DATA REQUIREMENTS FOR GROUNDWATER MODELLING

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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.

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, hydrogeologogical 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:

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

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:

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

where,

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

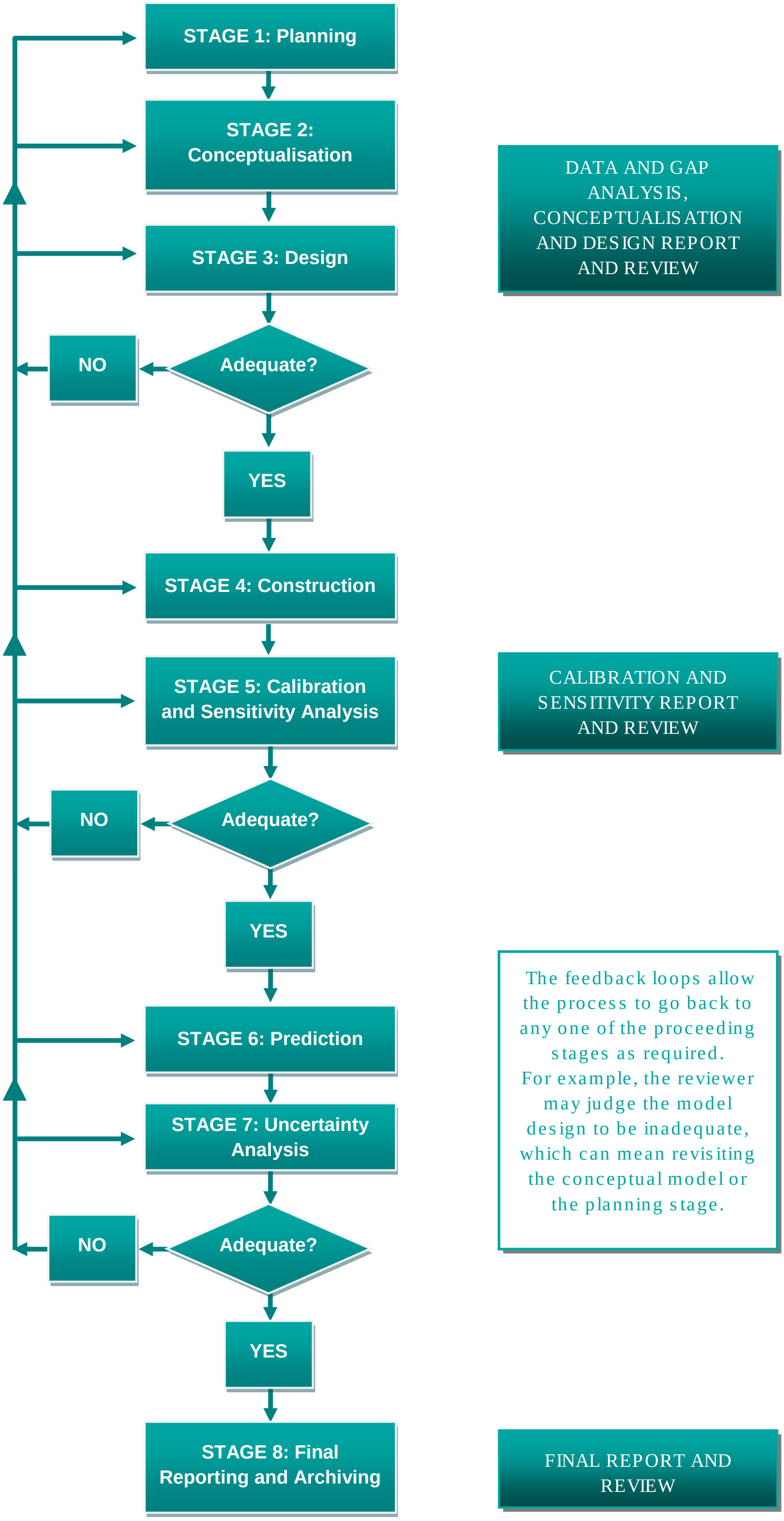
An understanding of these equations and their associated boundary and initial conditions is necessary before a modelling problem can be formulated. Basic processes, that are considered, include groundwater flow, solute transport and heat transport. Most groundwater modelling studies are conducted using 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.

