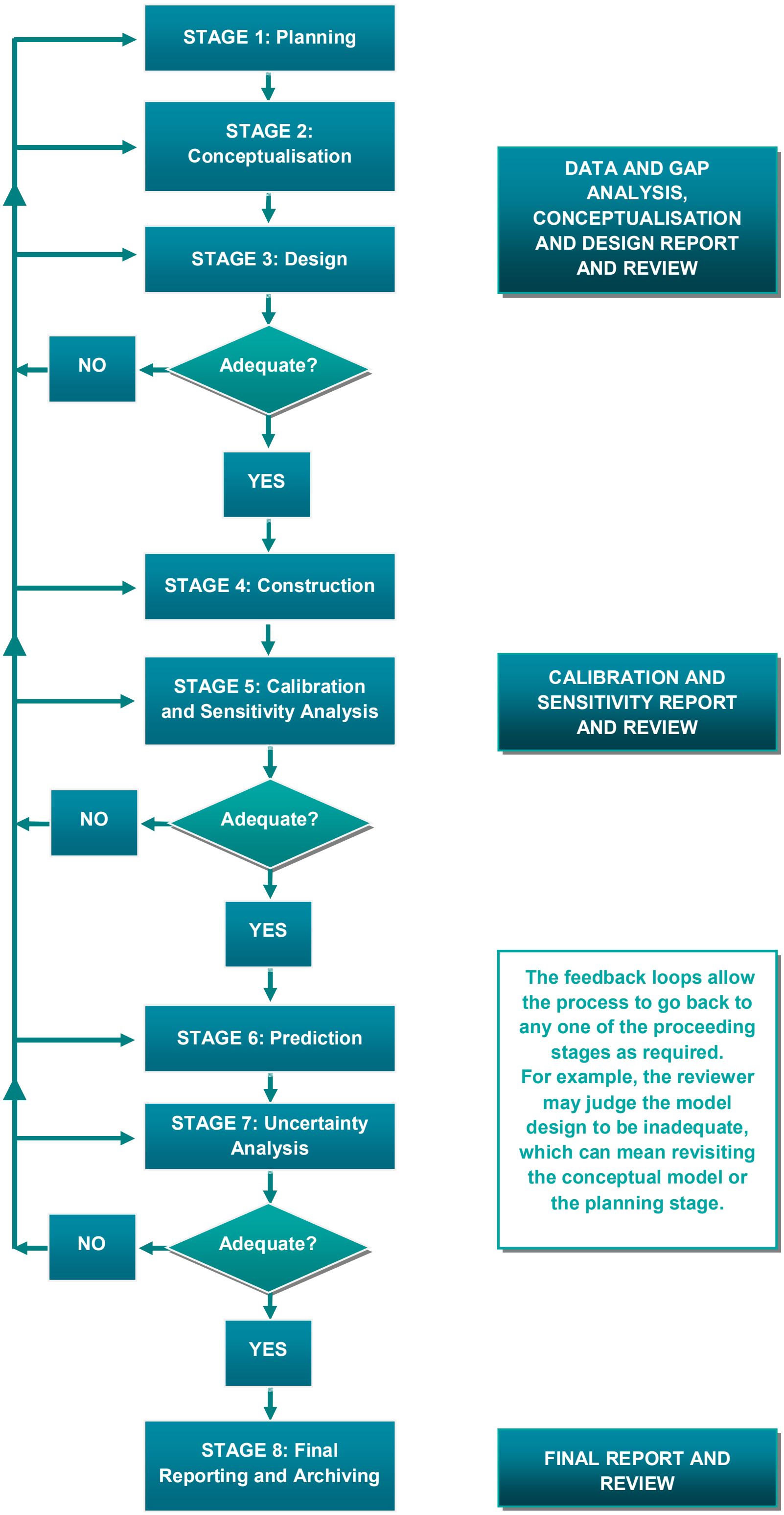

Figure 1: Groundwater Modelling Process (modified after MDBC, 2001 and Yan et al., 2010)

The *calibration and sensitivity analysis* of the model occurs through a process of matching model outputs to a historical record of observed data. It is recommended that a calibration and sensitivity analysis report be prepared and reviewed at this point in the process.

Predictions comprise those model simulations that provide the outputs to address the questions defined in the modelling objectives. The predictive analysis is followed by an analysis of the implications of the *uncertainty* associated with the modelling outputs.

Clear communication of the model development and quality of outputs through *model reporting and review* allows stakeholders and reviewers to follow the process and assess whether the model is fit for its purpose, that is, meets the modelling objectives.

The process is one of continual iteration and review through a series of stages. For example, there is often a need to revisit the conceptual model during the subsequent stages in the process. There might also be a need to revisit the modelling objectives and more particularly reconsider the type of model that is desired once calibration has been completed. Any number of iterations may be required before the stated modelling objectives are met. Accordingly, it is judicious at the planning stage to confirm the iterative nature of the modelling process so that clients and key stakeholders are receptive to and accepting of the approach.

4. DATA REQUIREMENTS FOR GROUNDWATER MODELLING

The first phase of any groundwater study consists of collecting all existing geological and hydrological data on the groundwater basin in question. This will include information on surface and subsurface geology, water tables, precipitation, evapotranspiration, pumped abstractions, stream flows, soils, land use, vegetation, irrigation, aquifer characteristics and boundaries, and groundwater quality. If such data do not exist or are very scanty, a program of field work must first be undertaken, for no model whatsoever makes any hydrological sense if it is not based on a rational hydrogeological conception of the basin. All the old and newly-found information is then used to develop a conceptual model of the basin, with its various inflow and outflow components.

A conceptual model is based on a number of assumptions that must be verified in a later phase of the study. In an early phase, however, it should provide an answer to the important question: does the groundwater basin consist of one single aquifer (or any lateral combination of aquifers) bounded below by an impermeable base? If the answer is yes, one can then proceed to the next phase: developing the numerical model. This model is first used to synthesize the various data and then to test the assumptions made in the conceptual model. Developing and testing the numerical model requires a set of quantitative hydrogeological data that fall into two categories:

- Data that define the physical framework of the groundwater basin
- Data that describe its hydrological stress

These two sets of data are then used to assess a groundwater balance of the basin. The separate items of each set are listed below.

Physical framework	***Hydrological stress***
1. Topography	1. Water table elevation
2. Geology	2. Type and extent of recharge areas
3. Types of aquifers	3. Rate of recharge
4. Aquifer thickness and lateral extent	4. Type and extent of discharge areas
5. Aquifer boundaries	5. Rate of discharge

6. Lithological variations within the aquifer
7. Aquifer characteristics

It is common practice to present the results of hydrogeological investigations in the form of maps, geological sections and tables - a procedure that is also followed when developing the numerical model. The only difference is that for the model, a specific set of maps must be prepared. These are:

- Contour maps of the aquifer's upper and lower boundaries
- Maps of the aquifer characteristics
- Maps of the aquifer's s net recharge
- Water table contour maps

Some of these maps cannot be prepared without first making a number of auxiliary maps. A map of the net recharge, for instance, can only be made after topographical, geological, soil, land use, cropping pattern, rainfall, and evaporation maps have been made.

The data needed in general for a groundwater flow modelling study can be grouped into two categories: (a) Physical framework and (b) Hydrogeologic framework (Moore, 1979). The data required under physical framework are:

1. Geologic map and cross section or fence diagram showing the areal and vertical extent and boundaries of the system.
2. Topographic map at a suitable scale showing all surface water bodies and divides. Details of surface drainage system, springs, wetlands and swamps should also be available on map.
3. Land use maps showing agricultural areas, recreational areas etc.
4. Contour maps showing the elevation of the base of the aquifers and confining beds.
5. Isopach maps showing the thickness of aquifers and confining beds.
6. Maps showing the extent and thickness of stream and lake sediments.

These data are used for defining the geometry of the groundwater domain under investigation, including the thickness and areal extent of each hydrostratigraphic unit.