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 feedback loops allow the process to go back to any one of the proceeding stages as required. For example, the reviewer may judge the model design to be inadequate, which can mean revisiting the conceptual model or the planning stage.

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

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.

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.

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.

The hydrogeological domain

The hydrogeological domain should be conceptualised to be large enough to cover the location of the key stresses on the groundwater system (both the current locations and those in the foreseeable future) and the area influenced or impacted by those stresses. It should also be large enough to adequately capture the processes controlling groundwater behaviour in the study area.

All hydrogeological systems are ‘open’ and it is debatable whether the complete area of influence of the hydrogeological system can be covered. As such, some form of compromise is inevitable in defining the hydrogeological domain.

The hydrogeological domain comprises the architecture of the hydrogeologic units (aquifers and aquitards) relevant to the location and scale of the problem, the hydraulic properties of the hydrogeological units, the boundaries and the stresses.

One of the difficult decisions early on in developing a conceptual model relates to the limits of the hydrogeological domain. This is best done so that all present and potential impacts on the groundwater system can be adequately accounted for in the model itself. The extent of the conceptual model can follow natural boundaries such as those formed by the topography, the geology or surface water features. It should also account for the extent of the potential impact of a given stress, for example pumping or injection. It is important that the extent of the hydrogeological domain is larger than the model domain developed during the model design stage.

Defining the hydrogeological domain involves:

- describing the components of the system with regard to their relevance to the problem at hand, such as *the hydrostratigraphy* and the *aquifer properties*
- describing the relationships between the components within the system, and between the system components and the broader environment outside of the hydrogeological domain
- defining the specific processes that cause the water to move from recharge areas to discharge areas through the aquifer materials
- defining the *spatial scale* (local or regional) and *time scale* (steady-state or transient on a daily, seasonal or annual basis) of the various processes that are thought to influence the water balance of the specific area of interest
- in the specific case of solute transport models, *defining the distribution of solute concentration* in the hydrogeological materials (both permeable and less

permeable) and the processes that control the presence and movement of that solute
- making simplifying assumptions that reduce the complexity of the system to the appropriate level so that the system can be simulated quantitatively. These assumptions will need to be presented in a report of the conceptualisation process, with their justifications.

Hydrostratigraphy

The layout and nature of the various hydrogeological units present within the system will guide the definition of the distribution of various units in the conceptual model. Generally, where a numerical simulation model is developed, the distribution of hydrogeologic layers typically provides the model layer structure. In this regard, the conceptualisation of the units should involve consideration of both the lateral and vertical distribution of materials of similar hydraulic properties.

Typical information sources for this data are from geological information such as geological maps and reports, drill-hole data and geophysical surveys and profiles. Where the data is to be used to define layers in numerical models, surface elevation data (usually from digital elevation models) is required.

A hydrostratigraphic description of the system will consist of:

- stratigraphy, structural and geomorphologic discontinuities (e.g. faults, fractures, karst areas)
- the lateral extent and thickness of hydrostratigraphic units
- classification of the hydrostratigraphic units as aquifers (confined or unconfined) or as aquitards
- maps of aquifer/aquitard extent and thickness (including structure contours of the elevation of the top and bottom of each layer)

Aquifer properties

The aquifer and aquitard properties control water flow, storage and the transport of solutes, including salt, through the hydrogeological domain. Quantified aquifer properties are critical to the success of the model calibration. It is also well understood that aquifer properties vary spatially and are almost unknowable at the detailed scale. As such, quantification of aquifer properties is one area where simplification is often applied, unless probabilistic parameterisation methods are applied for uncertainty assessment. Hydraulic properties that should be characterised include hydraulic conductivity (or transmissivity), specific storage (or storativity) and specific yield.

Conceptual boundaries

The conceptualisation process establishes where the boundaries to the groundwater flow system exist based on an understanding of groundwater flow processes. The conceptualisation should also consider the boundaries to the groundwater flow system in the light of future stresses being imposed (whether real or via simulations). These boundaries include the impermeable base to the model, which may be based on known or inferred geological contacts that define a thick aquitard or impermeable rock.

Assumptions relative to the boundary conditions of the studied area should consider:

- where groundwater and solutes enter and leave the groundwater system
- the geometry of the boundary; that is, its spatial extent
- what process(es) is(are) taking place at the boundary, that is, recharge or discharge
- the magnitude and temporal variability of the processes taking place at the boundary. Are the processes cyclic and, if so, what is the frequency of the cycle?

Stresses

The most obvious anthropogenic stress is groundwater extraction via pumping. Stresses can also be those imposed by climate through changes in processes such as evapotranspiration and recharge. Description and quantification of the stresses applied to the groundwater system in the conceptual domain, whether already existing or future, should consider:

- if the stresses are constant or changing in time; are they cyclic across the hydrogeological domain?
- what are their volumetric flow rates and mass loadings?
- if they are localised or widespread (i.e. point-based or areally distributed).

Fundamental to a conceptual groundwater model is the identification of recharge and discharge processes and how groundwater flows between recharge and discharge locations. As for many features of a groundwater model, the level of detail required is dependent on the purpose of the model. The importance attached to individual features such as recharge and discharge features in any given study area should be discussed among the project team.

Representation of surface water - groundwater interaction is required in increasing detail in modelling studies. An interaction assessment should outline the type of interaction between surface water and groundwater systems in terms of their connectedness and whether they are gaining or losing systems. Techniques such as hydraulic measurements, tracer tests, temperature measurements and mapping, hydrogeochemistry and isotopic methods may be used. The need to account for spatial and temporal variability, for example during flood events, in describing interaction between surface water and groundwater should also be assessed.

Physical processes

The processes affecting groundwater flow and/or transport of solutes in the aquifer will need to be understood and adequately documented in the model reporting process. Description of the actual processes, as opposed to the simplified model representation of processes, is required to facilitate third-party scrutiny of the assumptions used in the model development. Flow processes within the hydrogeological domain need to be described, including the following:

- the equilibrium condition of the aquifer, that is, whether it is in steady state or in a transient state. This is established by investigating the historical records in the form of water-level hydrographs, groundwater-elevation surfaces made at different times, or readings from piezometers.
- the main flow direction(s). Is groundwater flowing in one direction predominantly? Is horizontal flow more significant than vertical flow?
- water properties such as density. Are they homogeneous throughout the aquifer? What are the effects of dissolved solutes and/or temperature? Can the flow field be assumed to be driven by hydraulic gradients only?

Additional tasks related to describing the flow processes include:

- creating flow nets from groundwater elevation contours. These will describe the directions of flow, and can be used in a semi-quantitative manner to derive flow volumes.
- quantifying the components of recharge and discharge to the hydrogeological domain, including all those related to point and diffuse recharge and discharge.
- undertaking analysis of the interactions between surface water and groundwater in the hydrogeological domain where it has been highlighted as a significant process.

A database (e.g. GIS-based) will capture all the data that has been collated, whether or not it has been used to develop the conceptual model, with data sources listed and references to previous studies.