Under the hydrogeologic framework, the data requirements are:

1. Water table and potentiometric maps for all aquifers.
2. Hydrographs of groundwater head and surface water levels and discharge rates.
3. Maps and cross sections showing the hydraulic conductivity and/or transmissivity distribution.
4. Maps and cross sections showing the storage properties of the aquifers and confining beds.
5. Hydraulic conductivity values and their distribution for stream and lake sediments.
6. Spatial and temporal distribution of rates of evaporation, groundwater recharge, surface water - groundwater interaction, groundwater pumping, and natural groundwater discharge.

The data collection and analysis stage of the modelling process involves:

- confirming the location and availability of the required data
- assessing the spatial distribution, richness and validity of the data
- data analysis commensurate with the level of confidence required. Detailed assessment could include complex statistical analysis together with an analysis of errors that can be used in later uncertainty analysis.
- developing a model project database. The data used to develop the conceptualisation should be organised into a database, and a data inventory should be developed, which includes data source lists and references.

- evaluating the distribution of all parameters/observations so that model calibration can proceed with parameters that are within agreed and realistic limits. Parameter distributions for the conceptual model are sometimes best represented as statistical distributions.
- justification of the initial parameter value estimates for all hydrogeological units
- quantification of any flow processes or stresses (e.g. recharge, abstraction).

Some of the compiled information will be used not only during the conceptualisation, but also during the design and calibration of the model. This includes the data about the model layers and hydraulic parameters as well as observations of hydraulic head, watertable elevation, and fluxes.

The conceptualisation stage may involve the development of maps that show the hydraulic heads in each of the aquifers within the study area. These maps help illustrate the direction of groundwater flow within the aquifers, and may infer the direction of vertical flow between aquifers.

The data used to produce maps of groundwater head is ideally obtained from water levels measured in dedicated observation wells that have their screens installed in the aquifers of interest. More often than not, however, such data is scarce or unavailable and the data is sourced from, or complemented by, water levels from production bores. These may have long well screens that intersect multiple aquifers, and be influenced by preceding or coincident pumping. The accuracy of this data is much less than that obtained from dedicated observation wells. The data can be further supplemented by information about surface expressions of groundwater such as springs, wetlands and groundwater-connected streams. It provides only an indication of the minimum elevation of the watertable (i.e. the land surface) in areas where a stream is gaining and local maximum elevation in areas where a stream is losing. As such, this data has a low accuracy, but can be very valuable nonetheless.

5. MODELLING SOFTWARE

Groundwater modelling sometimes requires the use of a number of software types. These include:

- the model code that solves the equations for groundwater flow and/or solute transport, sometimes called simulation software or the computational engine
- a GUI that facilitates preparation of data files for the model code, runs the model code and allows visualisation and analysis of results (model predictions)
- software for processing spatial data, such as a geographic information system (GIS), and software for representing hydrogeological conceptual models
- software that supports model calibration, sensitivity analysis and uncertainty analysis
- programming and scripting software that allows additional calculations to be performed outside or in parallel with any of the above types of software.

Some software is public domain and open source (freely available and able to be modified by the user) and some is commercial and closed (only available in an executable form that cannot be modified by the end user).

Some software fits several of the above categories, for example, a model code may be supplied with its own GUI, or a GIS may be supplied with a scripting language. Some GUIs support one model code while others support many. Software packages are increasingly being coupled to other software packages, either tightly or loosely.

Table 1 lists some examples of modelling software commonly used.