Boundary conditions

Groundwater flow models require information about the head and/or head gradient at the boundaries of the model domain. There are three types of boundary conditions:

- *Type 1, Dirichlet or specified head boundary condition*: The head of a boundary cell or node is specified. When the head is specified along a section of the model boundary, the flow across this model boundary section is calculated.
- *Type 2, Neumann or specified head-gradient boundary condition*: The gradient of the hydraulic head is specified at the boundary, which implies that the flow rate across the boundary is specified.
- *Type 3, Cauchy or specified head and gradient boundary condition*: Both the head and the head gradient are specified. In flow models this type of boundary condition is implemented in an indirect manner by specifying a head and a hydraulic conductance or resistance. Both represent effects of features that are located outside the model domain. For example, if a confined aquifer underlies a lake, the flow between the aquifer and the lake can be represented by a Type 3 boundary condition in which the specified head represents the lake level, and the conductance is that of the aquitard that separates the aquifer from the lake.

All three types of model boundary conditions can be assigned as either constant or variable with time. For example, rivers can be modelled as Type 3 Cauchy boundary conditions with time-varying river stages obtained from water-level records.

Groundwater stresses are defined as those processes that lead to the removal or addition of water from or to a groundwater domain. Stresses are typically separated into those associated with the climate (rainfall infiltration and evapotranspiration) and those associated with human activity (such as groundwater extraction). Groundwater stresses are often considered or treated as boundary conditions both by modellers and model GUIs alike. Technically they are ‘sink and source’ terms that are included in the equations that describe water movement and storage in the model.

Most groundwater model codes and GUIs allow the modeller to implement boundary conditions and stresses that are tailored to represent typical near-surface groundwater phenomena such as rainfall-derived recharge, interaction with rivers or lakes and evapotranspiration fluxes from shallow or outcropping groundwater.

Initial conditions

Initial conditions in a transient simulation should be obtained, wherever possible, from a previous model run (e.g. a steady state solution) to avoid spurious results at early times in the transient model run.

Initial conditions define the groundwater conditions present at the start of the model run. In practice, the modeller must define initial heads in all model cells. The choice of initial conditions for a steady state model does not influence the model outcome, but the steady state solution is obtained more rapidly when initial conditions are defined that are reasonably close to the final solution.

For a transient groundwater model, the initial conditions are part of the mathematical problem statement and will influence the model outcomes during the subsequent time steps. It is therefore important that the models are chosen so that they are consistent with the boundary conditions and stresses. When field data is used to define the initial conditions there is a risk that the assigned heads (and solute concentrations) are not in equilibrium with the boundary conditions and stresses applied to the model. Remedies to this problem include:

- allowing for an initial model equilibration time. After a certain amount of time the influence of the initial heads on the calculated heads becomes negligible
- using the results of a steady state model with the boundary conditions and stresses, as they are believed to be at the start of the transient simulation. This approach is only strictly valid if the system can be assumed to be in a steady state at some point in time. In practice, however, it can provide a useful initial condition that is both stable and close to the correct starting condition for a transient model
- using the results of another variant of the model. This is appropriate, for example, when the model is used for predictive simulations; the calculated heads from the (calibrated) model are used to define the initial heads of the predictive model.

Initial estimates of model parameters

All available information should be used to guide the parameterisation and model calibration. All parameters should initially be considered to be uncertain. Before a model can be run it is necessary to assign initial values to all model parameters.

Parameter values representing hydrogeological properties are normally chosen based on aquifer tests undertaken in the area of interest or through simple calculations that use observed groundwater behaviour to indicate key parameter values. Where parameter values have not been calculated they are typically estimated from values reported in the literature for the hydrostratigraphic units being modelled or from text books that provide more generic ranges of values for the type of sediments or rocks included in the model.

Even when aquifer tests provide values for hydraulic conductivity and storage parameters for some of the hydrogeological units being modelled, these parameters are typically variable within an individual unit. As a result the initial values of hydrogeological parameters should be considered as approximate guides only and subsequent adjustment or modification of these parameters during the calibration process is expected.

Solute transport data

All available solute concentration data should be used during conceptualisation to determine the spatial distribution of solutes, identify source zones and migration pathways, and to determine appropriate boundary conditions. An assessment of the relative importance of advection, diffusion and dispersion should be made during the conceptualisation stage, and a decision should be made on which processes are to be included in the solute transport model. The importance of variable-density flow should be assessed with a quantitative analysis using all available head and concentration data. Conceptualisation for the purpose of solute transport involves:

- collection of solute concentration data, and solute conditions at the start of transient simulations
- identification of solute transport processes
- delineation of the area of interest (which may be different from that of the flow model) and an assessment of the relevant time scales
- identification of solute concentration boundary conditions and sources and sinks of solutes
- assessment of the spatial variability (i.e. heterogeneities) in the aquifer’s geological properties
- quantification of solute transport parameters to be used in simulations.

All available solute concentration data should be used during conceptualisation to determine the spatial distribution of solutes, identify source zones and migration pathways, and to determine appropriate boundary conditions.

Measurements of the spatial distribution and temporal variations of solute concentrations are essential elements of the conceptualisation process. Solute concentration data is also required to determine the initial conditions for transient solute transport models and during the calibration stage. Solute concentrations should be obtained from all available sources within the study area, including pumping bores, injection wells, monitoring wells, surface water bodies and rainfall. If insufficient solute concentration data is available for an adequate site characterisation, new data collection efforts should be undertaken.

Solute concentration boundary conditions

Similar to flow models, boundary conditions must be defined for transport models, and similar considerations apply in the selection of their location, that is, preferably coinciding with physical features and sufficiently far away from the area of interest. There are three types of solute concentration boundary conditions.

- *Type 1, Dirichlet or specified concentration boundary condition*. The concentration of a boundary cell or node is specified. Solute mass can be added or removed through Dirichlet boundaries by advection and/or diffusion and dispersion.
- *Type 2, Neumann or specified concentration gradient boundary condition*. The gradient of the solute concentration is specified at the boundary, which implies that the diffusive/dispersive flux across the boundary is specified.
- *Type 3, Cauchy or specified concentration and gradient boundary condition*. Both the concentration and the gradient are specified.

The specified mass flux boundary condition can be implemented as either a Type 2 or a Type 3 boundary condition, depending on which transport process dominates. If dispersive and diffusive mass transport across the boundary is small, which is often a defensible assumption, the concentration gradient across the boundary can be set to zero. The specified mass flux is the product of the specified flow rate and the solute concentration of groundwater entering the system.

Specified boundary concentrations and fluxes can be constant during the entire duration of the simulation or vary as a function of time. The type of boundary condition may even change during a simulation, which could occur where surface water features are variable in extent, or where tidal fluctuations occur on a sloping beach face.

Sources and sinks

Sources and sinks either add water to or remove water from the model domain, and the water entering or leaving the model has an associated solute concentration that must be known or approximated. Sources can be injection wells, rivers, lakes or recharge. Abstraction wells are one example of a sink, and the concentration of the water leaving the model domain in this way is typically considered to be equal to that of the groundwater immediately adjacent to the well. Evapotranspiration represents a sink of water, but not of solutes, and causes an increase in solute concentrations. This is typically encountered in the simulation of groundwater discharge in riparian zones or salt lakes.

In coastal aquifers, the source of saline groundwater may not always be modern seawater, but may reflect other sources such as rock dissolution, connate water entrapped in marine deposits, paleo-seawater that intruded during land surface inundations, and/or anthropogenic contaminants. Also, tidal creeks, rivers and estuaries may also be sources of salt water in coastal aquifers, and knowledge of their tidal limits and the annual salinity variations along their lengths is usually required. Failing to account for these factors may result in a flawed conceptual understanding of the system, leading to erroneous model outcomes. The data collection effort during the conceptualisation stage must therefore allow for various hypotheses to be evaluated, for example, by collecting information on various hydrochemical and isotope tracer techniques that can identify solute origins.