Table 1: Groundwater Modelling Software Commonly Used

Name of Software	Type of Software	Description
MODFLOW	Simulation of saturated flow	Open source software developed by the USGS, based on a block-centred finite difference algorithm. Relies on a large number of modular packages that add specific capabilities. Most packages are also open source and can therefore be modified by end users. Can be coupled to MT3DMS and other codes to simulate solute transport, as well as MIKE 11 for flow in river and stream networks.
FEFLOW	Simulation of saturated and unsaturated flow, transport of mass (multiple solutes) and heat, with integrated GUI	Commercial software based on the finite element method. Several versions with different capabilities. Extendable using plug-ins that can be developed by end users to expand the capabilities, during or after computations. Can be coupled to MIKE 11 to simulate flow in river and stream networks.
SUTRA	Simulation of saturated and unsaturated flow, transport of mass and heat	Open source software based on the finite element method, designed for density-coupled flow and transport.
MT3DMS	Simulation of transport of multiple reactive solutes in groundwater	Open source software that can be coupled with MODFLOW to compute coupled flow and transport.
SEAWAT	Simulation of saturated flow and transport of multiple solutes and heat	Open source software combining MODFLOW and MT3DMS for density-coupled flow and transport.
MIKE SHE	Integrated catchment modelling, with integrated GUI	Commercial software that uses the finite difference method for saturated groundwater flow, several representations of unsaturated flow, including the 1D Richards equation, MIKE 11 for flow in river and stream networks and the 2D diffusive-wave approach for overland flow.
Visual MODFLOW	GUI	Commercial software. Supports MODFLOW (with many packages), MODPATH, SEAWAT, MT3DMS, MT3D99, RT3D, PHT3D, MGO, PEST, MODFLOW-SURFACT, MIKE 11.

Groundwater Vistas	GUI	Commercial software. Supports MODFLOW (with many packages), MODPATH, SEAWAT, MT3DMS, PEST, MODFLOW-SURFACT.
GMS	GUI	Commercial software. Supports MODFLOW (with many packages), MODPATH, MODAEM, SEAWAT, MT3DMS, RT3D, SEAM2D, PEST, SEEP2D, FEMWATER.
PMWIN	GUI	Commercial software. Supports MODFLOW (with many packages), MODPATH, SEAWAT, MT3DMS, PHT3D, PEST.
ArcGIS	GIS	Commercial software to manage spatial data. Capabilities can be extended using ArcPy, an implementation of the Python scripting language.
Surfer	Gridding and contouring	Commercial software to manage and plot spatial data.
Hydro GeoAnalyst	Management of hydrogeological data	Visualisation of bore logs, fence diagrams. Creation of hydrostratigraphic layers. Incorporates elements of ArcGIS.
RockWorks	Management of hydrogeological data	Visualisation of bore logs, fence diagrams. Creation of hydrostratigraphic layers. Can be linked to ArcGIS.
ArcHydro Groundwater	Management of hydrogeological data	Visualisation of bore logs, fence diagrams. Creation of hydrostratigraphic layers. Tightly linked with ArcGIS.
PEST	Parameter estimation and uncertainty analysis	Open-source software designed to allow parameter estimation for any model. Available in many implementations to support specific groundwater models and GUIs.

6. CONCLUDING REMARKS

It is generally agreed that modelling and model calibration should utilise and take into account all available information. In the context of groundwater flow modelling, available information includes:

- observations of watertable elevations and piezometric heads (at depth)
- prior estimates of hydrogeological properties obtained following aquifer tests, slug tests and even permeameter tests on cores
- geophysical data, including seismic and ground-based or airborne electromagnetic data used to define stratigraphy
- downhole geophysics leading to understanding of fracture density and orientation
- records of pumping abstraction and irrigation rates
- estimates of recharge and evapotranspiration
- measurements of streamflow or water quality in losing and gaining streams
- concentrations of solutes and tracers that could provide insights about flow directions and/or groundwater age.

Some of this data are measurements of state variables (e.g. head or concentration), some are observations of quantities derived from state variables (e.g. flux of water or solute) and some are observations of hydrogeological properties or boundary conditions represented by model parameters.

Historical measurements may reflect the behaviour of a groundwater system subject only to natural stresses, and with head gradients and flows that are much smaller than after development of the project (e.g. a water supply borefield, an irrigation scheme or a mine). The changes in levels of stress on an aquifer mean that the future behaviour of the groundwater-flow model depends on different model parameters. Calibration may lead to good estimates of some model parameters that have little influence on the accuracy of predictions and such estimates will not improve the level of confidence in predictions.

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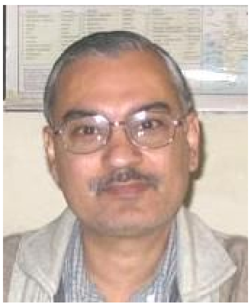

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