Heterogeneity

Groundwater flow conceptualisation usually involves identification and delineation of the primary hydrostratigraphic units, and the heterogeneities in hydraulic conductivity and porosity within geological strata are often neglected or implicitly incorporated (e.g. through an anisotropic hydraulic conductivity field). While this is usually a reasonable approach for determining the distribution of aquifer heads and for estimating average groundwater flows, aquifer heterogeneities within geological units have a more profound influence on solute transport. Therefore, solute transport models generally require a higher resolution of geological information, in particular in the vertical direction.

An assessment must be made of the extent to which solute concentration patterns are influenced by heterogeneities, by considering the existence of preferential flow pathways, aquitard windows, dual-porosity effects, and the degree of the variability of porosity and permeability within aquifers. Heterogeneities are usually characterised from various data sources, such as geological maps, borehole logs, geophysical surveys, solute concentration distributions, aquifer tests and slug tests, and knowledge about the depositional environment or fracture density, connectivity and aperture. The depositional environments of some unconsolidated aquifers can result in heterogeneities that impose considerable effects on concentration distributions. These include unconsolidated aquifers comprising fluvial sediments, where permeable sand and/or gravel may alternate with relatively impermeable clay layers over short distances.

Solute transport parameters

Solute transport models require input parameters that describe the combined effect of advection, dispersion and diffusion. This typically involves quantification of the following parameters:

- effective porosity
- longitudinal and transverse dispersivity
- diffusion coefficient
- an equation(s) of state (for variable density problems).

Solute transport models require the *effective porosity* and spatial variations thereof to be specified. The porosity has a dual role in solute transport models: it determines the advective flow rate, and it determines the volume of water in the model for storage of solute mass. Total porosity values are relatively easy to quantify when undisturbed cores are available. If this is not the case, values can sometimes be obtained from geophysical logs or estimated from the literature. A range of values exist for different lithological units, but the variability of this parameter is not as large as the hydraulic conductivity variability.

The processes associated with the spreading of solute plumes are challenging to reproduce explicitly (i.e. in a process-based way) because of the small scale of many dispersive factors. The associated transport parameters (such as *dispersivity*) are equally difficult to quantify, especially under field conditions, and the approach to solute transport parameterisation is usually one where transport parameters are modified so that field observations are optimally reproduced by the transport model. The transverse dispersivity is usually much lower than the longitudinal dispersivity, and the sparse data that exists suggest that (i) the horizontal transverse dispersivity is about one order of magnitude lower than the longitudinal dispersivity and (ii) the vertical transverse dispersivity is one or two orders of magnitude smaller than the horizontal transverse dispersivity (Zheng and Bennett 2002).

Diffusion can be an important transport process in solute transport problems (i) at the local (i.e. metres or less) scale; (ii) in low-permeability units (e.g. shale, clay); or (iii) at long timescales (i.e. centuries or more) in stagnant groundwater systems. Unless these problems are being considered, the value of the diffusion coefficient has little effect on the simulation outcomes. The parameterisation of diffusion depends on the solute of interest. The value of the diffusion coefficient is dependent on temperature, and varies for different solute species. However, the diffusion coefficient of chloride, which only ranges between 10^{-9} and 2×10^{-9} m^2/s in pure water, can be used as a good approximation under most circumstances for solutes like major ions, or in a simulation that considers an aggregate solute concentration, like total dissolved solids, or salinity. Specialised application could require the use of different diffusion coefficients for individual ions, for example, with long-term transport processes in clay layers (e.g. safety assessment of nuclear waste repositories).

Variable-density problems further require an *equation of state* that relates the water density to concentration, temperature, and/or pressure. The equation of state couples the groundwater flow equation to the advection–dispersion equation. The flow is affected by the density, and the flow affects the concentrations, and through this, the density. Equations of state are typically linear or exponential functions, and their parameters are readily available in the literature and the supporting documentation of model codes. The parameter values depend on the chemical composition of the groundwater, and the modeller needs to evaluate which relationships are appropriate for the system under consideration.

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.

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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